

PRESUMED AND TRANSPORTED PDF METHODS
APPLIED TO TURBULENT PREMIXED FLAMES

LARS MAGNUS PERSSON
M.Sc.

THESIS SUBMITTED FOR
THE DEGREE OF DOCTOR OF PHILOSOPHY
OF
IMPERIAL COLLEGE LONDON

THERMOFLUIDS SECTION
DEPARTMENT OF MECHANICAL ENGINEERING
IMPERIAL COLLEGE LONDON
SOUTH KENSINGTON CAMPUS
LONDON SW7 2AZ
UNITED KINGDOM

FEBRUARY 2011

To my family & Linda

“Röd vallmo växer även på slitets gråa åker”

Declaration of Originality

I Magnus Persson hereby declare that this thesis is my own work and that the thesis has not been submitted in any other form for another degree or diploma. Information derived from published or unpublished work of others has been acknowledged in the text and a list of references is given in the bibliography.

Magnus Persson, February 2011

Abstract

The current study focuses on the modelling of turbulent premixed or partially premixed flames over a wide range of combustion regimes using various fuels. Opposed flows featuring fractal-generated turbulence are examined using different classes of models. The reacting case is in the flamelet regime of combustion and two-scalar joint β -bimodal presumed PDF and transported PDF approaches are applied for scalar statistics. In the isothermal case the $k - \epsilon$ model works comparatively well, in contrast to previous studies, while in the reacting case the second moment closures are outperforming the eddy viscosity based closures. The transported PDF approach indicates an under-prediction of the turbulent burning velocity in this flow. The latter approach is therefore applied to compute freely propagating turbulent premixed flames using comprehensive chemistry. Turbulent burning velocities are extracted and compared with experimental data. The computed cases are covering the laminar flamelet to the distributed reaction zone regime. The mixture reactivity is also varied through different fuel/air mixtures and explored in terms of the Zeldovich number. The fuel/air composition studied include fuel-lean CH_4 , stoichiometric CH_4 and C_2H_6 and fuel-rich H_2 mixtures. The impact of molecular transport is investigated through the inclusion of an explicit analytical formulation. A multi-scale scalar dissipation rate closure that accounts for the influence of the Da number is extended in a simple manner to include Le number effects. An industrial swirl-stabilised partially premixed fuel-rich CH_4 flame is simulated at realistic gas turbine conditions using the node-based Eulerian transported PDF approach coupled with a second moment closure for the velocity field. The case is in the well stirred reactor regime and the chemical kinetics is modelled using a global reaction scheme for hydrocarbon combustion. The flow field is initialised and compared with the predictions of the two-scalar joint β -bimodal presumed PDF approach.

Acknowledgements

First of all, I would like to express my sincere gratitude to my supervisor Prof. R. P. Lindstedt for his excellent guidance, constant support and encouragement throughout this work. I appreciate his high standards, thoroughness and eye for details and also, his patience and flexibility regarding my work in industry.

I would also like to express my gratitude to my industrial supervisor and former colleague Dr. Vladimir Milosavljevic for teaching me the engineering side of science. I really appreciate his support and encouragement and his patience with me. Special thanks to Dr. Evangelos Váos who have taught me so much about turbulent flows and has given me many hours of his time for support and discussions.

Thanks to friends, former and current colleagues in London. Mark Potter, Tek-Seang Kuan, Nadeem Malik, Henri-Charles Ozarovsky, Ruddy Vincent, Andreas Kempf, Oliver Stein, Konstantinos Gkagkas, Jeremy Floyd, Valentini Markaki, Konstantina Vogiatzaki, Darren Luff, Despoina Chatzikyriakou, Pankaj Vaishnavi, Fabian Cerru, Roger Robinson, Jayesh Bhatt, Matt Cleary, Andrew Wandel, Antonino Tomasello, Marco Montini, Nakul Prasad, Nicholas Vaughan, Sandeep Saha, Laura Nicolaou, Mike Leaford, Michele Bonnani, Sung-Woo Park, Kok Hin Henry Goh, Bharat Lad, Abdel Rabhiou, Marie Kirsten, Josephine Jones, Elefteria Laughland, Florian Finger. A special thanks to Dr. Philipp Geipel for being a very supportive friend and for proof-reading this manuscript.

I would like to acknowledge the financial support of Siemens Industrial Turbomachinery AB. Thanks to Thomas Andersson and Dr. Christian Troger who made this work possible in the first place, Annette Joelsson, Dr. Jenny Larfeldt, Henrik Hull and Thomas Lindgren for supporting me and giving me the time to finalise this. The preparation of Fig. 4.2 by Olle Lindman and the proof-reading support of Dr. Darioush Gohari Barhagi is much appreciated.

I am most grateful to my family for their support throughout this work. Finally, my thanks to Linda Joki for all the weekends and holidays when I was working and for the constant love and support through the difficult times.

Contents

List of Tables	17
List of Figures	19
Nomenclature	31
1 Overview	39
1.1 Introduction	39
1.1.1 Premixed turbulent combustion	42
1.2 The governing equations	44
1.2.1 Direct numerical simulation	50
1.2.2 Moment methods	51
1.2.2.1 Gradient diffusion closures	53
1.2.2.2 Mean reaction rate closures	54
1.2.3 Large eddy simulation	57
1.2.4 Transported PDF methods	62
1.3 The present contribution	63
1.3.1 Objectives	63
1.3.2 Outline	64
2 Second moment closures	69
2.1 Introduction	69
2.2 The governing equations	70
2.3 Redistributive pressure strain	72

2.3.1	Dissipation model considerations	74
2.3.2	Specific models	75
2.3.2.1	The generalised Langevin model of Haworth & Pope	75
2.3.2.2	The model of Jones & Musonge	77
2.3.2.3	Acceleration redistribution and scrambling models .	79
2.4	Triple moments & pressure transport	80
2.5	Turbulent kinetic energy dissipation	81
2.6	Closures in the flamelet regime of combustion	82
2.6.1	Pressure dilatation models	84
3	Transported PDF methods	87
3.1	Introduction	87
3.2	Transport equation for the joint scalar PDF	88
3.3	Modelling and solution algorithm	90
3.3.1	The method of fractional steps	92
3.3.2	Transport in physical space	93
3.3.3	Diffusion in scalar space (mixing)	95
3.3.3.1	Mixing models	96
3.3.4	Convection in scalar space (reaction)	99
4	Isothermal and reacting opposed flows	101
4.1	Introduction	101
4.1.1	The present contribution	104
4.2	Flow configuration	104
4.3	Closure considerations	106
4.3.1	A conserved passive scalar — the mixture fraction	106
4.3.1.1	A joint β -bimodal presumed PDF approach	111
4.3.2	Eulerian joint scalar PDF	113
4.3.2.1	Transport in physical space	114
4.3.2.2	Diffusion in scalar space	115
4.3.2.3	Convection in scalar space	115

4.4	Numerical procedure	118
4.4.1	The presumed PDF approach	119
4.4.1.1	Spatial discretisation of convective terms	120
4.4.2	The transported PDF approach	121
4.4.3	Boundary conditions	121
4.5	Results	123
4.5.1	Isothermal opposed flow	125
4.5.2	Reacting opposed flow	132
4.5.2.1	The presumed PDF approach	132
4.5.2.2	The transported PDF approach	140
4.6	Summary	143
5	Burning velocity predictions using transported PDF methods	145
5.1	Introduction	145
5.1.1	The present contribution	147
5.2	Analytical work on burning velocities	147
5.3	Closure considerations	149
5.3.1	The scalar dissipation rate	150
5.3.2	The impact of closures for molecular transport and chemical reaction	153
5.3.2.1	Laminar reaction rates	155
5.3.2.2	Mixture reactivity	158
5.3.2.3	Molecular transport terms	161
5.4	Numerical procedure	168
5.5	Experimental data	170
5.6	Results	171
5.6.1	Standard closure for the scalar dissipation rate	172
5.6.2	Extended closure for the scalar dissipation rate	173
5.6.3	Implicit impact of molecular transport	176
5.6.4	Explicit impact of molecular transport	178

5.7	Summary	184
6	Simulation of a partially premixed flame in an industrial burner	185
6.1	Introduction	185
6.1.1	The present contribution	187
6.2	Flow configuration	187
6.3	Closure considerations	188
6.4	Numerical procedure	189
6.4.1	Initialisation	190
6.4.2	The PDF solver	192
6.4.3	Boundary conditions	193
6.5	Results	194
6.6	Summary	210
7	Summary and concluding remarks	213
7.1	The present contributions and conclusions	213
7.2	Suggestions for future work	218
	Appendices	221
A	Reduced and detailed mechanisms	223
B	Global activation energies	231
C	Transformation to the $t - \omega$ coordinate system	233
	Bibliography	237

List of Tables

4.1	Global hydrocarbon mechanism	116
5.1	Summary of precomputed parameters at atmospheric conditions and 328 K	152
5.2	Global activation energies and Zeldovich numbers from literature . .	160
5.3	Computed global activation energies and Zeldovich numbers as pre- dicted in the current work.	160
A.1	Reduced hydrocarbon mechanism	223
A.2	Detailed hydrogen mechanism	229
B.1	Computed global activation energies based on stoichiometric CH_4 mixtures with N_2 dilution.	231
B.2	Computed global activation energies based on slightly lean ($\phi = 0.88$) CH_4 mixtures with N_2 dilution.	231
B.3	Computed global activation energies based on stoichiometric C_2H_6 mixtures with N_2 dilution.	232
B.4	Computed global activation energies based on fuel rich ($\phi = 1.6$) H_2 mixtures with N_2 dilution.	232

List of Figures

1.1	Classical turbulent combustion diagram. Stoichiometric CH_4 flames presented in Chapter 5, $0.25 < u' < 16$ m/s, $u_L^0 = 0.45$ m/s, $l_T = 40$ mm and $\delta_L = 1$ mm ($\circ$).	43
4.1	Two counterflowing jets with streamlines shown. Location of the flame is indicated by temperature contours.	102
4.2	The current opposed jet configuration	105
4.3	The laminar burning velocity as a function of equivalence ratio for CH_4 at 1 Atm and 298 K (—) [102].	112
4.4	The adiabatic flame temperature as a function of equivalence ratio for CH_4 at 1 Atm and 298 K (—) [102].	113
4.5	The unstructured mesh featuring 3.5×10^5 non-uniform hexahedral cells.	119
4.6	Predictions using the $k - \epsilon$ model along the centreline. Top left (TL): Mean axial velocity component, top right (TR): Turbulent kinetic energy, bottom left (BL): Axial velocity fluctuation and bottom right (BR): Radial velocity fluctuation. Predictions (—) and experimental data ($\circ$).	126
4.7	Predictions using the $k - \epsilon$ model along the centreline. Left: Mean axial velocity component normalised by u_b . Right: Turbulent kinetic energy normalised by u_b^2 . Fractal generated turbulence, $u_b = 4.0$ m/s, predictions (—) and experimental data ($\circ$). Perforated plates, $u_b = 3.4$ m/s, predictions (- - -) and experimental data ($\square$).	127

4.8	Predictions using the $k - \epsilon$ model along the stagnation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions (—) and experimental data (o).	127
4.9	Predictions using the $k - \epsilon$ model 1.5 mm downstream of the nozzle exit. TL: Mean axial velocity component, TR: Mean radial velocity component, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions (—) and experimental data (o).	128
4.10	Predictions using Reynolds stress models along the centreline. TL: Mean axial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions using the model of Haworth & Pope (—), Jones & Musonge (- - -) and experimental data (o).	129
4.11	Predictions using Reynolds stress models along the stagnation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions using the model of Haworth & Pope (—), Jones & Musonge (- - -) and experimental data (o).	130
4.12	Predictions using Reynolds stress models 1.5 mm downstream of the nozzle exit. TL: Mean axial velocity component, TR: Mean radial velocity component, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions using the model of Haworth & Pope (—), Jones & Musonge (- - -) and experimental data (o).	131
4.13	Predictions using $k - \epsilon$ /gradient diffusion models along the centreline. TL: Mean axial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions (—) and experimental data (o).	133

4.14	Predictions using $k-\epsilon$ /gradient diffusion models along the centreline. Left: Mean reaction progress variable profile. Right: Mean reaction progress variable variance. Conventional averages (—), Favre aver- ages (- - -) and experimental data ($\circ$).	133
4.15	Predictions using $k-\epsilon$ /gradient diffusion models along the stagnation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluc- tuation. Predictions (—) and experimental data ($\circ$).	134
4.16	Predictions using HP/gradient diffusion models along the centreline. TL: Mean axial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions (—) and experimental data ($\circ$).	135
4.17	Predictions using HP/gradient diffusion models along the centreline. Left: Mean reaction progress variable profile. Right: Mean reaction progress variable variance. Conventional averages (—), Favre aver- ages (- - -) and experimental data ($\circ$).	135
4.18	Predictions using HP/gradient diffusion models along the stagnation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluc- tuation. Predictions (—) and experimental data ($\circ$).	136
4.19	Predictions using HP/scalar flux models along the centreline. TL: Mean axial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Con- ventional averages (—), Favre averages (- - -) and experimental data ($\circ$).	137
4.20	Predictions using HP/scalar flux models along the centreline. Left: Mean reaction progress variable profile. Right: Mean reaction progress variable variance. Conventional averages (—), Favre averages (- - -) and experimental data ($\circ$).	137

4.21	Predictions using HP/scalar flux models along the stagnation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Conventional averages (—), Favre averages (- - -) and experimental data (○).	138
4.22	Predictions using HP/extended scalar flux models along the centre- line. TL: Mean axial velocity component, TR: Turbulent kinetic en- ergy, BL: Axial velocity fluctuation and BR: Radial velocity fluctua- tion. Conventional averages (—), Favre averages (- - -) and experi- mental data (○).	139
4.23	Predictions using HP/extended scalar flux models along the centre- line. Left: Mean reaction progress variable profile. Right: Mean re- action progress variable variance. Conventional averages (—), Favre averages (- - -) and experimental data (○).	139
4.24	Predictions using HP/extended scalar flux models along the stag- nation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial veloc- ity fluctuation. Conventional averages (—), Favre averages (- - -) and experimental data (○).	140
4.25	Predictions using HP/transported PDF along the centreline. TL: Mean axial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Pre- dictions (—) and experimental data (○).	141
4.26	Predictions using HP/transported PDF along the centreline. Left: Mean reaction progress variable profile. Right: Mean reaction progress variable variance. Conventional averages (—), Favre averages (- - -) and experimental data (○).	141

4.27	Predictions using HP/transported PDF along the stagnation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions (—) and experimental data (○).	142
5.1	Evolution of the laminar burning velocity for a stoichiometric CH_4 flame.	154
5.2	Flamelet reaction rates at 328 K in reaction progress variable space for the hydrocarbon fuels. Stoichiometric C_2H_6 (—), stoichiometric CH_4 (- - -) and $\phi = 0.88$ CH_4 (- · -).	156
5.3	Flamelet reaction rate at 328 K in reaction progress variable space for hydrogen. $\phi = 1.6$ H_2 (—).	156
5.4	Flamelet reaction rates at 328 K in reaction progress variable space for the rich ($\phi = 1.6$) H_2 (—), stoichiometric CH_4 (- - -) and C_2H_6 (- · -) assuming equal diffusivities.	159
5.5	Arrhenius plot of the computed laminar burning rate of the diluted lean ($\phi = 0.88$) methane-oxygen-nitrogen flames (—), stoichiometric methane-oxygen-nitrogen flames (- - -), stoichiometric ethane-oxygen- nitrogen flames (- · -) and rich ($\phi = 1.6$) hydrogen-oxygen-nitrogen flames (···).	159
5.6	Laminar diffusion terms at 328 K in reaction progress variable space for a stoichiometric CH_4 flame. CH_4 (—), O_2 (- - -), CO_2 (- · -) and H_2O (···).	162
5.7	Laminar diffusion terms at 328 K in reaction progress variable space for a stoichiometric CH_4 flame. H_2 (—) and CO (- - -).	162
5.8	Laminar diffusion terms at 328 K in reaction progress variable space for a stoichiometric CH_4 flame. H (—), O (- - -), OH (- · -), HO_2 (· - -) and CH_3 (···).	163
5.9	Laminar diffusion terms at 328 K in reaction progress variable space for a stoichiometric CH_4 flame. C_2H_2 (—), C_2H_4 (- - -) and C_2H_6 (- · -).	164

5.10	Laminar diffusion terms at 328 K in reaction progress variable space for a stoichiometric CH_4 flame assuming a global reaction step. CH_4 (—), O_2 (- - -), CO_2 (- · -) and H_2O (···).	165
5.11	Reaction progress variable profiles in η -space at 328 K. Computed profile using detailed chemistry and equal diffusivities, spatial coordinate normalised by $\delta_L = 1$ mm (—), functional form of Eq. (5.31) with $A = 12$ (- - -).	166
5.12	Laminar diffusion terms in reaction progress variable space at 328 K. Computed profile using detailed chemistry and equal diffusivities (—), diffusion term model of equations (5.30) - (5.33) (- - -) with $A = 12$, $A_\mu = 1.0$, $\tau = 6.0$, $\delta_L = 1$ mm and $\mu_u = 1.9 \times 10^{-5}$ kgm ⁻¹ s ⁻¹	166
5.13	1D simulations schematically shown in the solved ω -space as given in Appendix C.	169
5.14	Predicted turbulent burning velocities for the rich ($\phi = 1.6$) hydrogen flames ($l_T = 40$ mm) using 1600 ppc. Experimental data, measured (○), corrected for fully developed flames (□) and error bars by Abdel-Gayed <i>et al.</i> [1]. Mixing time scale expression given by Eq. (3.41) with $C_\phi = 2.0$ (—).	172
5.15	Predicted turbulent burning velocities for the rich ($\phi = 1.6$) hydrogen flames. Measured (○), corrected for fully developed flames (□) [1]. $l_T = 40$ mm; τ_ϕ^{-1} via Eq. (5.13) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$, 1600 ppc (···); τ_ϕ^{-1} via Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$, 800 ppc (- · -); τ_ϕ^{-1} via Eq. (5.15); $C_\phi = 0.0$ and $C_\phi^* = 2.4$, 800 ppc (—); $l_T = 20$ mm; $C_\phi = 0.0$ and $C_\phi^* = 2.4$, 800 ppc (- - -).	174
5.16	Predicted turbulent burning velocities for stoichiometric ($\phi = 1.0$) methane flames ($l_T = 40$ mm) using 1600 ppc. Experimental data, measured (○), corrected for fully developed flames (□) and error bars by Abdel-Gayed <i>et al.</i> [1]. τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (—)	174

5.17	Predicted turbulent burning velocities for the stoichiometric ethane flames ($l_T = 40$ mm) using 1600 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed <i>et al.</i> [1]. τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (—).	175
5.18	Predicted average normalised turbulent reaction rate for stoichiometric methane (---) and stoichiometric ethane (— · —) using 1600 ppc, $u' = 4$ m/s, $l_T = 40$ mm, τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$. Normalised progress variable variance, $\tilde{c}(1 - \tilde{c})$ (—). . . .	175
5.19	Predicted turbulent burning velocities for lean ($\phi = 0.88$) methane flames ($l_T = 40$ mm) using 200 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed <i>et al.</i> [1]. τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (—).	176
5.20	Predicted turbulent burning velocities for stoichiometric ($\phi = 1.0$) methane flames ($l_T = 40$ mm) using 200 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed <i>et al.</i> [1]. τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (—)	177
5.21	Predicted turbulent burning velocities for stoichiometric ($\phi = 1.0$) ethane flames ($l_T = 40$ mm) using 200 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed <i>et al.</i> [1]. τ_ϕ^{-1} given by: Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (—), Eq. (5.15) with $C_\phi = 0.0$ and $C_\phi^* = 2.4$ (---). . . .	177
5.22	Predicted turbulent burning velocities for the stoichiometric methane flames ($l_T = 40$ mm) using extracted diffusion terms and 200 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed <i>et al.</i> [1]. τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (—).	179

5.23	Predicted turbulent burning velocities for the stoichiometric methane flames ($l_T = 40$ mm) using 200 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed <i>et al.</i> [1]. Reaction rate expression given by Eq. (5.36) with $A_c = 12$ and $\delta_L = 1$ mm. τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$, $A_\mu = 1.0$ ($\cdots$), $A_\mu = 0.5$ (- - -). τ_ϕ^{-1} given by Eq. (5.15) with $C_\phi = 0.0$ and $C_\phi^* = 2.4$, $A_\mu = 1.0$ (—).	179
5.24	Predicted turbulent burning velocities for the slightly lean ($\phi = 0.88$) methane flames ($l_T = 40$ mm) using 200 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed <i>et al.</i> [1]. Reaction rate expression given by Eq. (5.36) with $A = 12$ $A_\mu = 1.0$ and $\delta_L = 1$ mm. τ_ϕ^{-1} given by Eq. (5.15) with $C_\phi = 0.0$ and $C_\phi^* = 2.4$ (—).	180
5.25	Predicted turbulent burning velocities for stoichiometric ethane flames ($l_T = 40$ mm) using 200 ppc. Symbols as in Fig. 5.24 except $\delta_L = 0.7$ mm.	180
5.26	Computed reaction progress variable profiles, $u' = 1$ m/s and $l_T = 40$ mm. Predicted profile with diffusion term correction of Eq. (5.36) with $A_c = 12$, $A_\mu = 1.0$, $\delta_L = 1$ mm and 200 ppc, τ_ϕ^{-1} given by Eq. (5.15) with $C_\phi = 0.0$ and $C_\phi^* = 2.4$ (—) and without diffusion term correction using 1600 ppc, τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (- - -).	181
5.27	Computed reaction progress variable variance profiles, $u' = 1$ m/s and $l_T = 40$ mm. Predicted variance with diffusion term correction of Eq. (5.36) with $A_c = 12$, $A_\mu = 1.0$, $\delta_L = 1$ mm and 200 ppc, τ_ϕ^{-1} given by Eq. (5.15) with $C_\phi = 0.0$ and $C_\phi^* = 2.4$ (—) and without diffusion term correction using 1600 ppc, τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (- - -) and theoretical maximum variance $\widetilde{c'^2} = \widetilde{c}(1 - \widetilde{c})$ ($\cdots$).	182

5.28	Predicted normalised turbulent reaction rates for stoichiometric CH_4 flames, $u' = 1$ m/s and $l_T = 40$ mm. No diffusion model, 1600 ppc, τ_ϕ^{-1} via Eq. (5.14), $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (- - -). Diffusion model of Eq. (5.36), 200 ppc, τ_ϕ^{-1} via Eq. (5.15), $C_\phi = 0.0$, $C_\phi^* = 2.4$, $A_c = 12$, $A_\mu = 1.0$ and $\delta_L = 1$ mm (—). Experimental data: Cheng & Shepherd [29] ($\circ$) and Lawn & Schefer [101] ($\bullet$).	183
6.1	The unstructured grid featuring 5.0×10^4 tetrahedral and hexahedral cells.	189
6.2	Fuel/air mixture temperature as a function of equivalence ratio at 23.8 bar, $T_O = 757$ K and $T_F = 300$ K (—).	190
6.3	Laminar burning velocity as a function of equivalence ratio for CH_4 at 23.8 bar and temperatures according to Fig. 6.2 (—) [102].	191
6.4	Adiabatic flame temperature as a function of equivalence ratio for CH_4 at 23.8 bar and temperatures according to Fig. 6.2 (—) [102].	191
6.5	Locations of the various cross sections	194
6.6	Computed axial velocity using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.	195
6.7	Computed turbulence intensity using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.	195
6.8	Computed mixture fraction using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.	196
6.9	Computed temperature using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.	196
6.10	Computed mass fractions of CH_4 using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.	197
6.11	Computed mass fractions of O_2 using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.	197
6.12	Computed mass fractions of H_2O using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.	198

6.13	Computed mass fractions of CO_2 using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.	198
6.14	Computed mass fractions of H_2 using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.	199
6.15	Computed mass fractions of CO using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.	199
6.16	Predictions at the first cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. Top left(TL): Mean axial velocity, top right (TR): Tur- bulence intensity, middle left (ML): Mixture fraction, middle right (MR): Temperature, bottom left (BL): Mass fraction of CH_4 , bottom right (BR): Mass fraction of O_2 . Presumed (- - -) and transported (—) PDF.	200
6.17	Predictions at the second cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. TL: Mean axial velocity, TR: Turbulence intensity, BL: Mixture fraction, BR: Temperature. Presumed (- - -) and transported (—) PDF.	201
6.18	Predictions at the second cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. Mass fractions of TL: CH_4 , TR: O_2 , ML: H_2O , MR: CO_2 , BL: H_2 , BR: CO . Transported PDF (—).	202
6.19	Predictions at the third cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. TL: Mean axial velocity, TR: Turbulence intensity, BL: Mixture fraction, BR: Temperature. Presumed (- - -) and transported (—) PDF.	203
6.20	Predictions at the third cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. Mass fractions of TL: CH_4 , TR: O_2 , ML: H_2O , MR: CO_2 , BL: H_2 , BR: CO . Transported PDF (—).	204
6.21	Predictions at the fourth cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. TL: Mean axial velocity, TR: Turbulence intensity, BL: Mixture fraction, BR: Temperature. Presumed (- - -) and transported (—) PDF.	205

6.22	Predictions at the fourth cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. Mass fractions of TL: CH_4 , TR: O_2 , ML: H_2O , MR: CO_2 , BL: H_2 , BR: CO . Transported PDF (—).	206
6.23	Predictions at the fifth cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. TL: Mean axial velocity, TR: Turbulence intensity, BL: Mixture fraction, BR: Temperature. Presumed (- - -) and transported (—) PDF.	207
6.24	Predictions at the fifth cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. Mass fractions of TL: H_2O , TR: CO_2 , BL: H_2 , BR: CO . Transported PDF (—).	207
6.25	Predictions at the sixth cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. TL: Mean axial velocity, TR: Turbulence intensity, BL: Mixture fraction, BR: Temperature. Presumed (- - -) and transported (—) PDF.	208
6.26	Predictions at the sixth cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. Mass fractions of TL: H_2O , TR: CO_2 , BL: H_2 , BR: CO . Transported PDF (—).	208
6.27	Time trace of the axial velocity at the swirler channel exit, left: PPDF, right: TPDF.	209
6.28	Dominant frequencies using the TPDF approach based on the axial velocity trace at the swirler channel exit. Left: Frequency peaks ranging roughly from 800 - 1100 Hz. Right: Unphysical frequency at around 70 kHz obtained as a result of the solution strategy.	209

Nomenclature

Latin symbols

A	pre-exponential factor
$\mathcal{A}$	area
A_c	reaction progress variable function parameter
A_i	particle rate of change
A_{jk}^i, A_{ij}	scaling tensors for acceleration redistribution and scrambling
A_μ	diffusion model parameter
a	speed of sound
a_k	acceleration vector
B	diffusion coefficient
B_{ijkl}	scaling tensor
b	temperature dependent exponent
$\underline{b}, b_{ij}$	normalised anisotropy tensor
C_0	Haworth & Pope turbulence model constant
$C_1, \dots, C_7$	Jones & Musonge turbulence model constants
C_{AR}, C_{AS}	acceleration redistribution and scrambling model constants
C_{EBU}	Eddy-Break-Up model constant
C_{ij}	scaling tensor
C_m	BML model parameter
C_R	Fractal model constant
C_S	Smagorinsky model constant
$C_{\epsilon_1}, \dots, C_{\epsilon_3}, C_{S_\epsilon}$	dissipation equation model constants

C_μ	turbulence model constant
C_ϕ	scalar to mechanical turbulence time scale ratio
$C_{\phi_1}, \dots, C_{\phi_5}$	Jones & Musonge scalar flux model constants
C'_{ϕ_1}	Jones & Musonge scalar flux model constant
c	reaction progress variable
c_{lim}	threshold value
c_p	specific heat
$c_{p\alpha}$	specific heat of species α
D	diffusion coefficient
$\mathcal{D}$	fractal dimension
D	nozzle diameter
D_i	drift coefficient
D_{ijk}	scaling tensor
D_α	diffusion coefficient of species α into the mixture of other species
$d\mathbf{W}(t)$	Wiener process
E_a	activation energy
$F_{u\phi}$	joint mass density function
$\mathcal{F}_{u\phi}$	joint distribution function
f	body force
f_ϕ	probability density function (PDF) of scalar ϕ
f_ϕ^N	discrete fine grained PDF of scalar ϕ
G	filter function
G_{ij}	turbulence model scaling tensor
g_i	gravity
H	nozzle separation
H_{ijkl}	Reynolds stress model scaling tensor
h	static mixture enthalpy
h	uniform random variable
h_α	static species enthalpy
I	identity operator

I_0	strain reduction factor
J_i^h	heat flux in coordinate direction i
J_i^α	mass molecular flux of species α in coordinate direction i
k	turbulent kinetic energy
k_j	rate constant of reaction j
k_r	residual turbulent kinetic energy
l_G	Gibson length scale
l_K	Kolmogorov length scale
l_T	turbulent integral length scale
M	molecular weight of mixture
M_α	molecular weight of species α
M_f^C	convective cell face flux
$\dot{m}$	mass flux
N	number of realisations/particles
n	particle number
n	total mole number
n_α	mole number of species α
n_{reac}	number of reactions
n_{sp}	number of species
$\mathbf{P}(\mathbf{A})$	probability of event $\mathbf{A}$
$P_1, \dots, P_3$	transported PDF processes
$P_{ij}, P_{ic}, P_{i\xi}$	Reynolds stress and turbulence scalar flux production terms
$P_{\xi\xi}$	mixture fraction variance production term
P_R	probability of reaction
p	pressure
q	heat source
R	universal gas constant, $R = 8314.3 \text{ J/kmolK}$
R_α	net rate of formation of species α
r	beta PDF parameter
S	chemical source term

$\mathcal{S}$	filtered characteristic rate of strain
S_{ic}	turbulence-reaction rate correlation
S_{ij}	strain rate
s	beta PDF parameter
T	temperature
$T_{ijk}, T_{ijc}, T_{ij\xi}$	Reynolds stress and turbulent scalar flux transport terms
$T_{i\xi\xi}$	mixture fraction variance transport term
$\mathcal{T}$	heat release parameter
t	time
$\bar{t}$	elapsed time divided by the Lagrangian eddy life time
$u_i = \{u, v, w\}$	velocity vector
u_L^0	unstrained laminar burning velocity
u_T	turbulent burning velocity
u_T^*	fully developed turbulent burning velocity
V	velocity sample space
V_K	Kolmogorov velocity
X_α	mole fraction of species α
x	number of C atoms
$x_i = \{x, y, z\}$	cartesian coordinate vector
Y_α	mass fraction of species α
y	number of H atoms
Z_γ	element mass fraction of element γ

Greek symbols

α_1, α_2	turbulence model constants
β	coupling function
$\beta_1, \dots, \beta_3$	turbulence model constants
β_ϕ	mixing model constant
Γ	diffusion coefficient

$\gamma_1, \dots, \gamma_6$	turbulence model constants
Δ	filter width
Δh_α^0	enthalpy of formation
Δt	time step
Δx	characteristic cell size (length)
δ_{ij}	Kronecker delta
δ_L	laminar flame thickness
ϵ	turbulent kinetic energy dissipation
ϵ_c	reaction progress variable scalar dissipation rate
ϵ_N	statistical error
ϵ_ξ	mixture fraction scalar dissipation rate
ϵ_ϕ	scalar dissipation rate
$\epsilon_{ij}, \epsilon_{ic}, \epsilon_{i\xi}$	viscous dissipation
ε	measurement scale
η	normalised coordinate
Θ_α	particle rate of change
λ	thermal conductivity
μ	dynamic viscosity
μ_T	eddy viscosity
ν	kinematic viscosity
ν_r	residual eddy viscosity
ν_α	stoichiometric coefficient of species α
$\Xi_{j\alpha}$	stoichiometric coefficient for species α in reaction j
ξ	mixture fraction
ξ_c	reaction progress variable cut-off
ξ_i	standardized joint normal random vector
$\xi_{j\alpha}$	concentration dependence for species α in reaction j
ρ	fluid density
Σ	flamelet surface to volume ratio
σ	scalar dimension

$\sigma_k, \sigma_\epsilon$	$k - \epsilon$ turbulence model constants
τ	turbulent time scale
τ_c	chemical time scale for the largest eddies
τ_K	Kolmogorov time scale
τ_r	residual turbulent time scale
τ_{ij}	viscous stress tensor
τ_{ij}^R	residual stress tensor
τ_{ij}^r	anisotropic residual stress tensor
τ_ϕ	mixing time scale
Υ	blending factor
$\Phi_{ij}, \Phi_{ic}, \Phi_{i\xi}$	effects of mean pressure gradients
ϕ	arbitrary scalar
ϕ	stoichiometric ratio
$\phi_{ij}, \phi_{ic}, \phi_{i\xi}$	pressure gradient correlation terms
$\phi_{ij}^A, \phi_{ic}^A, \phi_{i\xi}^A$	acceleration redistribution and scrambling tensors
ϕ_α	molar concentration of species α
Ψ	scalar sample space
ω_α	reactive-diffusive rate of species α

Superscripts

CD	constant density
f	forward
L	Lagrangian
r	reverse
$'$	difference between instantaneous and conventional mean value
$''$	difference between instantaneous and Favre averaged mean value
$\imath$	difference between instantaneous and filtered value
$\imath\imath$	difference between instantaneous and Favre filtered value

Subscripts

b	burnt gas
F	fuel
I	inert
K	Kolmogorov
L	laminar
O	oxidizer
P	products
st	stoichiometric value
T	turbulent
u	unburnt gas

Others

$\langle \phi \rangle$	conventional mean value of ϕ
$\tilde{\phi}$	Favre averaged mean value of ϕ
$\bar{\phi}$	filtered value of ϕ
$\tilde{\bar{\phi}}$	Favre filtered value of ϕ
$\langle a b \rangle$	conditional average of a on b

Dimensionless numbers

$Da = \tau/\tau_c$	Damköhler number
$Ka = \tau_c/\tau_K$	Karlowitz number
$Le = \lambda/c_p\rho D$	Lewis number
$Ma = u/a$	Mach number
$Pe = \rho u \Delta x/\Gamma$	Peclet number
$Re = ul/\nu$	Reynolds number
$Re_T = u'l_T/\nu$	turbulent Reynolds number

$Sc = \mu/\rho D$ Schmidt number

$\beta = E_a(T_b - T_u)/RT_b^2$ Zeldovich number

$\sigma = c_p\mu/\lambda$ Prandtl number

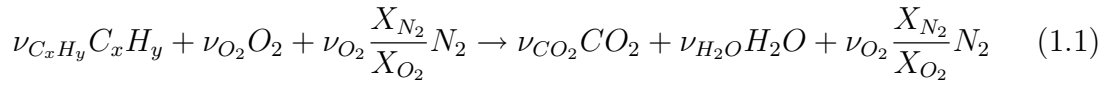
Chapter 1

Overview

1.1 Introduction

Combustion, one of the oldest technologies of mankind, is still responsible for more than 80% of worldwide energy production. Today, and for some time to come, combustion of fossil and perhaps renewable fuels will be the main energy source for domestic heating, electric power generation and transportation. A major concern is the rapid increase in fossil fuel consumption and the unavoidable formation of carbon dioxide (CO_2). The latter was, for a long time, considered to be harmless, but is now believed to be a major contributor to global warming through the greenhouse effect. Since pre-industrial times, the amount of carbon dioxide in the atmosphere has increased by 30% and is increasing on average by 0.4% each year [72]. Carbon dioxide generated by the combustion of fossil fuels is the only man-made source, but a part of the increase is due to deforestation. Besides CO_2 , nitric oxide, soot and unburnt hydrocarbons are further pollutants also formed during the combustion process. The main oxides of nitrogen (NO and NO_2) are collectively called NO_x and contribute to the formation of smog and ozone in urban air and the removal of the ozone layer in the stratosphere [175]. The introduction of new legislations forces industries to reduce the formation of these pollutants. A major step forward was achieved through a change of the combustion mode in many practical devices. A common classification of combustion is based on the level of mixing of fuel and oxidiser prior to ignition.

In a non-premixed or diffusion flame, the fuel and air are completely separated, and are mixed on a molecular level by the flow. The diffusion flame stabilises around the stoichiometric point in a mixing layer. In premixed combustion, fuel and air are perfectly mixed (no concentration gradients) at a certain stoichiometric ratio before reaching the flame front. Stoichiometric combustion occurs when fuel and oxidiser completely consumes each other to form combustion products only. Considering a general global hydrocarbon reaction step



where ν_α represent the stoichiometric coefficients of the reaction. The stoichiometric coefficients of oxygen, carbon dioxide and water are defined as $\nu_{O_2} = (x + y/4)\nu_{C_xH_y}$, $\nu_{CO_2} = x\nu_{C_xH_y}$ and $\nu_{H_2O} = (y/2)\nu_{C_xH_y}$, respectively. If the stoichiometric coefficient of fuel is one ($\nu_{C_xH_y} = 1$), one mole of fuel reacts with $(x + y/4)$ moles of oxygen to form combustion products. The number of moles of each species in the mixture, the mole number (n_α), may be used to define the mole fraction (X_α)

$$X_\alpha = \frac{n_\alpha}{n} \quad \text{where} \quad n = \sum_{\alpha=1}^{n_{sp}} n_\alpha \quad (1.2)$$

where n is the total mole number in the mixture. For dry air $X_{N_2} \approx 3.762X_{O_2}$ assuming an oxygen content of 21%. The mass fraction Y_α is related to the mole fraction through

$$Y_\alpha = \frac{X_\alpha M_\alpha}{M} \quad \text{where} \quad M = \sum_{\alpha=1}^{n_{sp}} X_\alpha M_\alpha \quad (1.3)$$

where M_α represent the molecular weight of species α and M is the molecular weight of the mixture. A measure of the stoichiometry of the mixture is given by the equivalence ratio ϕ

$$\phi = \frac{Y_F Y_{O,st}}{Y_O Y_{F,st}} \quad (1.4)$$

where subscripts F and O represent fuel and oxidiser (air), respectively. The ratio $Y_{O,st}/Y_{F,st}$ is the stoichiometric air-to-fuel ratio. The mixture is said to be stoichiometric when $\phi = 1$, fuel-lean (lean) when $\phi < 1$ and fuel-rich (rich) when $\phi > 1$. For a stoichiometric methane-air mixture the fuel mole fraction is 9.5% while the mass fraction is 5.5%. The latter gives a stoichiometric air-to-fuel ratio of 17.2.

In contrast to a diffusion flame, a characteristic feature of a premixed flame is that it has a propagation velocity. The premixed flame propagates normal to the fresh reactant mixture and its velocity is usually called the burning velocity and is proportional to the consumption rate of the mixture. The laminar burning velocity u_L is a function of composition, temperature of the fresh mixture and the pressure. The laminar burning velocity increases with increased preheat temperature while it is decreasing with elevated pressure [175]. In the turbulent case, the turbulent burning velocity u_T is predominantly a function of the turbulence parameters. In general, $u_T \gg u_L$ since the flame front area increases with turbulence and as a consequence leads to an increase in the consumption rate. The premixed flame will stabilise where the flow velocity is equal to the burning velocity.

One of the major motivations of applying combustion in a premixed mode in practical devices is the potential to reduce emissions such as oxides of nitrogen (NO_x). Industrial gas turbines are usually operated with an excess of air. A lean mixture of fuel and air leads to a reduction in flame temperature compared to traditional diffusion flame techniques. The reduced flame temperature significantly reduces the NO_x production. On the other hand, the lean mixtures make the combustion system sensitive to flow instabilities that may be amplified by the combustion process. These flow instabilities may also lead to local or global extinction and re-ignition phenomena induced for example by shear layer instabilities. To deal with these issues, sophisticated numerical and experimental techniques are a necessity for successful predictions at an early stage in the design phase of industrial devices/combustors.

1.1.1 Premixed turbulent combustion

A turbulent reacting flow field is covering a wide range of length and time scales. The different length and time scales may be combined to form dimensionless numbers that to some extent characterises the flow in question. A dimensionless measure of the level of turbulence may be obtained by the turbulent Reynolds number (Re_T),

$$Re_T = \frac{u' l_T}{\nu} \quad (1.5)$$

where u' is a characteristic velocity fluctuation, ν the kinematic viscosity and l_T the turbulent integral length scale representing a measure of the size of the largest eddies in the turbulent flow field. A relative measure between the turbulent (τ) and the chemical (τ_c) time scales for the largest eddies is given by the Damköhler number (Da)

$$Da = \frac{\tau}{\tau_c} = \frac{l_T u_L^0}{\delta_L u'} \quad (1.6)$$

where u_L^0 is the unstrained laminar burning velocity and δ_L represents the laminar flame thickness. The Karlovitz number (Ka) on the other hand relates the chemical time scale to the smallest eddies defined by the Kolmogorov scales. The Karlovitz number is defined as the ratio between the chemical time and the Kolmogorov time (τ_K),

$$Ka = \frac{\tau_c}{\tau_K} = \frac{\delta_L \sqrt{\epsilon}}{u_L^0 \sqrt{\nu}} = \left(\frac{l_T}{\delta_L} \right)^{-1/2} \left(\frac{u'}{u_L^0} \right)^{3/2} \quad (1.7)$$

where ϵ represents the turbulent kinetic energy dissipation rate. Lines of $Re_T = 1$, $Da = 1$ and $Ka = 1$ may now be plotted as function of lengths (l_T/δ_L) and velocities (u'/u_L^0) in a combustion diagram as shown in Fig. 1.1. This combustion diagram is known as the classical turbulent combustion diagram or Borghi diagram [17, 136, 175]. The lines of $Re_T = 1$, $Da = 1$ and $Ka = 1$ in the diagram roughly separate different regimes of premixed turbulent combustion. The area in the lower left corner separated by the line $Re_T = 1$ is laminar combustion. The area to the right of laminar combustion and below the line $Ka = 1$ represents the laminar flamelet regime of combustion. This regime is further split into two regions, wrinkled and

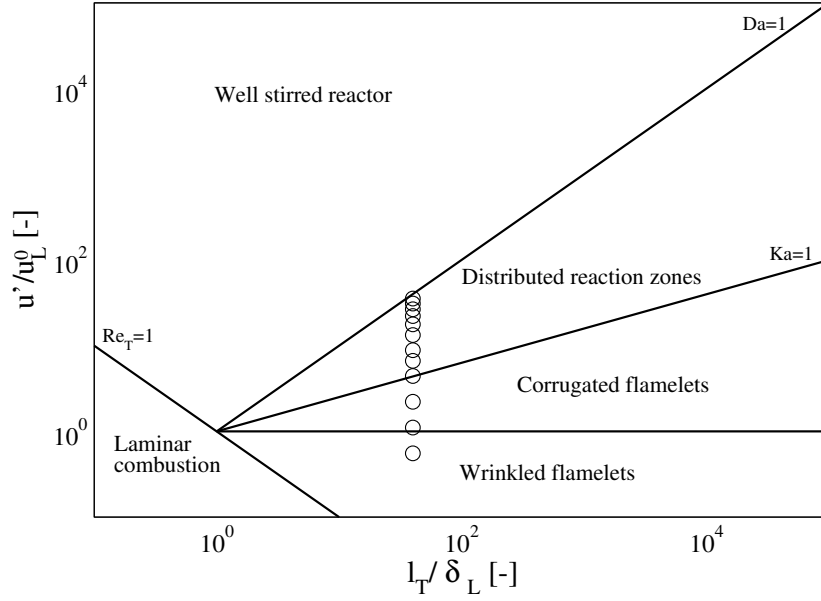


Figure 1.1: Classical turbulent combustion diagram. Stoichiometric CH_4 flames presented in Chapter 5, $0.25 < u' < 16$ m/s, $u_L^0 = 0.45$ m/s, $l_T = 40$ mm and $\delta_L = 1$ mm ($\circ$).

corrugated flamelets, by the line $u' = u_L^0$. In the flamelet regime where $Da > 1$ and $Ka < 1$, all the chemical time scales are shorter than any turbulent time scale and the flame thickness is smaller than the smallest scale of turbulence, the Kolmogorov scale, so the inner structure of the turbulent flame resembles that of a laminar flame but wrinkled by turbulent motions. Above the line $Ka = 1$, but below the line $Da = 1$, is the distributed reaction zones regime where $Ka > 1$ and $Da > 1$. In this regime, the smallest scales of turbulence can enter the inner structure of the flame and, as a consequence, the flame can not be identified as laminar. Finally, above the line $Da = 1$, the area characterised by $Ka > 1$ and $Da < 1$, is the well stirred reactor regime where all scales of turbulence can enter the inner structure of the turbulent premixed flame. The chemical time scales are longer than any turbulent time scales, the overall reaction rate is solely controlled by chemical kinetics. Included in the diagram are also the computed stoichiometric CH_4 flames assuming $0.25 < u' < 16$ m/s, $u_L^0 = 0.45$ m/s, $l_T = 40$ mm and $\delta_L = 1$ mm presented in Chapter 5.

1.2 The governing equations

Conservation principles are fundamental to reacting fluid flows since all such flows obey conservation laws for mass, momentum and scalars. The conservation laws, together with an equation of state, are used for the mathematical description of a turbulent reacting flow field. For completeness, boundary and initial conditions must be supplied to the set of transport equations. Conservation of mass is given in differential form by the continuity equation [103],

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \quad (1.8)$$

where ρ represents the fluid density, $u_i = \{u, v, w\}$ the velocity vector and $x_i = \{x, y, z\}$ the Cartesian coordinate vector. Conservation of momentum [103]

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i \quad (1.9)$$

is derived from Newton's second law and relates the fluid element acceleration, represented by the two terms on the left hand side (LHS), to the surface and body forces acting on that fluid element. The surface forces are represented by the pressure p and the viscous stress tensor τ_{ij} while the body force of interest is the gravity g_i . Given that conservation of momentum is described by the Navier-Stokes equations presented above, the gas mixture may be treated as a Newtonian fluid, then the resulting viscous stress tensor [103] is given by

$$\tau_{ij} = \mu \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right] \quad (1.10)$$

assuming negligible bulk viscosities, where δ_{ij} is the Kronecker delta and μ is the dynamic viscosity coefficient. The dynamic viscosity coefficient is a function of composition and temperature. The remaining transport equations are related to scalar quantities, the conservation of individual species and conservation of energy.

The conservation of individual species, the mass fractions Y_α [104], is described by

$$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho u_i Y_\alpha}{\partial x_i} = -\frac{\partial J_i^\alpha}{\partial x_i} + \rho S_\alpha \quad (1.11)$$

where J_i^α is the molecular flux and S_α the chemical source/sink term representing creation/consumption of species α . In the general case, the molecular flux consists of three contributions [175], ordinary diffusion, thermal diffusion and pressure diffusion. Mass transport caused by temperature and pressure gradients, the thermal diffusion (Soret) and the pressure diffusion respectively, are usually small and are therefore omitted [103, 104, 175]. The multi-component molecular flux is given by [81, 82]

$$J_i^\alpha = -\rho D_\alpha \left(\frac{\partial Y_\alpha}{\partial x_i} - Y_\alpha \frac{1}{n} \frac{\partial n}{\partial x_i} \right) - \rho v_c Y_\alpha \quad (1.12)$$

where D_α is the diffusion coefficient of species α into a mixture of other species and v_c is the correction velocity. The correction velocity term is used in the expression for the flux term to ensure that the diffusive flux sum to zero ($\sum_{\alpha=1}^{n_{sp}} Y_\alpha v_c = 0$). In turbulent reacting flows, especially in high Reynolds number flows, the mass molecular flux is of secondary importance [104] and is usually approximated by Fick's law of diffusion [71]

$$J_i^\alpha = -\rho D \frac{\partial Y_\alpha}{\partial x_i} \quad (1.13)$$

where D is a single diffusion coefficient. Insertion of Eq. (1.13) into Eq. (1.11) results in

$$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho u_i Y_\alpha}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\rho D \frac{\partial Y_\alpha}{\partial x_i} \right] + \rho S_\alpha. \quad (1.14)$$

The chemical source term of Eq. (1.14) may be expressed as

$$\rho S_\alpha = R_\alpha M_\alpha. \quad (1.15)$$

The net rate of formation R_α of species α is given by [81, 82]

$$R_\alpha = \sum_{j=1}^{n_{reac}} \Xi_{j\alpha} \left[k_j^f \prod_{\beta=1}^{n_{sp}} \phi_\beta^{\xi_{j\alpha}} - k_j^r \prod_{\beta=1}^{n_{sp}} \phi_\beta^{\xi_{j\alpha}} \right] \quad (1.16)$$

In the expression above, $\Xi_{j\alpha}$ is the stoichiometric coefficient for species α in reaction j , k_j is the forward (f) and reverse (r) rate constants of reaction j , ϕ_β is the molar concentration of species β , $\xi_{j\alpha}$ is the concentration dependence for species α in reaction j and n_{reac} is the number of reactions. The forward rate constant is given by the extended Arrhenius law [175],

$$k^f = AT^b \exp\left(-\frac{E}{RT}\right) \quad (1.17)$$

where A is the pre-exponential factor, b the temperature dependent exponent and E the activation energy. The reverse rate constant is related to the forward rate constant through the equilibrium constant. The transport equation representing conservation of energy can be formulated in various ways with a number of alternatives for the principle variable. For low Mach number ($Ma = u/a$, where a represents the speed of sound) flows, conservation of energy may be represented by the static enthalpy of the mixture h [103] which is the mass weighted sum of the species enthalpies h_α

$$h = \sum_{\alpha=1}^{n_{sp}} Y_\alpha h_\alpha \quad (1.18)$$

and the species enthalpies are given by

$$h_\alpha = \Delta h_\alpha^0 + \int_{T_0}^T c_{p\alpha} dT \quad (1.19)$$

where Δh_α^0 is the enthalpy of formation at the reference state p_0 , T_0 and $c_{p\alpha}$ is the specific heat of species α at temperature T and constant pressure. The enthalpy of formation is defined as the change in enthalpy during the formation of 1 mole of a substance from its constituent elements usually at the reference state $p_0 = 1$ bar and $T_0 = 298.15$ K. The specific heat of the mixture follows from the mass weighted sum of the species specific heat

$$c_p = \sum_{\alpha=1}^{n_{sp}} Y_\alpha c_{p\alpha}. \quad (1.20)$$

The transport equation for the static enthalpy of the mixture is given by [136]

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_i h}{\partial x_i} = \frac{Dp}{Dt} - \frac{\partial J_i^h}{\partial x_i} + \tau_{ij} \frac{\partial u_i}{\partial x_j} + q + \rho f \quad (1.21)$$

where the first term on the right hand side (RHS) is written in terms of the substantial derivative [97]

$$\frac{D(\cdot)}{Dt} = \frac{\partial(\cdot)}{\partial t} + u_i \frac{\partial(\cdot)}{\partial x_i}. \quad (1.22)$$

For low Mach number flows, the $u_i \partial p / \partial x_i$ term is small [103, 134] and is therefore neglected. Furthermore, at constant pressure, Libby & Williams [104] and Peters [134] argue that the $\partial p / \partial t$ term may be neglected at low Ma numbers. J_i^h represents the heat flux and consists of three contributors [175], flux caused by heat conduction, flux caused by concentration gradients (Dufour effect) and flux caused by diffusion. The Dufour effect is usually negligible in combustion processes [103, 175] and is therefore omitted. The heat flux term may then be written in terms of contributions from conduction and diffusion

$$J_i^h = -\lambda \frac{\partial T}{\partial x_i} + \sum_{\alpha=1}^{n_{sp}} h_{\alpha} J_i^{\alpha} = -\lambda \frac{\partial T}{\partial x_i} - \sum_{\alpha=1}^{n_{sp}} \rho h_{\alpha} D \frac{\partial Y_{\alpha}}{\partial x_i} \quad (1.23)$$

where λ represents thermal conductivity and T the temperature. The third term in Eq. (1.21) is the viscous heating source term which is small in low speed flows [103, 134]. The fourth term is a heat source term related to radiant flux and is omitted in the present work. The last term is related to body forces (gravity) which are small compared to the thermal energy produced through chemical reactions [103]. Further simplifications are possible by differentiating Eq. (1.18) with respect to T and include Eqs. (1.19) and (1.20)

$$\frac{\partial h}{\partial T} = \sum_{\alpha=1}^{n_{sp}} \left(h_{\alpha} \frac{\partial Y_{\alpha}}{\partial T} + Y_{\alpha} \frac{\partial h_{\alpha}}{\partial T} \right) = c_p + \sum_{\alpha=1}^{n_{sp}} h_{\alpha} \frac{\partial Y_{\alpha}}{\partial T} \quad (1.24)$$

and rewrite the expression to get

$$\partial T = \frac{1}{c_p} \partial h - \frac{1}{c_p} \sum_{\alpha=1}^{n_{sp}} h_{\alpha} \partial Y_{\alpha} \quad (1.25)$$

Applying Eq. (1.25) to Eq. (1.23)

$$J_i^h = -\frac{\lambda}{c_p} \frac{\partial h}{\partial x_i} - \sum_{\alpha=1}^{n_{sp}} h_{\alpha} \left(\rho D - \frac{\lambda}{c_p} \right) \frac{\partial Y_{\alpha}}{\partial x_i} \quad (1.26)$$

and introducing the result into Eq. (1.21) together with the simplifications discussed above and the Schmidt ($Sc = \mu/\rho D$) and Prandtl ($\sigma = c_p \mu/\lambda$) numbers results in Eq. (1.27). Eq. (1.27) represents the balance equation for the static enthalpy suitable for low Ma number flows [104].

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_i h}{\partial x_i} = \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i} \left[\frac{\mu}{\sigma} \frac{\partial h}{\partial x_i} + \mu \sum_{\alpha=1}^{n_{sp}} \left(\frac{1}{Sc} - \frac{1}{\sigma} \right) h_{\alpha} \frac{\partial Y_{\alpha}}{\partial x_i} \right] \quad (1.27)$$

At this point it may be noted that a significant simplification is possible if the Lewis ($Le = Sc/\sigma$) number is unity. The latter assumptions remove the last term of the equation.

Finally, an equation of state that relates pressure, density and temperature is given, assuming ideal gases, by [104]

$$p = \frac{\rho R T}{M} = \rho R T \sum_{\alpha=1}^{n_{sp}} \frac{Y_{\alpha}}{M_{\alpha}} \quad (1.28)$$

where R is the universal gas constant. The equations presented above represent in principle a mathematical description of reacting fluid flows. If the discussion now is restricted to premixed combustion, Eqs. (1.14) and (1.27) may be replaced by one single equation, the transport equation for the reaction progress variable (c). Bray [12] assumes the following, combustion is controlled by a global and irreversible reaction step, the specific heat is constant at constant pressure and the molecular weight of the mixture is constant. Furthermore, pressure fluctuations are assumed to

be small, the σ and Sc numbers are both unity, there are no heat losses (adiabatic) and the Ma number is small compared to unity. Under these conditions the reaction progress variable may be defined as

$$c = \frac{T - T_u}{T_b - T_u} = \frac{Y_{F,u} - Y_F}{Y_{F,u} - Y_{F,b}} \quad (1.29)$$

where subscripts u and b denote properties in the unburnt and burnt gases, respectively, and Y_F represents the fuel mass fraction. Due to its definition, the reaction progress variable takes on values between zero and unity where 0 represents unburnt gases and 1 burnt gases and values in between represent a mixture undergoing chemical reaction. The fluid density may be obtained as

$$\rho = \frac{\rho_u}{1 + \mathcal{T}c} \quad (1.30)$$

where $\mathcal{T}$ represents the heat release parameter

$$\mathcal{T} = \frac{T_b}{T_u} - 1. \quad (1.31)$$

From the definition of the reaction progress variable, the mass fractions of oxidiser Y_O and products Y_P follows from the global reaction step

$$Y_O = Y_{O,u}(1 - c) \quad (1.32)$$

$$Y_P = cY_{P,b} \quad (1.33)$$

while the inert mass fraction Y_I is given by

$$Y_I = 1 - Y_F - Y_O \quad (1.34)$$

since by definition the sum of mass fraction equals unity. As shown above, mass fractions, temperature and density are all uniquely related to the reaction progress variable c . The problem of solving a minimum of four transport equations to obtain

T , Y_F , Y_O , Y_P and Y_I has been reduced to a single equation, the transport equation for the reaction progress variable

$$\frac{\partial \rho c}{\partial t} + \frac{\partial \rho u_i c}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\rho D \frac{\partial c}{\partial x_i} \right] + \rho S \quad (1.35)$$

which has the same general form as Eq. (1.14).

1.2.1 Direct numerical simulation

Direct numerical simulation (DNS) is conceptually the modelling approach that is easiest to understand — the governing equations are directly solved using numerical methods. Since the method does not rely on any modelling assumptions all scales of motion are resolved, hence providing an outstanding accuracy and level of description for one realisation of the flow. The numerical representation of all scales of motion requires high resolution in both space and time. The resolution in space rises rapidly with the Reynolds number and scales as $N^3 \propto Re^{\frac{9}{4}}$, while the Courant number needs to be of the order of 1/20 in practical simulations. Based on these numbers, Pope [143] estimates that the required time in days to perform DNS of isotropic turbulence is proportional to $(Re/800)^3$. This estimate assumes that the duration of the simulation (number of time steps) is four times the turbulence time scale, that 1000 floating point operations are needed for each grid point and that the computing rate is one gigaflop. This means that at $Re = 96000$ the simulation time is of the order of 5000 years of which more than 99% is spent on resolving the smallest scales, i.e the dissipation range. This approach is clearly limited to low or moderate Reynolds numbers. A further limitation is the vast amount of information provided by DNS. Poinso & Veynante [136] argue that DNS is still out of reach for practical flows especially reacting flows and that simplifications are necessary.

Nevertheless, DNS provides valuable information for modelling purposes, information that might be very difficult or impossible to extract from experiments. Eswaran & Pope [46] studied the mixing of an inert passive scalar in homogenous turbulence using DNS. Starting from a bimodal-like initial field, it was found that

the PDF of the scalar evolve continuously and tends to, as expected, a Gaussian distribution. The variance decay will continuously increase the value of the PDF at the mean and at the limit $t \rightarrow \infty$, converges to a δ function. The evolution of the scalar PDF is important for modelling purposes of the molecular mixing term in transported PDF methods. The DNS results suggest that a successful model should allow the Gaussian distribution as a solution.

1.2.2 Moment methods

A numerically tractable approach is a necessity for the successful application to practical devices. The dominating method of choice in industry is still, and for some time to come, computational methods based on a statistical description of the flow field where moments are evaluated. The latter can be obtained by solving the mean conservation equations using RANS (Reynolds Averaged Navier Stokes) approaches. The basic advantage of a statistical description is that all the turbulent scales are comparable to the dimensions of the solution domain, which makes the grid requirements manageable. On the other hand, the averaging techniques applied to the governing equations inevitably results in an unclosed set of equations. The starting point is the Reynolds decomposition of an instantaneous variable ϕ into mean $\langle \phi \rangle$ and fluctuation ϕ' parts

$$\phi = \langle \phi \rangle + \phi' \quad \text{and} \quad \langle \phi' \rangle = 0. \quad (1.36)$$

In variable density flows it is advantageous to use a density-weighted Favre average [80] of the dependent variable

$$\phi = \frac{\langle \rho \phi \rangle}{\langle \rho \rangle} + \phi'' = \tilde{\phi} + \phi'' \quad \text{and} \quad \langle \phi'' \rangle = -\frac{\langle \rho' \phi' \rangle}{\langle \rho \rangle} \neq 0 \quad (1.37)$$

where $\tilde{\phi}$ and ϕ'' denotes Favre averaged mean and fluctuation respectively. The mean part of Eq. (1.36) may be obtained as a time average for statistically stationary

flows [140]

$$\langle \phi \rangle \equiv \lim_{\Delta t \rightarrow \infty} \frac{1}{\Delta t} \int_0^{\Delta t} \phi(t) dt \quad (1.38)$$

or as an ensemble average

$$\langle \phi \rangle_N \equiv \frac{1}{N} \sum_{i=1}^N \phi^{(i)} \quad (1.39)$$

where N denotes the number of realisations. An alternative definition of the mean, the mathematical expectation [140], can be given in terms of the probability density function (PDF) f_ϕ of ϕ

$$\langle \phi \rangle \equiv \int_{\Psi} \Psi f_\phi(\Psi) d\Psi \quad \text{or} \quad \tilde{\phi} \equiv \int_{\Psi} \Psi \tilde{f}_\phi(\Psi) d\Psi \quad \phi \in \Psi \quad (1.40)$$

where Ψ represents the allowable (sample space) region in ϕ -space. The mathematical expectation of the ensemble average $\langle \phi \rangle_N$ of Eq. (1.39) is simply the average of ϕ ($\langle \langle \phi \rangle_N \rangle = \langle \phi \rangle$).

Application of the decomposition to the conservation equations (1.8), (1.9) and (1.35) followed by averaging, yields the mean equations for mass, momentum and reaction progress variable at high Re number

$$\frac{\partial \langle \rho \rangle}{\partial t} + \frac{\partial \langle \rho \rangle \tilde{u}_j}{\partial x_j} = 0 \quad (1.41)$$

$$\frac{\partial \langle \rho \rangle \tilde{u}_i}{\partial t} + \frac{\partial \langle \rho \rangle \tilde{u}_j \tilde{u}_i}{\partial x_j} = - \frac{\partial \langle p \rangle}{\partial x_i} - \frac{\partial \langle \rho \rangle \widetilde{u_i'' u_j''}}{\partial x_j} + \langle \rho \rangle g_i \quad (1.42)$$

$$\frac{\partial \langle \rho \rangle \tilde{c}}{\partial t} + \frac{\partial \langle \rho \rangle \tilde{u}_i \tilde{c}}{\partial x_i} = - \frac{\partial \langle \rho \rangle \widetilde{u_i'' c''}}{\partial x_i} + \langle \rho \rangle \tilde{S}. \quad (1.43)$$

The resulting mean equations for momentum and scalars contain turbulent transport correlations, the Reynolds stresses ($\widetilde{u_i'' u_j''}$) and turbulent scalar fluxes ($\widetilde{u_i'' c''}$), while the last term in Eq. (1.43) is a source term representing the mean turbulent reaction rate. All latter terms are unknown and in order to solve the equations above, closures need to be obtained.

1.2.2.1 Gradient diffusion closures

The most commonly adopted closure assumption is based on dimensional analysis of unknown terms. A typical example is eddy viscosity/gradient diffusion type closures [57, 79] where the unknown terms are closed by an algebraic expression containing known quantities and the turbulence kinetic energy (k) and its dissipation rate (ϵ)

$$\langle \rho \rangle \widetilde{u_i'' u_j''} = -\mu_T \left(\frac{\partial \widetilde{u_i}}{\partial x_j} + \frac{\partial \widetilde{u_j}}{\partial x_i} \right) + \frac{2}{3} \left(\langle \rho \rangle \widetilde{k} + \mu_T \frac{\partial \widetilde{u_k}}{\partial x_k} \right) \delta_{ij} \quad (1.44)$$

$$\langle \rho \rangle \widetilde{u_i'' c''} = -\frac{\mu_T}{\sigma_T} \frac{\partial \widetilde{c}}{\partial x_i} \quad (1.45)$$

where σ_T represents the turbulent Prandtl number and is of the order of unity and μ_T is closed by [104]

$$\mu_T = C_\mu \langle \rho \rangle \frac{\widetilde{k}^2}{\widetilde{\epsilon}} \quad (1.46)$$

and $\widetilde{k}$ is half of the trace of the Reynolds stress tensor ($\widetilde{k} = \widetilde{u_k'' u_k''}/2$). It should be noted that μ_T is a property of the flow rather than the fluid. The turbulence kinetic energy and its dissipation are usually obtained through their respective modelled transport equations, here represented in their standard high Reynolds number form [79]

$$\frac{\partial \langle \rho \rangle \widetilde{k}}{\partial t} + \frac{\partial \langle \rho \rangle \widetilde{u_i k}}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\frac{\mu_T}{\sigma_k} \frac{\partial \widetilde{k}}{\partial x_i} \right] + P_k - \langle \rho \rangle \widetilde{\epsilon} \quad (1.47)$$

$$\frac{\partial \langle \rho \rangle \widetilde{\epsilon}}{\partial t} + \frac{\partial \langle \rho \rangle \widetilde{u_i \epsilon}}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\frac{\mu_T}{\sigma_\epsilon} \frac{\partial \widetilde{\epsilon}}{\partial x_i} \right] + C_{\epsilon 1} P_k \frac{\widetilde{\epsilon}}{\widetilde{k}} - C_{\epsilon 2} \langle \rho \rangle \frac{\widetilde{\epsilon}^2}{\widetilde{k}}. \quad (1.48)$$

The source term P_k is the trace of the Reynolds stress production term

$$P_k = - \langle \rho \rangle \widetilde{u_i'' u_j''} \frac{\partial \widetilde{u_i}}{\partial x_j} \quad (1.49)$$

and the model constants of the standard $k - \epsilon$ model following Jones & Launder [79]

$$\sigma_k = 1.0 \quad \sigma_\epsilon = 1.3 \quad C_\mu = 0.09 \quad C_{\epsilon 1} = 1.44 \quad C_{\epsilon 2} = 1.92. \quad (1.50)$$

The basic advantage of the algebraic closure for the turbulent transport terms, is computational simplicity compared to the more complex second moment closures. The reported applications of eddy viscosity/gradient diffusion type closures are numerous [7, 9, 31, 38, 57, 74, 98, 99, 137] and while they are often capable of providing good results they do have limitations, for example their incapability of reproducing swirling motions and the effects of strong streamline curvature.

1.2.2.2 Mean reaction rate closures

The averaging technique applied to the governing equations makes it problematic to model the mean reaction rate $\langle \rho \rangle \tilde{S}_\alpha$ due to the highly non-linear chemical kinetics involved in the reaction rate expression. Consider an idealised forward reaction step



where fuel and oxidiser reacts and form combustion products. The mean rate of reaction for the fuel may then be written [103] as

$$\begin{aligned} \langle \rho \rangle \tilde{S}_F = & - \langle \rho \rangle \tilde{k}^f (\langle \rho \rangle \tilde{Y}_F \tilde{Y}_O + \langle \rho Y_F'' Y_O'' \rangle) \\ & - \langle \rho (\rho k^f)'' Y_O'' \rangle \tilde{Y}_F - \langle \rho (\rho k^f)'' Y_F'' \rangle \tilde{Y}_O - \langle \rho (\rho k^f)'' Y_F'' Y_O'' \rangle \end{aligned} \quad (1.52)$$

where the first term on the RHS is related to mean quantities only and the remaining five terms represent turbulence-chemistry interaction correlations. The turbulent terms are unknown and require modelling. In addition, an expression for the forward Favre averaged rate constant $\tilde{k}^f$ is needed. Since the rate constant is an exponential function of temperature, the only tractable approximation is to derive a power series of the exponential function, which introduces additional unknown turbulent temperature fluctuation terms. It should, however, be noted that, according to Eq. (1.16), for this reaction, the production rate depends only on ρ , T , Y_F and Y_O and the mean reaction rate of Y_F may be obtained as [103]

$$- \langle \rho \rangle \tilde{S}_F = \int_0^\infty \int_0^\infty \int_0^1 \int_0^1 \rho^2 k^f Y_F Y_O f_\phi(\rho, T, Y_F, Y_O; x) dY_F dY_O dT d\rho \quad (1.53)$$

if the joint scalar probability density function (PDF) $f_\phi(\rho, T, Y_F, Y_O; x)$ is known.

As indicated above, a simplified and more practical approach is required to close the mean reaction rate. One possible way forward is to limit the applicability of the model to certain combustion regimes. In the laminar flamelet regime of combustion, reactants and products are separated by thin interfaces. These thin interfaces should have thicknesses less than the Kolmogorov scale of turbulence and resemble that of a strained laminar flame. In this regime the mean reaction rate may be written in the following generic form [15]

$$\langle \rho \rangle \tilde{S} = \rho_u u_L^0 I_0 \Sigma \quad (1.54)$$

where I_0 represents a strain reduction factor and Σ is the flamelet surface to volume ratio. Algebraic or transport equation based closures [134] for Σ have been proposed. The latter approach requires a number of unknown terms to be modelled and increases the computational expense. Lindstedt & Sakthitharan [106] obtain a simple algebraic expression by assuming that the flamelet geometry being fractal — a concept introduced by Gouldin [59] in the context of turbulent burning velocity models. Following Lindstedt & Sakthitharan [106], if ε is a measurement scale and L^3 denotes a volume measure, the flamelet surface to volume ratio is proportional to

$$\Sigma \equiv \frac{\mathcal{A}}{L^3} \propto \frac{1}{L} \left(\frac{\varepsilon}{L} \right)^{2-\mathcal{D}} \quad (1.55)$$

where $\mathcal{A}$ is an area measure and $\mathcal{D}$ being the fractal dimension between 2 and 3 for homogeneous turbulence [133]. Lindstedt & Sakthitharan [106] assumes the inner cut-off to be equal to the Kolmogorov length scale $l_K = (\nu^3 \epsilon^{-1})^{1/4}$ and outer cut-off to be equal to the turbulent integral length scale [59] ($l_T = k^{3/2} \epsilon^{-1}$) and the fractal dimension to be $\mathcal{D} = 7/3$. The resulting expression for the flamelet surface to volume ratio is given by

$$\Sigma \propto \frac{1}{(\nu \tilde{\epsilon})^{1/4}} \frac{\tilde{\epsilon}}{k} P_R = \frac{1}{V_K} \frac{\tilde{\epsilon}}{k} P_R \quad (1.56)$$

where V_K is the Kolmogorov velocity and P_R is the probability of reaction assumed proportional to the reaction progress variable variance $\widetilde{c''^2}$ [108]. An algebraic expression for the variance is given in Section 2.6. Thus, the resulting mean reaction rate expression takes the following form

$$\langle \rho \rangle \tilde{S} = C_R \rho_u \frac{u_L^0}{V_K} \frac{\tilde{\epsilon}}{\widetilde{c''^2}}. \quad (1.57)$$

The strain reduction factor (I_0) is assumed to be unity, though more sophisticated expressions are available [15]. Bray et al. [22] evaluated a number of different closures for the mean reaction rate and concluded that none of the models, except the model given by Eq. (1.57), could be tuned to work satisfactorily. Lindstedt & Város [108] performed turbulent burning velocity calculations using the aforementioned mean reaction rate closure and obtained a desired scaling behaviour in response to length scale variations in the flamelet regime of combustion.

Peters [133] used the Gibson scale $l_G = (u_L^0)^3/\epsilon$ instead of the Kolmogorov scale as the inner cut-off. Following the fractal analysis given by Eqs. (1.55)-(1.57) and using the Gibson scale as the inner cut-off results in a flamelet surface to volume ratio expression given by

$$\Sigma \propto \frac{1}{u_L^0} \frac{\tilde{\epsilon}}{\widetilde{c''^2}} P_R \quad (1.58)$$

that essentially represents The Eddy-Break-Up (EBU) model first proposed by Spalding [161, 162] as shown by Lindstedt & Sakthitharan [106]. The model is attractive due to its simplicity and is given by

$$\langle \rho \rangle \tilde{S} = C_{EBU} \langle \rho \rangle \tau^{-1} \widetilde{c''^2} = C_{EBU} \langle \rho \rangle \frac{\tilde{\epsilon}}{\widetilde{c''^2}} \quad (1.59)$$

where τ represents a characteristic turbulent time scale of the largest eddies and C_{EBU} a model constant. At this point it should be noted that the mean reaction rate expression given by the EBU model can be proportional to the square root of the reaction progress variable variance [175]. Dimensional arguments were initially the basis of the introduction of this alternative model form, which may lead to

mathematical difficulties [136]. The EBU model is applicable in the high Re number and Da number limit and it is assumed that the rate of reaction is solely controlled by turbulence. The latter assumption is also one of the major drawbacks since the model does not contain any chemical kinetics information.

A different class of models are based on a closure of the turbulent burning velocity (u_T). The idea originates from the level set approach, where a passive scalar represents an iso-scalar surface, the flame front, which propagates at the turbulent burning velocity. Zimont et al. [183] applies the idea from the level set approach and formulates a mean reaction progress variable equation of the form

$$\frac{\partial \langle \rho \rangle \tilde{c}}{\partial t} + \frac{\partial \langle \rho \rangle \tilde{u}_i \tilde{c}}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\langle \rho \rangle D_T \frac{\partial \tilde{c}}{\partial x_i} \right) + \rho_u u_T \left| \frac{\partial \tilde{c}}{\partial x_i} \right| \quad (1.60)$$

where the last term represents the closure for the mean reaction rate. This model is for some reason popular in commercial software packages [184, 185] although being mathematically incorrect. Peters [134] have shown that Eq. (1.60) has no solution for a steady planar turbulent premixed flame.

1.2.3 Large eddy simulation

Large eddy simulation (LES) is a method that is becoming increasingly popular, probably due to the rapid increase in computational power. LES may be viewed as a spatially filtered DNS and its computational costs are between those of moment methods and DNS. In DNS, most of the computational expense is spent on resolving the smallest scales, whereas in LES the dynamics of the large scales are resolved and computed explicitly and the small scales are modelled. The value of the approach is accordingly reduced when key phenomena occur on the small (unresolved) scales. The large scales are not universal, but strongly case (geometry) dependent, while the smallest turbulent scales may be regarded as universal. Traditionally, simple models are applied to represent the small scale turbulence. The method is regarded to be more accurate compared to moment methods (second moment closures) in flows dominated by large scale motions [144]. The LES equations are derived from

the Navier-stokes equations and the basis is the filtering operation applied to the instantaneous variable that decomposes it into filtered (resolved) $\bar{\phi}(\underline{x}, t)$ and residual (subgrid) $\phi^i(\underline{x}, t)$ parts, respectively

$$\phi^i(\underline{x}, t) = \phi(\underline{x}, t) - \bar{\phi}(\underline{x}, t). \quad (1.61)$$

At this point it is worth to note, that $\bar{\phi}(\underline{x}, t)$ is random and that $\bar{\phi}^i(\underline{x}, t) \neq 0$ in general. The filtered variable is obtained from [143]

$$\bar{\phi}(\underline{x}, t) = \int G(\underline{x}^*, \underline{x}) \phi(\underline{x} - \underline{x}^*, t) d\underline{x}^* \quad \text{and} \quad \int G(\underline{x}^*, \underline{x}) d\underline{x}^* = 1 \quad (1.62)$$

where integration is over the entire flow domain and G is a specified filter function. Common filter functions are the box filter and the Gaussian filter in physical space [136, 143]. In variable density fluid flows it is convenient to use a Favre filtering function [136]

$$\bar{\rho} \tilde{\phi}(\underline{x}, t) = \int \rho G(\underline{x}^*, \underline{x}) \phi(\underline{x} - \underline{x}^*, t) d\underline{x}^*. \quad (1.63)$$

Similar to Eq. (1.61), the instantaneous variable decomposes into a Favre filtered $\tilde{\phi}(\underline{x}, t)$ and a Favre residual $\phi^n(\underline{x}, t)$

$$\phi^n(\underline{x}, t) = \phi(\underline{x}, t) - \tilde{\phi}(\underline{x}, t) \quad \text{and} \quad \tilde{\phi}^n(\underline{x}, t) \neq 0. \quad (1.64)$$

Application of the Favre filtering function to the instantaneous conservation equations results in

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = 0 \quad (1.65)$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{u}_i}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} - \frac{\partial}{\partial x_j} \left(\widetilde{\bar{\rho} u_i u_j} - \bar{\rho} \tilde{u}_i \tilde{u}_j \right) + \bar{\rho} g_i \quad (1.66)$$

$$\frac{\partial \bar{\rho} \tilde{c}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{c}}{\partial x_i} = -\frac{\partial \bar{J}_i}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\widetilde{\bar{\rho} u_i c} - \bar{\rho} \tilde{u}_i \tilde{c} \right) + \bar{\rho} \tilde{S} \quad (1.67)$$

where $(\widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j)$ and $(\widetilde{u_i c} - \tilde{u}_i \tilde{c})$ represent the residual stress τ_{ij}^R and scalar flux terms which require modelling. Also, the last term of Eq. (1.67), the filtered reaction

rate, requires modelling. The residual kinetic energy k_r may be obtained from

$$k_r = \frac{1}{2} \tau_{ii}^R \quad (1.68)$$

and the anisotropic residual stress tensor τ_{ij}^r is given by

$$\tau_{ij}^r = \tau_{ij}^R - \frac{2}{3} k_r \delta_{ij}. \quad (1.69)$$

The isotropic part of the residual stress tensor is usually included in the filtered pressure

$$\bar{p} = \bar{p} + \frac{2}{3} k_r. \quad (1.70)$$

Combining Eqs. (1.68)-(1.70) and rewrite Eq. (1.66) to get

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{u}_i}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} - \frac{\partial \bar{\rho} \tau_{ij}^r}{\partial x_j} + \bar{\rho} g_i. \quad (1.71)$$

In analogy with moment methods, the most common adopted closure assumptions are based on gradient diffusion approximations. The simplest model, the Smagorinsky model [143], may be viewed as an LES version of the $k - \epsilon$ model and is given by

$$\tau_{ij}^r = -\nu_r \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) = -2\nu_r \tilde{S}_{ij} \quad (1.72)$$

where $\tilde{S}_{ij}$ is the Favre filtered rate of strain and the eddy viscosity ν_r is given by

$$\nu_r = (C_S \Delta)^2 \tilde{\mathcal{S}}. \quad (1.73)$$

In the above, $\tilde{\mathcal{S}} = (2\tilde{S}_{ij}\tilde{S}_{ij})^{1/2}$ represents the characteristic Favre filtered rate of strain, Δ the filter width and C_S is a model constant. The model is attractive due to its simplicity but is known to be very dissipative [136]. The Germano dynamic model, on the other hand, estimates the dissipation of the small scales from the resolved scales and dynamically adjusts the model constant [136] to reduce the dissipative nature of the Smagorinsky model. The scalar flux term is usually closed

through a gradient diffusion approximation [136]

$$\widetilde{u_i c} - \tilde{u}_i \tilde{c} = -\frac{\nu_r}{Sc_r} \frac{\partial \tilde{c}}{\partial x_i} \quad (1.74)$$

where Sc_r is a subgrid scale Schmidt number. It has been argued that this closure is sufficient and that it is possible to capture counter-gradient transport through the large scales [87]. However, preferential acceleration effects depend on pressure gradients that act across all scales. Finally, the filtered reaction rate needs to be closed. As in the case of the simple residual stress and scalar flux models, a classical moment method model, such as the EBU model, can be rewritten into a version suitable for LES

$$\bar{\rho} \tilde{S} = C_{EBU} \bar{\rho} \frac{1}{\tau_r} \tilde{c}(1 - \tilde{c}) \quad (1.75)$$

where τ_r represents a residual turbulent time scale and is estimated as

$$\tau_r \approx \frac{\Delta}{\sqrt{k_r}}. \quad (1.76)$$

The lack of chemical kinetics information prevails in the LES-EBU model. A more important and general issue for the closure of the filtered reaction rate is the turbulent flame thickness in respect to the filter (mesh) width. Consider a premixed turbulent flame in the flamelet regime (see Section 1.1.1 for details) with a flame thickness smaller than the Kolmogorov scale. In order to resolve the flame front, the filter width has to be smaller than the Kolmogorov scale and then the LES approaches DNS in computational expense. A way to avoid the unresolved flame front is to artificially thicken [135] the flame to suit the filter width while maintaining the burning velocity characteristics. This changes the flame dynamics in a potentially inaccurate way and the approach is more of a practical nature rather than based on physical arguments.

Several LES studies featuring premixed reactants has been carried out. Kim et al. [87] performed swirling flow simulations of a gas turbine combustion chamber using a dynamic residual stress model and the G-equation (level-set) flamelet

approach. A coarse grid was used, but the general trends agreed well with experimental data. Nottin et al. [132] solved an acoustically excited premixed turbulent flame using the artificial thickened flame approach and the Smagorinsky residual stress model. The large coherent structures seen in the experimental data were well reproduced by the LES. The peak values of the reaction rate, on the other hand, were not predicted in the right locations. Selle et al. [156] used a compressible LES formulation to compute both non-reacting and reacting flows in a gas turbine combustion chamber. The methane-air combustion was represented by a reduced two-step mechanism coupled with the artificially thickened flame model. In general, predictions in the non-reacting case were better than in the reacting case. Sommerer et al. [159] simulated atmospheric lean premixed swirl stabilised propane flames in an experimental gas turbine combustion chamber using the artificially thickened flame model. Qualitative comparisons with OH-radical measurements were done for different equivalence ratios and flow rates resulting in different flame locations including flashback. Freitag & Janicka [50] computed the isothermal and reacting flow of an unconfined swirl burner using a dynamic Smagorinsky model. In the reacting case, the premixed flame was modelled using the level-set approach. A good agreement with experimental data was obtained for both cases. Nogenmyr et al. [131] simulated unconfined low-swirl lean premixed methane flames in a low-speed air co-flow using the Smagorinsky residual stress model and the G-equation flamelet approach. Velocity and temperature predictions agreed reasonably well with experimental data, while the lift-off height of the flame was, in general, underpredicted by the LES. Sengissen et al. [157] studied the influence of additional pilot flames on the flame stability. The case features a lean premixed swirling main flame with a central fuel pilot. At low levels of pilot fuel, a processing vortex core is observed, while an increase in pilot fuel had a stabilising effect. A similar study was performed by Milosavljevic et al. [129] in the context of second moment closures where an increase in pilot fuel changed the entire flow structure and had a stabilising effect. Wang & Bai [174] computed a bluff-body stabilised premixed propane flame using the level-set flamelet approach to study the effect of filtered and residual eddies on

the flame wrinkling. A simple test case is used to evaluate the effect of the residual stress model and it is shown that it has a major impact on flame wrinkling and thereby the burning velocity.

1.2.4 Transported PDF methods

In transported probability density function (PDF) methods, a transport equation is derived for the PDF itself and, as a consequence, no *a priori* assumption has to be made of the shape of the PDF. The approach offers significant advantages over the more traditional presumed PDF approach since finite rate chemistry effects are naturally included. The inclusion of finite rate chemistry effects offers the possibility to predict emission levels [96, 109, 113] and to study for example extinction and re-light phenomena [111] that are well separated from the high Da number limit. Furthermore, transported PDF methods offer, in principle, a general realisable [155] multiple scalar description of turbulent reacting flows in a combustion regime and flame type independent manner [140]. The transported PDF equation may for example be closed at the joint velocity-scalar level or at the joint scalar level. In the case of a closure at the joint velocity-scalar level, the PDF provides a complete one-point statistical description of a turbulent reactive flow field. The one-point description contains, however, no length or time scale information and such information must therefore be supplied. In the joint velocity-scalar PDF transport equation conditional expectations appear that needs to be modelled. The conditional expectations represent transport in velocity space by the viscous stresses, the fluctuating pressure gradient and transport in scalar space by the molecular fluxes, commonly known as mixing. The transport of the PDF in physical space appears in closed form. This is equivalent to a second moment closure [142] where the triple moments appear in closed form. In the joint scalar PDF transport equation the unknown terms comprise the molecular mixing term and transport of the PDF in physical space. Transport in physical space is usually closed by a gradient diffusion type model. It is, however, remarkable to note that in both of the aforementioned approaches the highly non-linear term representing chemical reaction appears in

closed form and can be treated without approximation [140]. The potentially large dimensionality of the PDF requires some special treatment. Numerical integration of the transported PDF equation using traditional finite volume techniques would be impractical since the computer requirements rises exponentially with the dimensionality of the PDF. Instead a *Monte Carlo*¹ technique is used where the requirements only rise linearly [140] with the number of variables.

The joint PDF closure as implemented in the context of LES/filtered density function (FDF) methods is also starting to be explored. Yilmaz et al. [180] applied a closure at the joint scalar level to compute a turbulent premixed flame stabilised on a Bunsen burner with encouraging results. Furthermore, McDermott and Pope [126] analysed the role of molecular transport in physical space alongside transport in composition space and showed that it is possible to produce FDF models that reduce to the DNS limit with vanishing filter width.

1.3 The present contribution

1.3.1 Objectives

In the present thesis, advanced modelling techniques of turbulent combustion with reactive scalars and heat release rates of practical relevance are examined. The closure level adopted features second moment closures coupled with both presumed and transported PDF methods for the scalar statistics. Attention is primarily focused on the predictive capabilities of such models in practical flow situations featuring premixed or partially premixed reactants.

The basis of the modelling techniques examined is that the variables of interest may be considered to be random. Random variables are completely defined by their statistical distribution through a probability density function (PDF). The PDF represents the probability per unit distance in sample space [143]. In the current work, the models can be divided in two categories and may be separated by the level of

¹Monte Carlo algorithms are computational algorithms that rely on repeated random sampling to compute their results.

closure of the scalar field. In the first category, the presumed PDF approach, the shape of the scalar variable PDF is assumed and determined *a priori*. Transport equations are solved for the first moment, the expected (mean) value and the second central moment (variance). The chemical kinetics is assumed to be fast compared to the relevant turbulent time scale and may be computed and tabulated beforehand as a pre-processing step. The fast chemistry assumption limits the method to regimes approaching the high Da number limit indicated as the flamelet regime in Fig. 1.1. *A priori* tabulation of the chemistry implies that the chemistry is decoupled from the flow solver. Consequently extinction and re-light phenomena are not possible to capture using this approach. In a second category, a transport equation is derived and solved for the PDF of the scalar statistics. Since the approach does not assume the shape of the PDF the method offers a general multiple scalar description of turbulent reacting flows in a combustion regime and flame type independent manner. In transported PDF methods, the turbulence-chemistry interaction is rigorously treated and the approach represents one of the most complete descriptions of turbulent reacting flows currently available [25]. It is remarkable that highly non-linear chemical reactions can be treated without approximation — the chemical source term appear in closed form. One of the key modelling aspects of the joint scalar transported PDF equation is to obtain closure of the molecular mixing term, the mixing model. In the current work, one of the most commonly adopted mixing models is evaluated in the context of turbulent premixed flames featuring multiple scalars and a number of key issues are identified. Transport in physical space is closed by a standard gradient diffusion type closure. In both cases, transport equations are derived and closed using first and second moment methods for the velocity field.

1.3.2 Outline

In Chapter 2, general modelling strategies for second moment closures are outlined. The starting point is the decomposition of the turbulent pressure strain terms in the Reynolds stress and scalar flux equations. Attention is primarily focused on the

redistributive part of the pressure strain correlation in the Reynolds stress equation and the corresponding scrambling term in the scalar flux equation. In turbulent reacting flows, the constant density models are usually recasted into a density weighted form. As shown by Lindstedt & Váos [108], this is not sufficient and variable density extensions of these terms are described. Furthermore, standard closures of the triple moments and pressure transport terms and the turbulence kinetic energy dissipation equation are outlined. Finally, closures applicable in the flamelet regime of combustion derived on the basis of the presumed PDF approach are described.

In Chapter 3 the transported PDF approach closed at the joint scalar level is outlined. The starting point is the transport equation supplemented with general definitions and the discrete representation of the PDF. Modelling strategies for the unclosed terms are outlined together with the solution algorithm originally proposed by Pope [140]. The solution algorithm includes the method of fractional steps allowing each process affecting the evolution of the transport equation to be treated separately. The unclosed terms represents transport in physical space and diffusion in scalar space. Closure for transport in physical space is achieved using a standard gradient diffusion type model while the mixing model is represented by The Modified Curl's model [41, 77]. The Modified Curl's model belongs to the class of particle interaction models. The Euclidean Minimum Spanning Tree (EMST) model [166] as well as deterministic and diffusion process type models are briefly described.

In Chapter 4 the models described in Chapters 2 and 3 are applied to compute isothermal and reacting opposed flows. Numerical studies have been performed of the experimental rig set-up of Geipel [52] and Geipel et al. [53]. In this geometry, the turbulent contribution is significantly increased compared to previous studies through fractal generated turbulence in addition to the traditional perforated plates. The mixture fraction variable is defined and the transport equations for the mean, scalar flux and variance are outlined. A joint β -bimodal presumed PDF approach involving two scalars, the mixture fraction and the reaction progress variable, are described. The two scalars are used to describe the effects of entrainment of air from the coflow and the progress of reaction. The node-based Eulerian joint scalar trans-

ported PDF is described and especially transport in physical space which differs to the Lagrangian approach. The chemistry is approximated by the global mechanism of Jones & Lindstedt [81, 82] and is described in detail. The scheme features four reactions and seven solved species (CH_4 , O_2 , H_2O , CO_2 , H_2 , CO and N_2). The models applied are ranging from the $k - \epsilon$ /gradient diffusion to full second moment closures coupled with a joint β -bimodal presumed PDF approach to the node-based Eulerian joint scalar transported PDF approach coupled with a second moment closure for the velocity field. The computational grid and spatial discretisation of convective terms are briefly described. The boundary conditions for this particular case is described in more detail as in-nozzle measurements are available in the isothermal case.

In Chapter 5 the joint scalar transported PDF approach is applied to compute freely propagating turbulent premixed flames with turbulent burning velocities determined for a range of turbulence intensities and fuel mixtures. The computed cases include lean and stoichiometric methane, stoichiometric ethane and rich hydrogen flames. The aim of the study is to investigate the sensitivity of predictions to different closure elements and to explore the predictive capabilities of the method for propagating turbulent premixed flames. The work features extended chemistry closures with the systematically reduced chemical mechanism applied to the methane and ethane flames featuring 142 reactions, 15 solved and 14 steady state species. A detailed sub-mechanism featuring 21 reactions and 9 solved species was used for the hydrogen flames.

In Chapter 6, the joint scalar transported PDF approach coupled with a second moment closure for the velocity field, is applied to compute the combustion process in a 3-dimensional industrial gas turbine burner geometry at realistic gas turbine conditions. The partially premixed flame is swirl-stabilised through the formation of a central recirculation zone. A joint β -bimodal presumed PDF approach is used to initialise the field for the PDF solver. The presumed PDF solution also act as a comparative solution due to the lack of experimental data at these conditions. The joint scalar transported PDF is closed at the node-based Eulerian level. The

chemistry is approximated by the global mechanism of Jones & Lindstedt [81, 82] featuring four reactions and seven solved species (CH_4 , O_2 , H_2O , CO_2 , H_2 , CO and N_2).

In Chapter 7 the general conclusions of the present work and suggestions for future work are summarised.

Chapter 2

Second moment closures

2.1 Introduction

In Section 1.2.2.1, the simplest complete turbulence model for turbulent reacting flows was presented — the Favre averaged standard $k - \epsilon$ and gradient diffusion models. The turbulence model is complete in the sense that modelled transport equations are solved to obtain the turbulence intensity and the turbulent integral length scale as compared to simpler one-equation turbulence models, where the latter is obtained from some typical flow dimension [176]. On the other hand, several authors [13, 85] have concluded that second moment closures represent the lowest level of closure for turbulent reacting flows, which are able to describe some important features of turbulence and combustion interaction. The model formulations are, however, not general with models for unclosed terms usually dictated by the assumed thermochemistry.

Applications featuring second moment closures for both velocity and scalar statistics in practical premixed reacting flow situations are somewhat limited. Bray [19] points out that it is difficult to obtain solutions to the BML (Bray-Moss-Libby) equations and suggests that the triple correlation may be replaced by gradient transport models. Lindstedt & Város [107, 108] successfully applied the latter type of model including variable density correction terms to reacting opposed flows.

2.2 The governing equations

The transport equations for the Reynolds stresses and turbulent scalar fluxes can be written [80]

$$\begin{aligned}
\frac{\partial \langle \rho \rangle \widetilde{u_i'' u_j''}}{\partial t} + \frac{\partial \langle \rho \rangle \widetilde{u_k u_i'' u_j''}}{\partial x_k} = & \underbrace{- \frac{\partial \langle \rho \rangle \widetilde{u_i'' u_j'' u_k''}}{\partial x_k}}_{\partial T_{ijk} / \partial x_k} \\
& - \underbrace{\langle \rho \rangle \left(\widetilde{u_i'' u_k''} \frac{\partial \widetilde{u_j}}{\partial x_k} + \widetilde{u_j'' u_k''} \frac{\partial \widetilde{u_i}}{\partial x_k} \right)}_{P_{ij}} \\
& - \underbrace{\left[\langle u_i'' \rangle \frac{\partial \langle p \rangle}{\partial x_j} + \langle u_j'' \rangle \frac{\partial \langle p \rangle}{\partial x_i} \right]}_{\Phi_{ij}} \quad (2.1) \\
& - \underbrace{\left[\langle u_i'' \frac{\partial p'}{\partial x_j} \rangle + \langle u_j'' \frac{\partial p'}{\partial x_i} \rangle \right]}_{\phi_{ij}} \\
& - \underbrace{\left[\langle \tau_{ik} \frac{\partial u_j''}{\partial x_k} \rangle + \langle \tau_{jk} \frac{\partial u_i''}{\partial x_k} \rangle \right]}_{\langle \rho \rangle \epsilon_{ij}}
\end{aligned}$$

$$\begin{aligned}
\frac{\partial \langle \rho \rangle \widetilde{u_i'' c''}}{\partial t} + \frac{\partial \langle \rho \rangle \widetilde{u_k u_i'' c''}}{\partial x_k} = & \underbrace{- \frac{\partial \langle \rho \rangle \widetilde{u_i'' u_k'' c''}}{\partial x_k}}_{\partial T_{ikc} / \partial x_k} \\
& - \underbrace{\langle \rho \rangle \left(\widetilde{u_k'' c''} \frac{\partial \widetilde{u_i}}{\partial x_k} + \widetilde{u_i'' u_k''} \frac{\partial \widetilde{c}}{\partial x_k} \right)}_{P_{ic}} \\
& - \underbrace{\langle c'' \rangle \frac{\partial \langle p \rangle}{\partial x_i}}_{\Phi_{ic}} - \underbrace{\langle c'' \frac{\partial p'}{\partial x_i} \rangle}_{\phi_{ic}} \quad (2.2) \\
& + \underbrace{\langle \rho \rangle \widetilde{u_i'' S_c}}_{S_{ic}} \\
& - \underbrace{\left[\langle \tau_{ik} \frac{\partial c''}{\partial x_k} \rangle - \langle J_{ck} \frac{\partial u_i''}{\partial x_k} \rangle \right]}_{\langle \rho \rangle \epsilon_{ic}}
\end{aligned}$$

and may be derived from the instantaneous conservation laws. Following Váos [170], the terms on the RHS of Eq. (2.1) represent, turbulent transport of the Reynolds

stresses (the triple moment term $\partial T_{ijk}/\partial x_k$), effects of mean strain (the production term P_{ij}), effects of mean pressure gradients (Φ_{ij}), the turbulent pressure strain term (ϕ_{ij}) and viscous dissipation ($\langle \rho \rangle \epsilon_{ij}$). Similarly, the terms on the RHS of Eq. (2.2) represent, turbulent transport of the scalar fluxes ($\partial T_{ikc}/\partial x_k$), the production term (P_{ic}), the effect of mean pressure gradient (Φ_{ic}), the pressure strain term (ϕ_{ic}), the turbulence-reaction rate correlation (S_{ic}) and viscous dissipation ($\langle \rho \rangle \epsilon_{ic}$). For modelling purposes, Lumley [122] decomposes the pressure strain correlation into a redistributive (ϕ_{ij}^R) and an isotropic part. The isotropic part is further decomposed into a pressure transport term (ϕ_{ij}^T) and a pressure dilatation term (ϕ_{ij}^D)

$$\begin{aligned} \phi_{ij} &= - \left[\langle u_i'' \frac{\partial p'}{\partial x_j} \rangle + \langle u_j'' \frac{\partial p'}{\partial x_i} \rangle - \frac{2}{3} \delta_{ij} \langle \frac{\partial p' u_k''}{\partial x_k} \rangle + \frac{2}{3} \delta_{ij} \langle \frac{\partial p' u_k''}{\partial x_k} \rangle \right] \\ &= - \underbrace{\left[\langle u_i'' \frac{\partial p'}{\partial x_j} \rangle + \langle u_j'' \frac{\partial p'}{\partial x_i} \rangle - \frac{2}{3} \delta_{ij} \langle \frac{\partial p' u_k''}{\partial x_k} \rangle \right]}_{\phi_{ij}^R} \\ &\quad - \underbrace{\frac{2}{3} \delta_{ij} \langle \frac{\partial p' u_k''}{\partial x_k} \rangle}_{\phi_{ij}^T} + \underbrace{\frac{2}{3} \delta_{ij} \langle p' \frac{\partial u_k''}{\partial x_k} \rangle}_{\phi_{ij}^D}. \end{aligned} \quad (2.3)$$

Similarly the pressure strain term in the scalar flux equation can be decomposed into a pressure transport (ϕ_{ic}^T) and a pressure scrambling term (ϕ_{ic}^S)

$$\phi_{ic} = - \langle c'' \frac{\partial p'}{\partial x_i} \rangle + \langle \frac{\partial p' c''}{\partial x_i} \rangle - \langle \frac{\partial p' c''}{\partial x_i} \rangle = - \underbrace{\langle \frac{\partial p' c''}{\partial x_i} \rangle}_{\phi_{ic}^T} + \underbrace{\langle p' \frac{\partial c''}{\partial x_i} \rangle}_{\phi_{ic}^S}. \quad (2.4)$$

In the exact Reynolds stress and scalar flux equations presented above unknown terms appear. In both equations, the turbulent transport term, the pressure strain term and the viscous dissipation term require modelling, while terms involving the turbulence-reaction rate correlation $\langle \rho \rangle \widetilde{u_i'' S_c}$ and the average density weighted fluctuations of velocity $\langle u_i'' \rangle$ and scalars $\langle c'' \rangle$ depend in general on the type of flow considered.

2.3 Redistributive pressure strain

The focal point in second moment closures is the modelling of the redistributive part of the pressure strain correlation. This correlation is traceless and serves only to redistribute energy among the Reynolds stress components while the total turbulent kinetic energy is unaltered. The redistribution process essentially amounts to minimising the anisotropy created by the production mechanism. In constant density flows, production by strain is the primary cause of anisotropy and the redistribution process is therefore scaled exclusively on mean strain. The extension to variable density flows is usually obtained through a re-derivation of constant density models in a density weighted form. This approach will result in models invariably taking the following form [164]

$$\phi_{ij}^{CD} = \langle \rho \rangle \left(\frac{\tilde{\epsilon}}{\tilde{k}} C_{ij}[\underline{b}] + B_{ijkl}[\underline{b}] \frac{\partial \tilde{u}_k}{\partial x_l} \right) \tilde{k} \quad (2.5)$$

$$\phi_{ic}^{CD} = \langle \rho \rangle \left(\frac{\tilde{\epsilon}}{\tilde{k}} C_{ij}[\underline{b}] + B_{ijkl}[\underline{b}] \frac{\partial \tilde{u}_k}{\partial x_l} \right) \widetilde{u_j'' c''} \quad (2.6)$$

where C_{ij} and B_{ijkl} are scaling tensor functions of the (normalised) anisotropy tensor b_{ij} for the “slow” and “rapid” redistribution and scrambling, respectively. The normalised anisotropy tensor is given by [143]

$$b_{ij} = \frac{\widetilde{u_i'' u_j''}}{\widetilde{u_k'' u_k''}} - \frac{1}{3} \delta_{ij}. \quad (2.7)$$

On the other hand, Jones [85] derives a Poisson type equation (ignoring viscous terms) for variable density flows of the fluctuating pressure component

$$\nabla^2 p' = -\frac{\partial^2}{\partial x_i \partial x_j} (2\rho u_i'' \tilde{u}_j + \langle \rho u_i'' u_j'' \rangle - \rho u_i'' u_j'') + \frac{\partial^2 \rho'}{\partial t^2} - \frac{\partial^2 \rho' \tilde{u}_i \tilde{u}_j}{\partial x_i \partial x_j} \quad (2.8)$$

revealing that the first three terms on the RHS are identical to the Poisson equation derived for constant density flows while the last two are due to variable density effects. Recasting of the constant density formulation into eqs. (2.5) and (2.6) would

be justified if the last two terms can be neglected. The complexity of the equation allows however limited information to be extracted [80, 85]. An order of magnitude analysis shows that the latter terms will make a significant contribution to the overall budget of the fluctuating pressure component and Jones [85] argues that modifications or additional terms may be required to accurately account for variable density effects in turbulent reacting flows. Further insight might be gained through an examination of the role of variable density effects in the production of turbulence. Bray et al. [13] have shown that, in combustions flows with substantial heat release, turbulence is produced through a buoyancy production mechanism associated with self-induced mean pressure gradients. This mechanism is related to preferential acceleration effects where mean pressure gradients act in different ways on pockets of heavy fresh gas and pockets of light burnt gas. The preferential acceleration mechanism is also responsible for counter-gradient transport. On the other hand, the importance of mean pressure gradient terms is not surprising since the average density weighted fluctuations of velocity and reaction progress variable may alternatively be interpreted as density correlation effects [80]

$$\langle u_i'' \rangle = -\frac{\langle \rho' u_i' \rangle}{\langle \rho \rangle} \quad \text{and} \quad \langle c_i'' \rangle = -\frac{\langle \rho' c_i' \rangle}{\langle \rho \rangle}. \quad (2.9)$$

With a substantial amount of heat release, turbulence production through preferential acceleration may dominate [13] over dilatation effects associated with mean velocity gradients in strain related terms, i.e. the production terms (P_{ij} , P_{ic}). Lindstedt & Város [108] argue that due to preferential acceleration effects coupled to mean pressure gradients, the rate at which energy is redistributed is substantially lower than the rate at which anisotropy is produced and that an additional element should be included in the model, thus

$$\phi_{ij}^R = \phi_{ij}^{CD} + \phi_{ij}^A \quad (2.10)$$

$$\phi_{ic}^S = \phi_{ic}^{CD} + \phi_{ic}^A \quad (2.11)$$

where the acceleration redistribution/scrambling tensors $(\phi_{ij}^A, \phi_{ic}^A)$ take the following general form

$$\phi_{ij}^A = -(A_{jk}^i[\underline{b}, <\underline{u}''>] + A_{ik}^j[\underline{b}, <\underline{u}''>]) <\rho> a_k \quad (2.12)$$

$$\phi_{ic}^A = -A_{ik}[\underline{b}, <\underline{u}''>, <\underline{c}''>] <\rho> a_k \quad (2.13)$$

and the acceleration vector (a_k) is given by

$$a_k = -\frac{1}{<\rho>} \frac{\partial <p>}{\partial x_k}. \quad (2.14)$$

Domingo & Bray [39] also argue the importance of the instantaneous and mean pressure gradient terms but adopt an alternative approach. The pressure gradient terms are decomposed into mean and fluctuating parts as in Eqs. (2.1) and (2.2). The fluctuating part (pressure strain) is then directly modelled in the laminar flamelet regime of combustion with an alternative decomposition as compared to Eqs. (2.3) and (2.4). The pressure strain terms are decomposed into reactant, product and flamelet parts and models for each contribution are derived. The resulting model is in good agreement with DNS data for low heat release flames in the flamelet regime of combustion. One of the major drawbacks of the latter approach is the loss of generality and the model of Lindstedt & Váos [108] is adopted in the present work.

2.3.1 Dissipation model considerations

The turbulent kinetic energy dissipation tensor may be decomposed into an isotropic and a deviatoric part [123]

$$\epsilon_{ij} = \left(\epsilon_{ij} - \frac{2}{3} \delta_{ij} \tilde{\epsilon} \right) + \frac{2}{3} \delta_{ij} \tilde{\epsilon}. \quad (2.15)$$

The latter decomposition does not apply to ϵ_{ic} since there are no isotropic first order tensors. In high Re number constant density flows it is usually assumed that the deviatoric part is negligible [143]. Jones [80] gives support to the latter assumption

in variable density flows as well and argues that density fluctuations are unlikely to change the fine scale dissipative motions. Therefore, it may be assumed that

$$\epsilon_{ij} = \frac{2}{3}\delta_{ij}\tilde{\epsilon} \quad (2.16)$$

and

$$\epsilon_{ic} = 0 \quad (2.17)$$

since ϵ_{ic} is not an invariant. Lumley [124] on the other hand argues that the deviatoric part of Eq. (2.15) does not represent an energy decay process, but a transfer of energy between the Reynolds stress components due to small scale anisotropy. The deviatoric part thus resembles a redistribution process that will occur in addition to the effect of pressure strain terms. The consequence of this, from a modelling point of view, is that redistribution from small scale anisotropy is modelled direct in terms of large scale quantities such as the normalised anisotropy tensor. The deviatoric part is absorbed in the redistribution model and the resulting form

$$\phi_{ij}^R - \langle \rho \rangle \epsilon_{ij} = \text{redistribution model} - \frac{2}{3}\delta_{ij} \langle \rho \rangle \tilde{\epsilon} \quad (2.18)$$

should be a valid approximation. The same arguments apply to the corresponding scrambling model in the scalar flux equation and

$$\phi_{ic}^S - \langle \rho \rangle \epsilon_{ic} = \text{scrambling model} \quad (2.19)$$

should also be valid.

2.3.2 Specific models

2.3.2.1 The generalised Langevin model of Haworth & Pope

The constant density part of the redistributive pressure strain term adopted in Chapter 4 is the generalised Langevin model of Haworth & Pope [66, 67]. An attractive feature of the model is that it satisfies realisability [155] and a consistent

closure for the corresponding scrambling term [142] may be derived. The model for the Reynolds stress equation is given by

$$\phi_{ij}^{CD} = \langle \rho \rangle G_{ik} \widetilde{u_k'' u_j''} + \langle \rho \rangle G_{jk} \widetilde{u_k'' u_i''} + \langle \rho \rangle \left(C_0 + \frac{2}{3} \right) \delta_{ij} \widetilde{\epsilon} \quad (2.20)$$

where C_0 is a constant assigned the value of 2.1 [66]. The corresponding model for the scalar flux equation is given below [142]

$$\phi_{ic}^{CD} = \langle \rho \rangle G_{ik} \widetilde{u_k'' c''} - \langle \rho \rangle \frac{\widetilde{\epsilon}_c}{\widetilde{c''^2}} \widetilde{u_i'' c''} \quad (2.21)$$

where $\widetilde{\epsilon}_c$ is the scalar dissipation rate. The functional form of G_{ij} proposed by Haworth & Pope [66], is linear in the normalised anisotropy tensor and in the mean velocity gradients, and is given by

$$G_{ij} = \frac{\widetilde{\epsilon}}{\widetilde{k}} (\alpha_1 \delta_{ij} + \alpha_2 b_{ij}) + H_{ijkl} \frac{\partial \widetilde{u}_k}{\partial x_l} \quad (2.22)$$

where

$$\begin{aligned} H_{ijkl} = & \beta_1 \delta_{ij} \delta_{kl} + \beta_2 \delta_{ik} \delta_{jl} + \beta_3 \delta_{il} \delta_{jk} \\ & + \gamma_1 \delta_{ij} b_{kl} + \gamma_2 \delta_{ik} b_{jl} + \gamma_3 \delta_{il} b_{jk} \\ & + \gamma_4 b_{ij} \delta_{kl} + \gamma_5 b_{ik} \delta_{jl} + \gamma_6 b_{il} \delta_{jk}. \end{aligned} \quad (2.23)$$

The model contains 11 unknown coefficients that are determined through mathematical constraints and matching experimental data. The model constants are given by [66]

$$\alpha_1 = - \left[\frac{1}{2} + \frac{3}{4} C_0 + \alpha_2 b_{ii}^2 + \left(\beta_2 + \beta_3 + \frac{1}{3} \gamma^* \right) I_1 + \gamma^* I_2 \right] \quad (2.24)$$

where

$$\begin{aligned} \gamma^* & \equiv \gamma_2 + \gamma_3 + \gamma_5 + \gamma_6 \\ I_1 & \equiv b_{ij} S_{ij}^* & S_{ij}^* & \equiv \frac{1}{2} \frac{\widetilde{k}}{\widetilde{\epsilon}} \left[\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i} \right] \\ I_2 & \equiv b_{ij}^2 S_{ij}^* & b_{ij}^2 & \equiv b_{il} b_{lj} \end{aligned} \quad (2.25)$$

and [142]

$$\begin{aligned}
\alpha_2 &= 3.78 & \beta_1 &= -0.2 & \beta_2 &= 0.8 & \beta_3 &= -0.2 \\
\gamma_1 &= 0.0 & \gamma_2 &= 1.04 & \gamma_3 &= -0.34 \\
\gamma_4 &= 0.0 & \gamma_5 &= 1.99 & \gamma_6 &= -0.76.
\end{aligned} \tag{2.26}$$

2.3.2.2 The model of Jones & Musonge

The constant density part of the redistributive pressure strain term derived by Jones & Musonge [83] is applied both in Chapters 4 and 6. In Chapter 4, the model is used to compute isothermal opposed flow and in Chapter 6 a swirl-stabilised partially premixed flame at realistic gas turbine conditions coupled with a presumed or joint scalar transported PDF approach. In the case of a presumed PDF approach, the Reynolds stress closure is coupled with a gradient diffusion model. Closures are presented here both for the Reynolds stress and scalar flux equations for completeness. Following Jones & Musonge [83], the redistribution term in the Reynolds stress equation is approximated by

$$\phi_{ij}^{CD} = -C_1 \frac{\tilde{\epsilon}}{\tilde{k}} \left(\widetilde{u_i'' u_j''} - \frac{2}{3} \delta_{ij} \tilde{k} \right) + H_{ijkl} \frac{\partial \tilde{u}_k}{\partial x_l} \tag{2.27}$$

where H_{ijkl} may be expressed by the fourth-rank linear tensor function

$$\begin{aligned}
H_{ijkl} &= C_2 \delta_{ij} \widetilde{u_k'' u_l''} + C_3 (\delta_{ki} \widetilde{u_l'' u_j''} + \delta_{kj} \widetilde{u_l'' u_i''}) + C_4 (\delta_{li} \delta_{kj} + \delta_{lj} \delta_{ki}) \tilde{k} \\
&\quad + C_5 \delta_{kl} \widetilde{u_i'' u_j''} + C_6 (\delta_{li} \widetilde{u_k'' u_j''} + \delta_{lj} \widetilde{u_k'' u_i''}) + C_7 \delta_{ij} \delta_{kl} \tilde{k}
\end{aligned} \tag{2.28}$$

where $C_1 - C_7$ represent model constants that needs to be determined. The constants C_5 and C_7 make no contribution in isothermal flows but are likely to be important in flows with variable density [83]. Since ϕ_{ij}^{CD} is traceless, $H_{iikl} = 0$ and the constants C_6 and C_7 may be expressed as

$$C_6 = -\frac{3}{2} C_2 - C_3 \quad \text{and} \quad C_7 = -\frac{2}{3} (C_4 + C_5) \tag{2.29}$$

and the model involves 5 independent constants for variable density flows. The revised model constants are given by [85]

$$C_1 = 3.0 \quad C_2 = -0.44 \quad C_3 = 0.46 \quad C_4 = -0.23 \quad C_5 = -\frac{2}{3}C_4. \quad (2.30)$$

Jones & Musonge [83] adopts an alternative approach to close the scalar flux equation. The turbulent pressure strain term is not decomposed into pressure transport and scrambling terms according to Eq. (2.4), instead the pressure strain term is modelled directly. In principle, the net effect of this decomposition in variable density flows is zero since pressure transport terms may be absorbed in the closure of the triple moments [124]. Here, the model is presented with the latter decomposition to maintain a consistent notation. The proposed model is given by

$$\phi_{ic}^{CD} = C_{\phi_1} \frac{\tilde{\epsilon}}{\tilde{k}(1 + C'_{\phi_1} \sqrt{b_{ij}b_{ij}})} \widetilde{u_i'' c''} + 2C_{\phi_2} b_{ij} \tilde{k} \frac{\partial \tilde{c}}{\partial x_j} + D_{ijk} \frac{\partial \tilde{u}_j}{\partial x_k} \quad (2.31)$$

where

$$D_{ijk} = C_{\phi_3} \delta_{ij} \widetilde{u_k'' c''} + C_{\phi_4} \delta_{ik} \widetilde{u_j'' c''} + C_{\phi_5} \delta_{jk} \widetilde{u_i'' c''} \quad (2.32)$$

where $C_{\phi_1} - C_{\phi_5}$ and C'_{ϕ_1} are model constants. As in the case of the velocity field model, the constant C_{ϕ_5} plays a role in variable density flows only. The model constants are given by [83]

$$C_{\phi_1} = C'_{\phi_1} = 3.0 \quad C_{\phi_2} = 0.12 \quad C_{\phi_3} = 1.09 \quad C_{\phi_4} = 0.51 \quad C_{\phi_5} = 1.0. \quad (2.33)$$

It should be noted that neither the proposed Reynolds stress closure nor the scalar flux closure satisfies realisability [155]. Jones & Musonge [83] argue that this concept requires, in essence, the model equations to remain “well behaved” as turbulence becomes two-dimensional and that these extreme states are beyond the scope of all second moment closures.

2.3.2.3 Acceleration redistribution and scrambling models

Váos [170] derived a general second order model form of the scaling tensors of the acceleration redistribution and scrambling models, but argues that the formulation probably is too complicated for practical flame calculations. Furthermore, the improvements in the predictions are not proportionate to the increased computational cost. Lindstedt & Váos [108] applied a simplified form obtained from the general formulation involving only Kronecker deltas to demonstrate the effect. Significant improvements could be seen with respect to scalar and turbulence predictions. The latter model formulation is given by

$$A_{ik}^j = f_1 \delta_{ik} \langle u_j'' \rangle + f_2 \delta_{ij} \langle u_k'' \rangle + f_3 \delta_{jk} \langle u_i'' \rangle \quad (2.34)$$

$$A_{ik} = h_1 \delta_{ik} \langle c'' \rangle \quad (2.35)$$

where $f_1 - f_3$ and h_1 are model constants which need to be determined. Since the acceleration redistribution model represents a variable density correction term in the redistribution/scrambling models given by Eqs. (2.10) and (2.11), it should have the same mathematical properties. Therefore, it is generally required that [170]

$$A_{ik}^j = A_{ki}^j \quad A_{ik}^i = 0 \quad A_{kk}^j = \langle u_j'' \rangle \quad (2.36)$$

and

$$A_{ik} = A_{ki} \quad A_{kk} = \langle c'' \rangle. \quad (2.37)$$

The latter constraints determine all the unknown coefficients

$$f_1 = \frac{2}{5} \quad f_2 = -\frac{1}{10} \quad f_3 = f_2 \quad h_1 = \frac{1}{3}. \quad (2.38)$$

Substitution of Eqs. (2.14), (2.34), (2.35) and (2.38) into Eqs. (2.12) and (2.13) gives

$$\phi_{ij}^A = -\frac{3}{10} \left[-\langle u_i'' \rangle \frac{\partial \langle p \rangle}{\partial x_j} - \langle u_j'' \rangle \frac{\partial \langle p \rangle}{\partial x_i} + \frac{2}{3} \delta_{ij} \langle u_k'' \rangle \frac{\partial \langle p \rangle}{\partial x_k} \right] \quad (2.39)$$

$$\phi_{ic}^A = -\frac{1}{3} \left[-\langle c'' \rangle \frac{\partial \langle p \rangle}{\partial x_i} \right] \quad (2.40)$$

or in terms of Φ_{ij} and Φ_{ic}

$$\phi_{ij}^A = C_{AR} \left(\Phi_{ij} - \frac{1}{3} \delta_{ij} \Phi_{kk} \right) \quad (2.41)$$

$$\phi_{ic}^A = C_{AS} \Phi_{ic} \quad (2.42)$$

where $C_{AR} = -3/10$ and $C_{AS} = -1/3$. The above form does not guarantee realizability and a slightly modified form is therefore used as proposed by Váos [170]

$$\phi_{ij}^A = C_{AR} \left(\Phi_{ij} - \frac{1}{3} \delta_{ij} \Phi_{kk} - b_{ij} \Phi_{kk} \right) \quad (2.43)$$

$$\phi_{ic}^A = C_{AS} \Phi_{ic} + C_{AR} \frac{1}{4} \frac{\widetilde{u_i'' c''}}{\widetilde{k}} \Phi_{kk}. \quad (2.44)$$

2.4 Triple moments & pressure transport

In the second moment equations, terms of third order appear and represent turbulent transport of the Reynolds stress and turbulent scalar flux through the divergence of the fluctuating velocity. In addition, Lumley [124] derived a closure for the pressure transport correlation and expressed them in terms of the triple moments

$$\langle p' u_i'' \rangle = -C^T \langle \rho \rangle \widetilde{u_i'' u_j'' u_j''} \quad \text{and} \quad \langle p' c'' \rangle = -C^T \langle \rho \rangle \widetilde{c'' u_j'' u_j''} \quad (2.45)$$

where C^T was assigned a value of 0.2. It then seems reasonable to model the triple moment and pressure transport terms jointly. Several models have been derived of various complexity, see for example Hanjalić [64]. The use of complex formulations seem a bit excessive since, in most flows, the diffusion terms do not provide a major contribution to the overall budget [85] in the transport equations. Furthermore, the more complex formulations have not been extensively tested. Therefore, in the current work, the most commonly adopted closure assumption, the gradient diffusion

formulation of Daly & Harlow [35]

$$\frac{\partial T_{ijl}}{\partial x_l} + \phi_{ij}^T = \frac{\partial}{\partial x_k} \left[C_s < \rho > \frac{\tilde{k}}{\tilde{\epsilon}} \widetilde{u_k'' u_l''} \frac{\partial \widetilde{u_i'' u_j''}}{\partial x_l} \right] \quad (2.46)$$

$$\frac{\partial T_{ilc}}{\partial x_l} + \phi_{ic}^T = \frac{\partial}{\partial x_k} \left[C_s < \rho > \frac{\tilde{k}}{\tilde{\epsilon}} \widetilde{u_k'' u_l''} \frac{\partial \widetilde{u_i'' c''}}{\partial x_l} \right] \quad (2.47)$$

is used, here generalised to include the scalar field. The constant C_s is assigned the value 0.22 [64].

2.5 Turbulent kinetic energy dissipation

The turbulent kinetic energy dissipation equation is arguably the least understood equation in moment methods. Inspection of the exact transport equation reveals a dependence of unknown double and triple correlations of fluctuating velocity and velocity gradients that are difficult to measure [176] accurately. The exact equation is therefore of little help for modelling purposes. Following Pope [143], the modelled turbulent kinetic energy dissipation equation is embedded with a lot of empiricism and is therefore best viewed as being entirely empirical. The most frequently used model equation is the high Re number version used in the framework of the standard $k - \epsilon$ model given by Eq. (1.48). Application of the model equation has shown that the model constants represent a compromise for a wide range of flows. Additional terms or adjustment of the constants for particular flows improves the result. Mohamed & LaRue [130] found that for grid generated decaying turbulence, a decay exponent of 1.3 was matching a wide range of decay data. A decay exponent of 1.3 is equivalent to adjusting the C_{ϵ_2} constant to 1.77. Other modifications of the ϵ -equation have been proposed, see for example Pope [137], Hanjalic & Launder [63], Launder [100] and Hanjalic et al. [65]. In second moment methods, the turbulent kinetic energy dissipation equation has the same general form as Eq. (1.48) but the production and diffusion terms are evaluated from the solved Reynolds stresses. For

variable density flows Jones [80] suggests that additional terms could be added,

$$\frac{\tilde{\epsilon}}{\tilde{k}} < u_i'' > \frac{\partial < p >}{\partial x_i} \quad \text{and} \quad < \rho > \tilde{\epsilon} \frac{\partial \tilde{u}_i}{\partial x_i} \quad (2.48)$$

but points out that the constants of proportionality might be difficult to obtain. In the present work the model equation applied to a range of flows by Lindstedt & Váos [108]

$$\begin{aligned} \frac{\partial < \rho > \tilde{\epsilon}}{\partial t} + \frac{\partial < \rho > \tilde{u}_l \tilde{\epsilon}}{\partial x_l} = \frac{\partial}{\partial x_k} \left[C_{s_\epsilon} < \rho > \frac{\tilde{k}}{\tilde{\epsilon}} \widetilde{u_k'' u_l''} \frac{\partial \tilde{\epsilon}}{\partial x_l} \right] \\ - C_{\epsilon_1} < \rho > \frac{\tilde{\epsilon}}{\tilde{k}} \widetilde{u_k'' u_l''} \frac{\partial \tilde{u}_k}{\partial x_l} - C_{\epsilon_2} \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{\epsilon} - C_{\epsilon_3} \frac{\tilde{\epsilon}}{\tilde{k}} < u_l'' > \frac{\partial < p >}{\partial x_l} \end{aligned} \quad (2.49)$$

is maintained and the model constants are

$$C_{\epsilon_1} = 1.44 \quad C_{\epsilon_2} = 1.92 \quad C_{\epsilon_3} = 1.44 \quad C_{s_\epsilon} = 0.18. \quad (2.50)$$

2.6 Closures in the flamelet regime of combustion

If the discussion is limited to the flamelet regime and the aerothermochemistry of premixed turbulent combustion is assumed to be given by the well known Bray-Moss-Libby (BML) model [14], analytic expressions may be derived for the remaining unclosed terms. In the BML model, the probability density function (PDF) of the reaction progress variable is presumed to have a bimodal shape

$$f(c; \underline{x}) = \alpha(\underline{x})\delta(c) + \beta(\underline{x})\delta(1 - c) + \gamma(\underline{x})f_r(c; \underline{x}, t) \quad (2.51)$$

where $\alpha(\underline{x})$, $\beta(\underline{x})$ and $\gamma(\underline{x})$ are functions that relate to the three possible states in the gas mixture, reactants, products and reacting gas. f_r is a reaction mode PDF normalised such that

$$\alpha(\underline{x}) + \beta(\underline{x}) + \gamma(\underline{x}) = 1. \quad (2.52)$$

In the laminar flamelet regime of combustion the reaction zone is thin ($\gamma \ll 1$) giving $\alpha + \beta + \mathcal{O}(\gamma) = 1$. The latter result allows the remaining functions to be computed [14]

$$\alpha(\underline{x}) = \frac{1 - \tilde{c}}{1 + \tau\tilde{c}} + \mathcal{O}(\gamma) \quad (2.53)$$

$$\beta(\underline{x}) = \frac{(1 - \tau)\tilde{c}}{1 + \tau\tilde{c}} + \mathcal{O}(\gamma). \quad (2.54)$$

The presumed PDF given by Eq. (2.51) may be extended to include joint velocity-scalar statistics.

$$f(\underline{u}, c; \underline{x}) = \alpha(\underline{x})\delta(c)f(\underline{u}, 0; \underline{x}) + \beta(\underline{x})\delta(1 - c)f(\underline{u}, 1; \underline{x}) + \mathcal{O}(\gamma) \quad (2.55)$$

The latter extension allows simple algebraic expressions to be derived for the average density weighted fluctuations of velocity and reaction progress variable

$$\langle u_i'' \rangle = \mathcal{T} \frac{\langle \rho \rangle}{\rho_u} \widetilde{u_i'' c''} \cong \frac{\mathcal{T} \widetilde{u_i'' c''}}{1 + \mathcal{T}\tilde{c}} \quad (2.56)$$

$$\langle c'' \rangle = \mathcal{T} \frac{\langle \rho \rangle}{\rho_u} \widetilde{c''^2} \cong \frac{\mathcal{T} \widetilde{c''^2}}{1 + \mathcal{T}\tilde{c}} \quad (2.57)$$

and as a consequence, the mean pressure gradient terms in Eqs. (2.1) and (2.2) appear in closed form and where $\mathcal{T}$ is given by Eq. (1.31). Furthermore, an algebraic expression may also be derived for the reaction progress variable variance $\widetilde{c''^2}$ and thereby avoiding the necessity of solving another transport equation. The variance is given by [14]

$$\widetilde{c''^2} = \tilde{c}(1 - \tilde{c}). \quad (2.58)$$

An expression for the turbulence-reaction rate correlation is also be obtained from the BML model [14]

$$\widetilde{u_i'' S} = \frac{\tilde{S}}{\widetilde{c''^2}} (C_m - \tilde{c}) \widetilde{u_i'' c''}. \quad (2.59)$$

Furthermore, Bray [12] have shown that the scalar dissipation rate may be expressed as

$$\frac{\widetilde{\tilde{\epsilon}_c}}{\widetilde{c''^2}} = \frac{\widetilde{S}}{\widetilde{c''^2}} \left(C_m - \frac{1}{2} \right). \quad (2.60)$$

Combining the two last expressions allows the dependence of the parameter C_m to be removed

$$- \langle \rho \rangle \frac{\widetilde{\tilde{\epsilon}_c}}{\widetilde{c''^2}} \widetilde{u_i'' c''} + \langle \rho \rangle \widetilde{u_i'' S} = \frac{\langle \rho \rangle \widetilde{S}}{\widetilde{c''^2}} \left(\frac{1}{2} - \tilde{c} \right) \widetilde{u_i'' c''} \quad (2.61)$$

and a closure for the scalar dissipation rate and the turbulence-reaction rate correlation is obtained.

2.6.1 Pressure dilatation models

Few models have been developed for the pressure dilatation term, Sarkar et al. [151] and Sarkar [152] derived a general expression for compressible turbulence where the final expression depends on the Ma number. It is shown that the term becomes important at $Ma > 0.5$.

Zhang & Rutland [181] and Hůlek & Lindstedt [69] derived pressure dilatation term models in the flamelet regime of combustion. The model of Zhang & Rutland

$$\phi_{ij}^D = \frac{1}{3} \delta_{ij} \rho_u u_L^3 \mathcal{T}^2 \Sigma \tilde{c} = \frac{1}{3} \delta_{ij} \langle \rho \rangle \tilde{S} (\mathcal{T} u_L)^2 \tilde{c} \quad (2.62)$$

showed reasonable agreement with their DNS data involving quite low values ($0.67 < \mathcal{T} < 1.5$) of the heat release parameter. Lindstedt & Város [108] applied the model and overpredicted the turbulence quantities in the flame ($\mathcal{T} = 5.5$) of Gulati and Driscoll [61]. A different pressure dilatation expression was obtained by Hůlek & Lindstedt [69] following assumptions consistent with the flamelet approach

$$\phi_{ij}^D = \frac{1}{3} \delta_{ij} \langle \rho \rangle \tilde{S} (\mathcal{T} u_L)^2 \left(\langle c \rangle - \frac{1}{2} \right) \quad (2.63)$$

and the magnitude of both models was compared with the overall turbulent kinetic

energy budget. It was concluded that these terms are of secondary importance in high expansion ratio flames. For this reason, no pressure dilatation term model is included in the present work.

Chapter 3

Transported PDF methods

3.1 Introduction

In transported PDF methods, a transport equation is modelled and solved for the joint scalar or the joint velocity-scalar PDF. The chemical source term appears in closed form [140] and requires no modelling — finite rate chemistry effects are naturally included. One of the major closure challenges in both joint velocity-scalar and joint scalar PDF approaches concerns the modelling of the molecular diffusion term and a range of models have been proposed [40, 41, 128, 138, 141, 166, 168, 169, 173] and compared [27, 32, 70, 127, 146, 170].

Typical combustion applications feature non-premixed flames. Saxena & Pope [154] solved a piloted jet diffusion flame to test the speed-up using *In-Situ Adaptive Tabulation* (ISAT) of the chemistry for different levels of the error tolerance. Lindstedt et al. [109] computed piloted jet diffusion flames using comprehensive chemistry including a NO_x submechanism. Modified Curl’s mixing model [41] was used to close the molecular mixing term. The flames ranged from weakly turbulent to conditions close to extinction. Xu & Pope [179] solved a series of methane diffusion flames using a closure at the joint velocity-turbulence-frequency-scalar level. The EMST mixing model of Subramaniam & Pope [166] was used and the impact of the time scale ratio (C_ϕ) parameter investigated. Lindstedt & Louloudi [111] applied a closure at the joint scalar level to compute a set of methanol flames. Again a parametric study was

performed to check the sensitivity to the velocity scalar time scale ratio as extinction was approached. Kuan & Lindstedt [96] solved a bluff body stabilised diffusion flame using comprehensive thermo-chemistry featuring 300 reactions, 20 solved and 28 steady state species. A closure at the joint scalar level for scalar statistics was coupled with a second moment closure for the velocity field. Molecular mixing was represented by the modified Curl's model. A similar approach was used by Lindstedt & Ozarovsky [113] to compute two non-piloted $CH_4/H_2/N_2$ diffusion flames including radiative heat losses. An extensive comparison with available experimental data was made that illustrates the ability of the approach to reproduce the flame structure. Cao et al. [26] applied a joint velocity-turbulence-frequency-scalar approach to model turbulent lifted flames in a coflow of combustion products. Three different mixing models and two different chemical mechanisms were used in the study. This particular flame showed a greater sensitivity to the different mechanisms than to the different mixing models. The same burner was simulated by Gkagkas & Lindstedt [58] using a closure at the joint scalar level and a detailed chemical mechanism including low temperature chemistry.

3.2 Transport equation for the joint scalar PDF

Let $(\underline{V}, \underline{\Psi})$ be the sample space, defining all the permissible values of the random vector $(\underline{u}, \underline{\phi})$. The joint distribution function $\mathcal{F}_{u\phi}(\underline{V}, \underline{\Psi}; \underline{x}, t)$ of the $(3+\sigma)$ -dimensional random vector $(\underline{u}, \underline{\phi})$ is defined by

$$\mathcal{F}_{u\phi}(\underline{V}, \underline{\Psi}; \underline{x}, t) \equiv \mathbf{P}(u_i < V_i, \phi_\alpha < \Psi_\alpha; \underline{x}, t) \quad (3.1)$$

where $\mathbf{P}(\mathbf{A})$ simply denotes the probability of the event $\mathbf{A} \equiv (u_1 < V_1, u_2 < V_2, u_3 < V_3, \phi_1 < \Psi_1, \phi_2 < \Psi_2, \dots, \phi_\sigma < \Psi_\sigma)$. At every point in the velocity-scalar space this distribution function has a value between zero and one. The joint velocity scalar PDF $f_{u\phi}(\underline{V}, \underline{\Psi}; \underline{x}, t)$ is the derivative of the distribution function:

$$f_{u\phi}(\underline{V}, \underline{\Psi}; \underline{x}, t) = \frac{\partial^{3+\sigma} \mathcal{F}_{u\phi}(\underline{V}, \underline{\Psi}; \underline{x}, t)}{\partial V_1 \partial V_2 \partial V_3 \partial \Psi_1 \partial \Psi_2 \dots \partial \Psi_\sigma}. \quad (3.2)$$

The following fundamental properties hold for $f_{u\phi}(\underline{V}, \underline{\Psi}; \underline{x}, t)$

$$f_{u\phi}(\underline{V}, \underline{\Psi}; \underline{x}, t) \geq 0 \quad (3.3)$$

$$\iint f_{u\phi}(\underline{V}, \underline{\Psi}; \underline{x}, t) d\underline{V} d\underline{\Psi} = 1. \quad (3.4)$$

The joint scalar PDF can be obtained through integration over the entire velocity space

$$\int f_{u\phi}(\underline{V}, \underline{\Psi}; \underline{x}, t) d\underline{V} = f_\phi(\underline{\Psi}; \underline{x}, t) \quad (3.5)$$

where $f_\phi(\underline{\Psi}; \underline{x}, t)$ is called the marginal PDF. In inhomogeneous variable density flows, the natural dependent variable is the mass density function (MDF) defined as

$$F_{u\phi}(\underline{V}, \underline{\Psi}; \underline{x}, t) \equiv \rho(\underline{\Psi}) f_{u\phi}(\underline{V}, \underline{\Psi}; \underline{x}, t) = \langle \rho \rangle \tilde{f}_{u\phi}(\underline{V}, \underline{\Psi}; \underline{x}, t). \quad (3.6)$$

The transport equation for the joint velocity scalar MDF may be obtained, following Pope [140], by consideration of the transport equations for mass, momentum and scalars. The resulting transport equation for the joint velocity scalar MDF reads

$$\frac{\partial F_{u\phi}}{\partial t} + \frac{\partial V_j F_{u\phi}}{\partial x_j} + \frac{\partial}{\partial V_j} [\langle A_j | \underline{V}, \underline{\Psi} \rangle F_{u\phi}] + \frac{\partial}{\partial \Psi_\alpha} [\langle \Theta_\alpha | \underline{V}, \underline{\Psi} \rangle F_{u\phi}] = 0 \quad (3.7)$$

where functional dependencies have been omitted for clarity. A_j and Θ_α are given by

$$\rho A_j(\underline{x}, t) \equiv \frac{\partial \tau_{ij}}{\partial x_i} - \frac{\partial p}{\partial x_j} + \rho g_j \quad \rho \Theta_\alpha(\underline{x}, t) \equiv -\frac{\partial J_i^\alpha}{\partial x_i} + \rho S_\alpha. \quad (3.8)$$

The conditional expectations appearing in Eq. (3.7) represent turbulent transport in velocity and scalar space respectively. These terms are not closed and require modelling. Integration over the entire velocity space (i.e. Eqs. (3.5) and (3.8)) yields the transport equation for the joint scalar MDF in its well known form

$$\frac{\partial F_\phi}{\partial t} + \frac{\partial \tilde{u}_i F_\phi}{\partial x_i} + \frac{\partial S_\alpha(\underline{\Psi}) F_\phi}{\partial \Psi_\alpha} = \frac{\partial}{\partial \Psi_\alpha} \left[\left\langle \frac{1}{\rho} \frac{\partial J_i^\alpha}{\partial x_i} \middle| \underline{\Psi} \right\rangle F_\phi \right] - \frac{\partial \langle u_i'' | \underline{\Psi} \rangle F_\phi}{\partial x_i} \quad (3.9)$$

where the instantaneous conditional velocity has been decomposed into an unconditional mean and a conditional fluctuation

$$\langle u_i | \underline{\Psi} \rangle = \tilde{u}_i + \langle u_i'' | \underline{\Psi} \rangle . \quad (3.10)$$

Inspection of the transport equation for the joint scalar MDF, Eq. (3.9), reveals that all terms on the LHS appear in closed form and are accounted for exactly. The first two terms represent the rate of change following a particle moving with the mean velocity $\tilde{u}_i$ and the third term represents convection in scalar space due to reaction. The terms containing conditional expectations on the RHS are unclosed and require modelling. These terms represent diffusion in scalar space due to mixing and transport in physical space due to velocity fluctuations.

The usefulness of the transport equation of the joint scalar MDF is clearly indicated by the fact that highly non-linear reactions can be accounted for exactly. Pope [140] devised a modelling strategy and a solution algorithm which will be discussed below.

3.3 Modelling and solution algorithm

The joint scalar transported MDF equation is a deterministic equation even though it is a MDF of random variables. The dynamics of this equation enters through the conditional expectations. Many stochastically equivalent systems can evolve by the same equation.

The general idea is to create a set of easily solved equations that evolve with the same MDF as that of fluid particles. A given fluid particle is defined by its position $\underline{x}^L$, its velocity $\underline{u}^L$ and composition $\underline{\phi}^L$ which can be represented by the state vector $\{\underline{x}^L, \underline{u}^L, \underline{\phi}^L; t\}$ at the time t . The evolution of the particle is described by the Lagrangian equations

$$\frac{\partial \underline{x}^L}{\partial t} = \underline{u}^L \quad \frac{\partial \underline{\phi}^L}{\partial t} = \underline{\Theta} \quad (3.11)$$

where $\underline{\Theta}$ is given by Eq. (3.8). Now, consider the transition density function $f^L(\underline{\Psi}, \underline{x}; t | \underline{\Psi}_0, \underline{x}_0)$ which is the Lagrangian joint PDF at time t conditioned upon the particle properties at time t_0 . The transition density function basically allows particle properties to be calculated at time t based on the knowledge of the particle properties at time t_0

$$F_\phi(\underline{\Psi}, \underline{x}; t) = \iiint f^L(\underline{\Psi}, \underline{x}; t | \underline{\Psi}_0, \underline{x}_0) F_\phi(\underline{\Psi}_0, \underline{x}_0; t_0) d\underline{\Psi}_0 d\underline{x}_0. \quad (3.12)$$

The transition density function is clearly a function of fundamental importance in transported PDF methods since as shown by Pope [140] the transport equation for the joint scalar MDF derived from a Lagrangian framework is the same as the one derived from the instantaneous conservation laws. The problem to determine $F_\phi(\underline{\Psi}, \underline{x}; t)$ has thus reduced to determining the state of a finite number of particles. The state of the particles are described by the solution of $(3+\sigma)$ ordinary differential equations for each particle for the joint scalar MDF. The discrete fine grained PDF is represented by a large number of stochastic particles N

$$f_\phi^N(\underline{\Psi}, \underline{x}; t) = \frac{1}{N} \sum_{n=1}^N \delta(\underline{\Psi} - \underline{\phi}^{(n)}) \delta(\underline{x} - \underline{x}^{(n)}) \quad (3.13)$$

where $(\underline{\phi}^{(n)}, \underline{x}^{(n)})$ can be thought of as simultaneously measured values of composition and position. The expectation of the discrete ensemble averaged PDF is the PDF f_ϕ itself

$$\langle f_\phi^N(\underline{\Psi}, \underline{x}; t) \rangle = f_\phi(\underline{\Psi}, \underline{x}; t). \quad (3.14)$$

This shows, however, the major disadvantage with the discrete Monte Carlo sampling since

$$f_\phi(\underline{\Psi}, \underline{x}; t) = \lim_{N \rightarrow \infty} f_\phi^N(\underline{\Psi}, \underline{x}; t). \quad (3.15)$$

Consider any function $Q(\underline{\phi}, \underline{x})$, the ensemble average (expectation) may be obtained

through

$$\langle Q(\underline{\phi}, \underline{x}) \rangle_N = \iint Q(\underline{\Psi}, \underline{x}) f_\phi^N(\underline{\Psi}, \underline{x}; t) d\underline{\Psi} d\underline{x} = \frac{1}{N} \sum_{n=1}^N Q(\underline{\phi}^{(n)}, \underline{x}^{(n)}) \quad (3.16)$$

where the fundamental shifting property of the δ -function has been used. The use of a finite number of particles, N , results in a statistical error ϵ_N

$$\langle Q(\underline{\phi}, \underline{x}) \rangle_N = \langle Q(\underline{\phi}, \underline{x}) \rangle + \epsilon_N \quad (3.17)$$

which approximates the expected value. The mean value of the statistical error is zero and the standard deviation, ϵ'_N , is given by:

$$\epsilon'_N = \sqrt{\frac{Q'^2}{N}} \quad \Rightarrow \quad \epsilon'_N \propto N^{-1/2}. \quad (3.18)$$

The above equation clearly indicates the slow convergence characteristics of the Monte Carlo approach — the number of particles needs to be increased by a factor of four in order to obtain half the statistical error.

3.3.1 The method of fractional steps

The joint scalar MDF transport equation, Eq. (3.9), may be written as

$$\frac{\partial F_\phi}{\partial t} = (P_1 + P_2 + P_3)F_\phi \quad (3.19)$$

where P_1 , P_2 and P_3 are operators corresponding to the different processes. The process P_1

$$P_1 = - \langle u_i | \underline{\Psi} \rangle \frac{\partial}{\partial x_i} - \frac{\partial \langle u_i | \underline{\Psi} \rangle}{\partial x_i} \quad (3.20)$$

corresponds to the turbulent transport of F_ϕ in physical space while the processes P_2 and P_3

$$P_2 = \left[\left\langle \frac{1}{\rho} \frac{\partial J_i^\alpha}{\partial x_i} \middle| \underline{\Psi} \right\rangle \right] \frac{\partial}{\partial \Psi_\alpha} + \frac{\partial}{\partial \Psi_\alpha} \left[\left\langle \frac{1}{\rho} \frac{\partial J_i^\alpha}{\partial x_i} \middle| \underline{\Psi} \right\rangle \right] \quad (3.21)$$

$$P_3 = -S_\alpha(\underline{\Psi}) \frac{\partial}{\partial \Psi_\alpha} - \frac{\partial S_\alpha(\underline{\Psi})}{\partial \Psi_\alpha} \quad (3.22)$$

correspond to diffusion (mixing) and convection (reaction) of F_ϕ in scalar space. The method of fractional step can be used to calculate each process affecting the evolution of F_ϕ separately [140] with first order accuracy during a sufficiently small time increment Δt

$$\begin{aligned} F_\phi^{(1)}(t) &\equiv (I + \Delta t P_1) F_\phi(t) \\ F_\phi^{(2)}(t) &\equiv (I + \Delta t P_2) F_\phi^{(1)}(t) \\ F_\phi(t + \Delta t) &\equiv (I + \Delta t P_3) F_\phi^{(2)}(t) \end{aligned} \quad (3.23)$$

where I is the identity operator. Elimination of $F_\phi^{(1)}$ and $F_\phi^{(2)}$ gives

$$F_\phi(t + \Delta t) = F_\phi(t) + \Delta t (P_1 + P_2 + P_3) F_\phi(t) + \mathcal{O}(\Delta t^2) \quad (3.24)$$

and a Taylor series expansion of F_ϕ around t gives a second expression for $F_\phi(t + \Delta t)$

$$F_\phi(t + \Delta t) = F_\phi(t) + \frac{\partial F_\phi}{\partial t} \Delta t + \mathcal{O}(\Delta t^2). \quad (3.25)$$

Equating Eqs. (3.24) and (3.25) shows that the resulting expression is identical to Eq. (3.19)

$$\frac{\partial F_\phi}{\partial t} = (P_1 + P_2 + P_3) F_\phi + \mathcal{O}(\Delta t) \quad (3.26)$$

except for the first order truncation error.

3.3.2 Transport in physical space

In the joint scalar transported MDF equation, the conditional expectation containing the velocity fluctuation $\langle u_i'' | \underline{\Psi} \rangle$ is unclosed and needs to be modelled. The most commonly adopted approach is to close this term using a gradient diffusion type model

$$\langle u_i'' | \underline{\Psi} \rangle F_\phi = -\frac{\mu_T}{\sigma_f} \frac{\partial}{\partial x_i} [F_\phi / \langle \rho \rangle] \quad (3.27)$$

where σ_f is the turbulent Prandtl/Schmidt number and μ_T originates from the isotropic eddy viscosity hypothesis. The turbulent viscosity may be obtained from the $\tilde{k} - \tilde{\epsilon}$ model [79] theory, where modelled transport equations are solved for $\tilde{k}$ and $\tilde{\epsilon}$ and the eddy viscosity is expressed as

$$\mu_T = \langle \rho \rangle C_\mu \frac{\tilde{k}^2}{\tilde{\epsilon}} \quad (3.28)$$

where C_μ is a model constant or, alternatively, $\tilde{k}$ may be obtained as the trace of the Reynolds stress tensor, $\tilde{k} = \frac{1}{2} \widetilde{u_i'' u_i''}$, if a second moment closure is used.

Insertion of Eq. (3.27) into Eq. (3.9) and setting reaction and mixing to zero (corresponding to the first fractional step) gives

$$\frac{\partial F_\phi}{\partial t} + \frac{\partial \tilde{u}_i F_\phi}{\partial x_i} - \frac{\partial}{\partial x_i} \left[\frac{\mu_T}{\sigma_f} \frac{\partial}{\partial x_i} [F_\phi / \langle \rho \rangle] \right] = 0. \quad (3.29)$$

The first fractional step is modelled by considering the diffusion process given by the Langevin equation

$$d\underline{x} = \underline{D}(\underline{x}, t)dt + [\underline{B}(\underline{x}, t)]^{1/2} d\underline{W}(t) \quad (3.30)$$

where $d\underline{W}(t)$ represents the Wiener process. The transport equation for the joint scalar MDF corresponding to the Langevin equation, Eq. (3.30), is given by the Fokker-Planck equation

$$\frac{\partial F_\phi}{\partial t} + \frac{\partial}{\partial x_i} [D_i F_\phi] - \frac{1}{2} \frac{\partial^2}{\partial x_i \partial x_i} [B F_\phi] = 0 \quad (3.31)$$

where D_i and B are the coefficients of drift and diffusion, respectively. In order to model Eq. (3.29) with the Fokker-Planck equation and the diffusion process, Eq. (3.30), the coefficients of drift and diffusion

$$D_i = \tilde{u}_i + \frac{1}{\langle \rho \rangle} \frac{\partial (\mu_T / \sigma_f)}{\partial x_i} \quad B = \frac{2(\mu_T / \sigma_f)}{\langle \rho \rangle} \quad (3.32)$$

are already determined. During a time interval Δt , transport in physical space is

achieved by moving each stochastic particle independently by

$$x_i(t + \Delta t) = x_i(t) + \Delta t \left[\tilde{u}_i + \frac{1}{\langle \rho \rangle} \frac{\partial(\mu_T/\sigma_f)}{\partial x_i} \right]_{x_i(t)} + \left[\frac{2(\mu_T/\sigma_f)\Delta t}{\langle \rho \rangle} \right]_{x_i(t)}^{1/2} \xi_i \quad (3.33)$$

where ξ_i is a standardised joint normal random vector with zero mean and unit variance.

It should be noted that modelling of the conditional expectation containing the velocity fluctuation is avoided in joint velocity scalar PDF approaches as this term appears in closed [140] form. Lindstedt & Város [110] performed turbulent burning velocity calculations using a single scalar joint scalar PDF approach. The approach featured both a gradient diffusion type closure and a closure at the second moment level for transport in physical space. The calculations showed that the gradient diffusion type closure produces lower values for the turbulent burning velocity. This is in agreement with the presumed PDF study of Lindstedt & Város [108], where the mean reaction rate constant had to be adjusted in combination with gradient diffusion type models.

3.3.3 Diffusion in scalar space (mixing)

Consider the joint scalar transport equation during the second fractional step, molecular mixing, in the absence of convection and reaction

$$\frac{\partial F_\phi}{\partial t} = \frac{\partial}{\partial \Psi_\alpha} \left[\left\langle \frac{1}{\rho} \frac{\partial J_i^\alpha}{\partial x_i} \middle| \underline{\Psi} \right\rangle F_\phi \right]. \quad (3.34)$$

As shown by O'Brien [145], Eq. (3.34) may be rewritten as

$$\frac{\partial F_\phi}{\partial t} = -\frac{\partial^2}{\partial \Psi^2} [\langle \epsilon_\phi | \underline{\Psi} \rangle F_\phi] \quad (3.35)$$

showing that the closure for the molecular mixing term essentially amounts to a model for the conditional scalar dissipation rate, $\langle \epsilon_\phi | \underline{\Psi} \rangle$. The scalar dissipation rate is a quantity of fundamental importance in turbulent reactive flows.

The molecular mixing term has received much attention since it is unclosed in

both joint scalar and joint velocity scalar PDF approaches. Hřlek [70] performed an extensive review of the existing mixing models and only important conclusions will be repeated here.

3.3.3.1 Mixing models

During the mixing process of a passive scalar, from any given initial condition, it is expected that the PDF will relax towards a Gaussian distribution. Eswaran & Pope [46] studied the mixing of an inert passive scalar in homogenous turbulence using DNS. Starting from a bimodal-like initial field, it was found that the PDF of the scalar evolve continuously and tends to a Gaussian distribution. The variance decay will continuously increase the value of the PDF at the mean and at the limit $t \rightarrow \infty$, converge to a δ function. A satisfactory mixing model should allow the Gaussian distribution as a solution for the case considered above. On the other hand many scalars are bounded quantities and so are their PDF's. A bounded PDF can not be exactly Gaussian.

The deterministic, Linear Mean Square Estimate (LMSE) model of Dopazo [40] uses the intuitive idea that the rate of change of particle properties are proportional to the distance from the mean in scalar space. The constant C_ϕ is chosen to give the correct decay rate of the variance. The model is attractive due to its simplicity, but for the case considered above, the PDF does not relax to a Gaussian distribution [70, 140] from an arbitrary initial field since the shape of the PDF is left unchanged during the decay.

Stochastic particle interaction models simulate scalar dissipation through a Poisson type process [140]. During a small time increment Δt , N_{pq} pairs of particles out of a total of N particles are randomly selected without replacement. The independent particles, denoted p and q , will mix and their values will change according to

-With probability $\Delta t/\tau_\phi$:

$$\begin{aligned}\phi^{(p)}[t + \Delta t] &= \phi^{(p)}[t] + h \frac{\phi^{(q)}[t] - \phi^{(p)}[t]}{2} \\ \phi^{(q)}[t + \Delta t] &= \phi^{(q)}[t] - h \frac{\phi^{(q)}[t] - \phi^{(p)}[t]}{2} \\ \text{for } p, q &\in \{1, 2, \dots, N\}, \quad p \neq q\end{aligned}\tag{3.36}$$

$$\phi^{(i)}[t + \Delta t] = \phi^{(i)}[t] \quad \text{for } i = 1, 2, \dots, N, \quad i \neq p, \quad i \neq q$$

-With probability $1 - \Delta t/\tau_\phi$:

$$\phi^{(i)}[t + \Delta t] = \phi^{(i)}[t] \quad \text{for } i = 1, 2, \dots, N,$$

where h is a uniform random variable between 0 and 1. N_{pq} is given by

$$N_{pq} = \frac{\beta_\phi N \Delta t}{\tau_\phi}\tag{3.37}$$

and the remaining $(N - 2N_{pq})$ particles do not change during the time step. β_ϕ is a constant assigned the value 3.0 in order to obtain the correct decay rate of the scalar variance. τ_ϕ represents a decay time scale for scalar fluctuations and models are usually constructed in simple flows — the evolution of the mean and variance of a passive scalar, ϕ , in constant density homogenous turbulence. The mean of the passive scalar considered remains constant, i.e.

$$\frac{d \langle \phi \rangle}{dt} = 0\tag{3.38}$$

while the evolution equation for the scalar variance is given by

$$\frac{d \langle \phi'^2 \rangle}{dt} = -2\epsilon_\phi\tag{3.39}$$

where

$$\epsilon_\phi = \frac{D}{\rho} \left\langle \frac{\partial \phi'}{\partial x_i} \frac{\partial \phi'}{\partial x_i} \right\rangle.\tag{3.40}$$

A turbulent time scale τ is usually defined in terms of the the ratio of the turbulent kinetic energy, $\tilde{k}$, and its dissipation, $\tilde{\epsilon}$. Similarly, a decay time scale for the scalar fluctuations can be defined. The turbulent time scale and the decay time scale for scalar fluctuations are usually assumed to be proportionally related

$$\tau_\phi^{-1} = \frac{\tilde{\epsilon}_\phi}{\tilde{\phi}''^2} = \frac{C_\phi}{2} \frac{\tilde{\epsilon}}{\tilde{k}} = \frac{C_\phi}{2} \tau^{-1} \quad (3.41)$$

where C_ϕ is constant with the “standard” value 2.0. Eq. (3.40) shows that ϵ_ϕ is a positive quantity which implies that the scalar variance decays. The particle interaction model described above is known as the modified Curl’s mixing model and was independently proposed by Dopazo [41] and Janicka *et al.* [77]. Hůlek [70] performed simulations of an initially dichotomic scalar field using the modified Curl’s mixing model. The PDF relaxed towards a bell shaped distribution which is related to the inability of the model to reproduce moments of higher order.

The binomial sampling model of Valiño & Dopazo [168] is based on a two step algorithm. In the first step, all particles undergo a deterministic LMSE step which leaves the PDF unchanged but the variance of the scalar decays. During the second step, randomly selected particles undergo a stochastic jump process which causes the PDF to relax to a binomial distribution which approximates the Gaussian distribution. The mean and the variance are left unchanged during the second step. A disadvantage with the model is that the PDF does not evolve in a continuous manner; the binomial distribution is discrete.

The latter authors also presented the binomial Langevin model [169] which is based on the Langevin equation, Eq. (3.30), wherein mixing is simulated through a stochastic diffusion process. In the binomial Langevin model, the Wiener process (Gaussian random variable) from the Langevin model is replaced by a binomial deviate to make the model applicable to bounded scalars. The original Langevin model is strictly applicable to unbounded scalars. Application of the model [70, 169] gives excellent results compared to the DNS data of Eswaran & Pope [46]. The computational expense of the model is, however, significantly higher than to the

models mentioned above and the extension to multiple scalars is not straightforward.

A particle interaction model which takes the distance between particles in composition space (localness) into account has been derived by Subramaniam & Pope [166]. The edges of Euclidean Minimum Spanning Trees (EMST) are constructed in composition space and particles interact along these edges — mixing occurs locally in scalar space. The EMST model appears to be a more accurate mixing model but the computational burden is, of course, higher compared to other, simpler particle interaction models.

Recently, Wandel & Lindstedt [173] derived a hybrid binomial Langevin-Multiple Mapping Conditioning (MMC) model for inhomogeneous flows. The approach offers the advantage that difficulties encountered with the binomial Langevin model in modelling scalars with non-elementary bounds is removed and the closure leads to locality in scalar space. The model was evaluated through application to a chemically reacting mixing layer.

McDermott & Pope [126] derived a model for the conditional molecular diffusion term in the context of filtered density function (FDF) methods. FDF methods are the LES analog of PDF methods. The proposed model takes differential diffusion effects into account and converges to a DNS at zero filter width.

3.3.4 Convection in scalar space (reaction)

One of the major motivations of using transported PDF methods is that highly non-linear chemical reactions can be treated without approximation. The closed chemical source term, as it appears in Eq. (3.9), allows the complex interaction of turbulence and chemistry, pollutant formation and extinction/re-light phenomena to be accurately modelled. In practical simulations, a reduced reaction mechanism is generally used, since the chemical source term is by far the most expensive to compute. In a reduced reaction mechanism, certain species are assumed to be in steady state where changes in concentrations are calculated via algebraic expression related to the solved species. The Monte Carlo simulation technique is, however, relatively cheap and the computational cost rises only linearly with the number of

solved scalars.

Cannon et al. [24] simulated a bluff-body stabilised lean methane/air flame in a combustor and applied a reduced 5-step mechanism to describe fuel oxidation, CO and NO chemistry. The major species (CH_4 , O_2 , CO_2 and H_2O) were reasonably well predicted while CO and NO differed by the order of 100% compared to experimental data. James et al. [74] solved a piloted jet diffusion flame using the joint scalar PDF method. A 16-species 41-step C_1 and a reduced 16-species 12-step C_2 mechanism were applied and it was concluded that a C_2 mechanism is a minimum requirement for accurate CO predictions. Lindstedt et al. [109] solved three diffusion flames using a mechanism featuring 20 solved and 28 steady state species. The mechanism takes full account of the C_2 chemistry and, in addition, the formation of oxides of nitrogen is treated by another 5 species sub-mechanism. Both CO and OH levels are well reproduced as compared to the experimental data while a slight over-prediction can be seen in the NO predictions, especially far down-stream. The same mechanism was applied by Kuan & Lindstedt [96] to model a bluff-body stabilised flame and it was concluded that a good representation of the thermochemistry is a necessity for accurate NO and CO predictions. Gkagkas & Lindstedt [58] applied a detailed mechanism featuring 44 solved species and 256 reactions to model a lifted CH_4 /air flame. The thermochemical structure was well reproduced and the case illustrates the ability of the approach and the potential to predict auto-ignition phenomena.

In the third fractional step, changes of the scalar properties of the particles during a small time interval, Δt , are calculated according to

$$\phi_\alpha[t + \Delta t] = \phi_\alpha[t] + R_\alpha \Delta t \quad \alpha = 1 \dots n_{sp} \quad (3.42)$$

where α is the species under consideration and n_{sp} the number of solved species. R_α is given by Eq. (1.16).

Chapter 4

Isothermal and reacting opposed flows

4.1 Introduction

Isothermal opposed or impinging flows and flames stabilised in stagnating turbulence have been studied both experimentally and numerically by several authors [20, 34, 78, 92, 93, 94, 150]. Stagnating turbulence is usually created by either letting the stream from a turbulent jet impinge onto a surface or from two counterflowing jets. The former case adds the complexity of the viscous sublayer including surface reactions and surface heat transfer close to the wall. A typical opposed jet configuration is schematically shown in Fig. 4.1.

Kostiuk et al. [90] used Laser Doppler Velocimetry (LDV) to measure the velocity field in non-reacting turbulent opposed flows. It is shown that the axial mean flow is self-similar for a range of turbulence and flow conditions in both opposing jet flow configurations and jets impinging onto a surface. The same authors also investigated premixed turbulent combustion of two opposing jets [91] and the self-similarity of the isothermal flow was recovered at conditions close to global extinction. Mastorakos [125] also applied LDV to measure the turbulent flow of reacting opposed jets. The experimental work covered diffusion, premixed and partially premixed flames. Lindstedt et al. [112, 116] on the other hand, used Particle Image

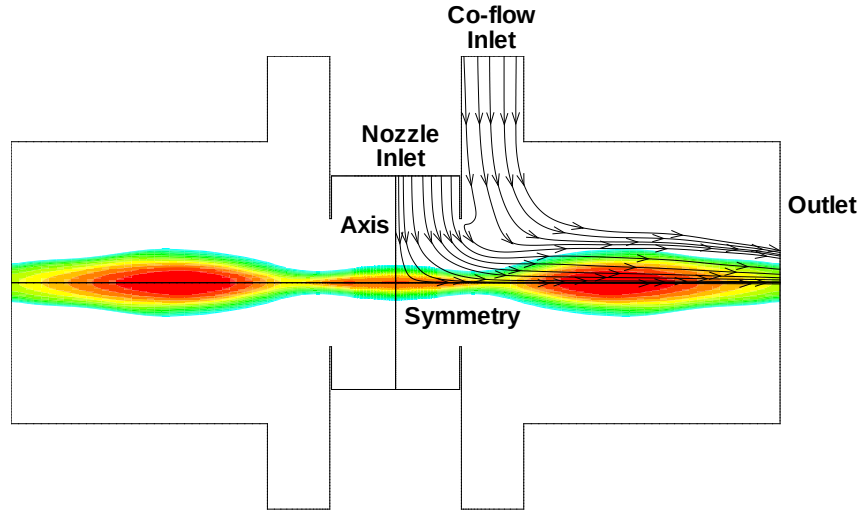


Figure 4.1: Two counterflowing jets with streamlines shown. Location of the flame is indicated by temperature contours.

Velocimetry (PIV) to characterise the velocity field of isothermal and reacting turbulent opposed flows. The experimental data was also compared with the predictive capabilities of second moment closures and eddy-viscosity based models. The impact of alternative ϵ -equation formulations was also explored. A common feature of the experimental configurations, is that all applied perforated plates upstream of the nozzle exits to ensure turbulent conditions. More recent investigations have been performed. Geipel [52] used the experimental set-up of Geyer et al. [56] and measured isothermal and reacting flows using the traditional perforated plates and additional fractal grids for turbulence level enhancement. The work of Geipel also covered liquid fuels like JP-10, cyclopentene and cyclopentane.

Bray et al. [16] applied the $\tilde{k} - \tilde{\epsilon}$ theory to analyse a premixed turbulent flame stabilised in stagnant turbulence. The stagnating turbulence was produced by the oncoming reactant stream impinging on an adiabatic surface. Craft et al. [33] compared the performance of four different turbulence models, one low Re number $k - \epsilon$ model and three second moment closures. Their test cases comprised turbulent jets impinging onto a wall and the inclusion of near wall effects in the pressure strain

correlation was emphasised. Dianat et al. [38] made a similar effort and applied a modified form of the Reynolds stress closure of Jones & Musonge [83] with the inclusion of a wall reflection term and a $k - \epsilon$ model to a range of impinging jet data. Wu & Bray [177, 178] closed the turbulent reaction rate through the solution of the transport equation for the mean flame surface density. The reaction rate closure was applied to model premixed combustion impinging on a wall [177] and a premixed flame stabilised in a counterflow geometry [178]. Lindstedt & Város [107, 108] simulated premixed flames stabilised in stagnating turbulence using second moment closures for both velocity and scalar statistics. The generalised Langevin model of Haworth & Pope [66, 67] was used to close the redistributive part of the pressure strain correlation and the corresponding scrambling term [142]. The closure was, however, suitably extended and included variable density correction terms for the pressure redistribution and the scrambling terms and the turbulence kinetic energy dissipation equation. Bray et al. [21] derived an alternative formulation for the Reynolds stress and scalar flux equations in the flamelet regime of combustion. The contributions of reactants, products and flamelets are modelled for the pressure gradient terms using an extended BML decomposition including the fluctuating pressure. The predictions are in good agreement with the experimental data. Most of the aforementioned numerical work indicates that second moment closures are outperforming eddy-viscosity based closures. Improvements are possible for two-equation models, but with the loss of generality. Geyer et al. [55] solved the joint scalar transported PDF equation supplemented with a second moment closure for the velocity field and compared with their LDV and Raman/Rayleigh data. The transported PDF predictions agreed well for all mixing models tested, but the EMST model of Subramaniam & Pope [166] improved the extinction limits compared to modified Curl's model [41] and the LMSE model [40]. Kempf et al. [86] simulated non-reacting and reacting opposed flows using LES. The burner geometry was that of Mastorakos [125] where one nozzle was supplied with air and the other methane. In general, predictions are in good agreement with experimental data. Geyer et al. [54, 56] applied LDV and Raman/Rayleigh spectroscopy to measure the velocity

and scalar fields of counterflow diffusion flames. The measurements were compared with reacting data using an LES solver. Predictions were in good agreement with measurements but significant deviations could be seen for the scalar dissipation rate at the rich side of the flame. Recently, Stein [165] performed an LES study of isothermal and premixed combustion in the opposed jet configuration of Lindstedt et al. [112, 116]. In general, predictions are in a reasonably good agreement with the experimental data, especially for isothermal flow conditions.

4.1.1 The present contribution

Opposing jet geometries present attractive configurations in which to explore the impact of strain effects on burning properties of laminar and turbulent flames. Previous studies featured comparatively low turbulence levels causing bulk strain to exceed the turbulent contribution. In the current work, numerical studies have been performed of the experimental rig set-up of Geipel et al. [53]. In the current geometry, the turbulent contribution is significantly increased through fractal generated turbulence in addition to the traditional perforated plates. Furthermore, the co-flow of air surrounding each nozzle and the ambient air require a minimum of two scalars, the mixture fraction and the reaction progress variable, to describe the flow in question. The objectives of the present study is to compare the predictive capabilities of different classes of models to this set of new boundary conditions and show the applicability of advanced turbulence closures to 3-dimensional geometries featuring unstructured meshes. The models applied are ranging from the $k - \epsilon$ /gradient diffusion to full second moment closures coupled with a joint β -bimodal presumed PDF approach to the node-based Eulerian joint scalar transported PDF approach coupled with a second moment closure for the velocity field.

4.2 Flow configuration

The current opposed jet configuration, schematically shown in Fig. 4.2, is based on the geometry described in detail by Geyer et al. [56], suitably modified to include

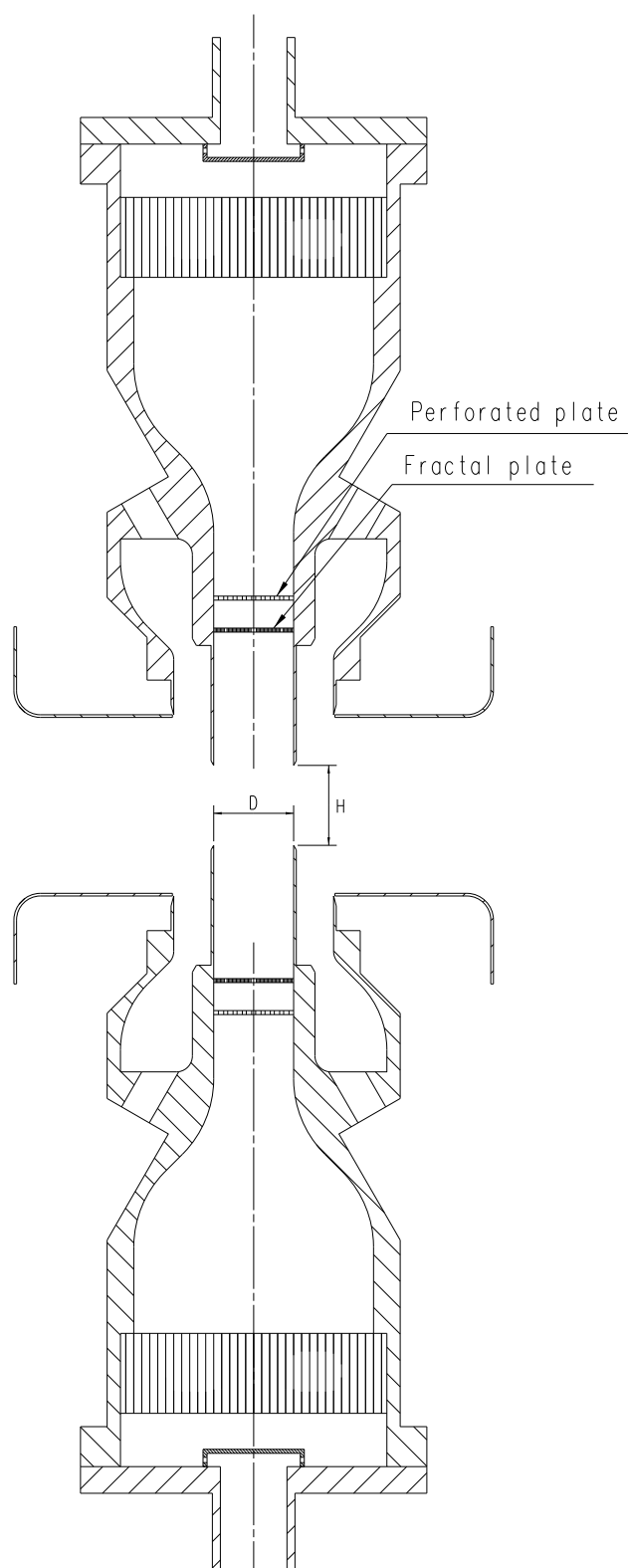


Figure 4.2: The current opposed jet configuration

fractal grids for turbulence level enhancement. The flow enters a short settling chamber through a half inch pipe followed by impingement plates. Downstream of the settling chamber are meshes placed to produce pure axial flow. The mesh was used in the isothermal case only. To reduce the thickness of the boundary layer, a contraction featuring an area contraction ratio of 9:1 is located downstream of the honeycomb flow straightener. In general, contraction contours usually follows a fifth order polynomial derived in the manner of Bell & Mehta [8] to avoid separation. The contraction connects to the nozzle of diameter (D) 30 mm and 60 mm upstream of the nozzle exit is a turbulence generating perforated plate featuring hexagonally arranged holes with a blockage ratio of 45% located. In addition, fractal grids are included 10 mm downstream of the turbulence generating perforated plate to increase turbulence levels. The fractal grid has a blockage ratio of 65%, a fractal dimension of 2.0 and a fractal bar width ratio of 4.0 [53]. The largest fractal bar width is 2 mm. The two identical, vertically positioned opposed nozzles are separated (H) by one nozzle diameter ($H = D$). Around each nozzle, a coflow of air of 30% of the nozzle bulk velocity is used to reduce bulk movement of the two opposed streams. The diameter of the annular coflow channel is 60 mm.

4.3 Closure considerations

4.3.1 A conserved passive scalar — the mixture fraction

From a modelling point of view, the presence of ambient air and a coflow of air adds complexity to the mathematical description. An additional scalar is required to describe the mixing pattern between the premixed fuel-air stream from the nozzles and the air stream from the surrounding coflow. From a numerical point of view, additional transport equations needs to be considered that increases the computational burden and the complexity. On the other hand, the entrainment of air will automatically limit the reaction zone compared to a fully premixed computational domain. The mixture fraction variable is commonly used to describe the combustion of non-premixed reactants where a fast chemistry assumption can be invoked [85].

To define the mixture fraction variable, a conserved quantity like the element mass fraction may be used. Let $a_{\alpha\beta}$ denote the number of atoms of element β in a molecule of species α and M_β the molecular weight of that atom. The mass of all atoms in the system may then be written as

$$m_\beta = \sum_{\alpha=1}^{n_{sp}} \frac{a_{\alpha\beta} M_\beta}{M_\alpha} m_\alpha \quad (4.1)$$

and the mass fraction of element β is then

$$Z_\beta = \frac{m_\beta}{m} = \sum_{\alpha=1}^{n_{sp}} \frac{a_{\alpha\beta} M_\beta}{M_\alpha} Y_\alpha. \quad (4.2)$$

Since element mass fractions are conserved, neither created nor consumed by chemical reactions, the following holds

$$\sum_{\alpha=1}^{n_{sp}} \frac{a_{\alpha\beta} M_\beta}{M_\alpha} S_\alpha = 0 \quad (4.3)$$

and the transport equation for element mass fraction may thus be written

$$\frac{\partial \rho Z_\beta}{\partial t} + \frac{\partial \rho u_i Z_\beta}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\rho D \frac{\partial Z_\beta}{\partial x_i} \right] \quad (4.4)$$

assuming equal diffusivities. If the system consists of two feeds, each of uniform composition, the mixture fraction may be defined as [10]

$$\xi \equiv \frac{Z_\beta - Z_{\beta_2}}{Z_{\beta_1} - Z_{\beta_2}} = \frac{\beta - \beta_2}{\beta_1 - \beta_2} \quad (4.5)$$

where 1 and 2 refers to the two feeds respectively. The coupling function

$$\beta = \frac{Z_C}{x M_C} + \frac{Z_H}{y M_H} - 2 \frac{Z_O}{\nu_{O_2} M_{O_2}} \quad (4.6)$$

is zero at stoichiometric conditions. In Eq. (4.6) the notation of the global reaction step given by Eq. (1.1) has been used. The normalised coupling function of Eq. (4.5)

gives Bilger's [11] definition of the mixture fraction

$$\xi = \frac{Z_C/(xM_C) + Z_H/(yM_H) + 2(Y_{O_2,2} - Z_O)/(\nu_{O_2}M_{O_2})}{Z_{C,1}/(xM_C) + Z_{H,1}/(yM_H) + 2Y_{O_2,2}/(\nu_{O_2}M_{O_2})} \quad (4.7)$$

which is often used to determine the mixture fraction from numerical or experimental data of mass fractions [134]. In Eq. (4.7), $Y_{O_2,2}$ refers to the mass fraction of oxygen in the oxidiser stream ($Y_{O_2,2} = 0.232$ for air). Peters [134] give an alternative definition where the mixture fraction is related to the mass flux, $\dot{m}$, of the two streams

$$\xi = \frac{\dot{m}_1}{\dot{m}_1 + \dot{m}_2} \quad (4.8)$$

where stream 1 refers to fuel and 2 to oxidiser, respectively. If equal diffusivities are assumed for fuel, oxygen and inert, the fuel and air may be related to the mixture fraction

$$Y_{F,u} = Y_{F,1}\xi \quad Y_{O_2,u} = Y_{O_2,2}(1 - \xi) \quad (4.9)$$

showing that for pure fuel ($Y_{F,1} = 1$) and oxidiser streams, ξ and $Y_{F,u}$ have the same value. Eq. (4.9) may be used to link ξ to the equivalence ratio through Eq. (1.4) [134]

$$\phi = \frac{\xi}{1 - \xi} \frac{(1 - \xi_{st})}{\xi_{st}} \quad (4.10)$$

where ξ_{st} is the stoichiometric mixture fraction value. Similarly to Eq. (4.4) the conservation equation for the mixture fraction is given by

$$\frac{\partial \rho \xi}{\partial t} + \frac{\partial \rho u_i \xi}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\rho D \frac{\partial \xi}{\partial x_i} \right]. \quad (4.11)$$

At this point it may be noted that Eq. (1.27) will reduce to Eq. (4.11) if $\partial p / \partial t$ can be neglected and if the Lewis number is unity. The latter simplifications allow the enthalpy to be linearly related to the mixture fraction

$$h = h_1 \xi + h_2 (1 - \xi). \quad (4.12)$$

The introduction of Reynolds decomposition and Favre averaging followed by averaging of Eq. (4.11) results in

$$\frac{\partial \langle \rho \rangle \tilde{\xi}}{\partial t} + \frac{\partial \langle \rho \rangle \tilde{u}_i \tilde{\xi}}{\partial x_i} = - \frac{\partial \langle \rho \rangle \widetilde{u_i'' \xi''}}{\partial x_i} \quad (4.13)$$

where a high Re number assumption is invoked. Again, an unknown term appears, the turbulent scalar flux which requires closure. The latter may be closed by a gradient diffusion type closure given by Eq. (1.45) or through a second moment closure as discussed in Chapter 2. The transport equation for the turbulent scalar flux involving the passive scalar is identical to Eq. (2.2) except for the turbulence-reaction rate correlation which is zero. For clarity, the equation is repeated here

$$\begin{aligned} \frac{\partial \langle \rho \rangle \widetilde{u_i'' \xi''}}{\partial t} + \frac{\partial \langle \rho \rangle \tilde{u}_k \widetilde{u_i'' \xi''}}{\partial x_k} = & - \frac{\partial \langle \rho \rangle \widetilde{u_i'' u_k'' \xi''}}{\partial x_k} \\ & - \langle \rho \rangle \left(\widetilde{u_k'' \xi''} \frac{\partial \tilde{u}_i}{\partial x_k} + \widetilde{u_i'' u_k''} \frac{\partial \tilde{\xi}}{\partial x_k} \right) \\ & - \langle \xi'' \rangle \frac{\partial \langle p \rangle}{\partial x_i} - \langle \xi'' \frac{\partial p'}{\partial x_i} \rangle \\ & - \left[\langle \tau_{ik} \frac{\partial \xi''}{\partial x_k} \rangle - \langle J_{\xi k} \frac{\partial u_i''}{\partial x_k} \rangle \right] \end{aligned} \quad (4.14)$$

where the terms on the RHS represent turbulent transport of the scalar fluxes ($T_{ik\xi}$), the production term ($P_{i\xi}$), the effect of mean pressure gradient ($\Phi_{i\xi}$), the pressure strain term ($\phi_{i\xi}$) and viscous dissipation ($\langle \rho \rangle \epsilon_{i\xi}$). The transport equation for the mixture fraction variance is given by [85]

$$\begin{aligned} \frac{\partial \langle \rho \rangle \widetilde{\xi''^2}}{\partial t} + \frac{\partial \langle \rho \rangle \tilde{u}_k \widetilde{\xi''^2}}{\partial x_k} = & - \frac{\partial \langle \rho \rangle \widetilde{u_k'' \xi''^2}}{\partial x_k} \\ & - 2 \langle \rho \rangle \widetilde{u_k'' \xi''} \frac{\partial \tilde{\xi}}{\partial x_k} - \langle \rho \rangle \tilde{\epsilon}_\xi \end{aligned} \quad (4.15)$$

where the terms on the RHS represent turbulent transport of the scalar variance ($T_{i\xi\xi}$), the production term ($P_{\xi\xi}$) and the scalar dissipation rate ($\tilde{\epsilon}_\xi$). As described in Chapter 2, $\phi_{i\xi}$ is decomposed into a pressure transport ($\phi_{i\xi}^T$) and a pressure scrambling ($\phi_{i\xi}^S = \phi_{i\xi}^{CD} + \phi_{i\xi}^A$) term. $T_{ik\xi}$ and $\phi_{i\xi}^T$ in the scalar flux equation and $T_{i\xi\xi}$

in the scalar variance equation are closed by the gradient diffusion formulation of Daly & Harlow [35] (see Section 2.4)

$$\frac{\partial T_{il\xi}}{\partial x_l} + \phi_{i\xi}^T = \frac{\partial}{\partial x_k} \left[C_s < \rho > \frac{\tilde{k}}{\tilde{\epsilon}} \widetilde{u_k'' u_l''} \frac{\partial \widetilde{u_i'' \xi''}}{\partial x_l} \right] \quad (4.16)$$

$$\frac{\partial T_{l\xi\xi}}{\partial x_l} = \frac{\partial}{\partial x_k} \left[C_s < \rho > \frac{\tilde{k}}{\tilde{\epsilon}} \widetilde{u_k'' u_l''} \frac{\partial \widetilde{\xi''^2}}{\partial x_l} \right] \quad (4.17)$$

here generalised to include the scalar field. The constant density part of the pressure scrambling term ($\phi_{i\xi}^{CD}$) is closed by the generalised Langevin model formulation of Haworth & Pope [66, 67]

$$\phi_{i\xi}^{CD} = < \rho > G_{ik} \widetilde{u_k'' \xi''} - < \rho > \frac{\tilde{\epsilon}_\xi}{\tilde{\xi''^2}} \widetilde{u_i'' \xi''} \quad (4.18)$$

where the scalar dissipation rate is obtained by assuming a constant scalar to mechanical turbulence time scale ratio [85, 142]

$$\tilde{\epsilon}_\xi = \frac{1}{2} C_\phi \frac{\tilde{\epsilon}}{\tilde{k}} \widetilde{\xi''^2} \quad (4.19)$$

where $(C_\phi/2)^{-1}$ is the time scale ratio with $C_\phi = 2.0$. G_{ik} is given in Section 2.3.2.1. The remaining unclosed term is the mean pressure gradient term in the scalar flux equation. A closure for $< \xi'' >$ may be obtained if the PDF of the mixture fraction is known [85]

$$< \xi'' > = < \rho > \int_0^1 \frac{(\xi - \tilde{\xi})}{\rho(\xi)} f_\xi(\xi) d\xi \quad (4.20)$$

where f_ξ is the mixture fraction PDF. Jones [85] argues that the contribution of the mean pressure gradient terms are small in many flows and Kuan [95] neglected the terms when applied to a bluff body stabilised non-premixed flame on the basis of this argument. In the current computations, the mean pressure gradient terms are included for two reasons. First the terms do not represent a closure problem if the PDF is known and secondly, Lindstedt & Váos [107, 108] argue the importance of the mean pressure gradient in turbulent premixed flames due to preferential acceleration

effects as discussed in Section 2.3.

4.3.1.1 A joint β -bimodal presumed PDF approach

If the joint PDF of the reaction progress variable and the mixture fraction $\tilde{f}(\xi, c)$ is known, the favre averaged mean can be obtained from

$$\tilde{\phi} = \int_0^1 \int_0^1 \phi(\xi, c) \tilde{f}(\xi, c) d\xi dc. \quad (4.21)$$

For the premixed case, the PDF is usually presumed to have a bimodal shape given by Eq. (2.51). In the non-premixed case, on the other hand, the mixture fraction is the primary variable and a β function PDF is widely used [85, 134]. The β function PDF is defined completely by the mixture fraction mean and variance and is given by [85]

$$\tilde{f}(\xi) = \frac{\xi^{r-1}(1-\xi)^{s-1}}{\int_0^1 \xi^{r-1}(1-\xi)^{s-1} d\xi} \quad 0 \leq \xi \leq 1 \quad (4.22)$$

where r and s are given by

$$r = \tilde{\xi} \left[\frac{\tilde{\xi}(1-\tilde{\xi})}{\tilde{\xi}^2} - 1 \right] \quad \text{and} \quad s = \frac{1-\tilde{\xi}}{\tilde{\xi}} r \quad (4.23)$$

and the mean and variance are both obtained from their modelled transport equations.

To close the problem certain assumptions have to be made regarding the statistical dependence between the mixture fraction and the reaction progress variable. In many cases it is assumed that the mixture fraction and the reaction progress variable are statistically independent — an assumption that is unlikely to be true [49] in general. On the other hand, *a priori* determination of the shape of the PDFs is a rather strong assumption.

In the current case, two opposing streams of premixed reactants are surrounded by a coflow of air. The flow is premixed along the centreline and at the vicinity of the stagnation point where the flame is stabilised. The shear layer formed between the coflow of air and the counterflowing jets successively leans the premixed streams

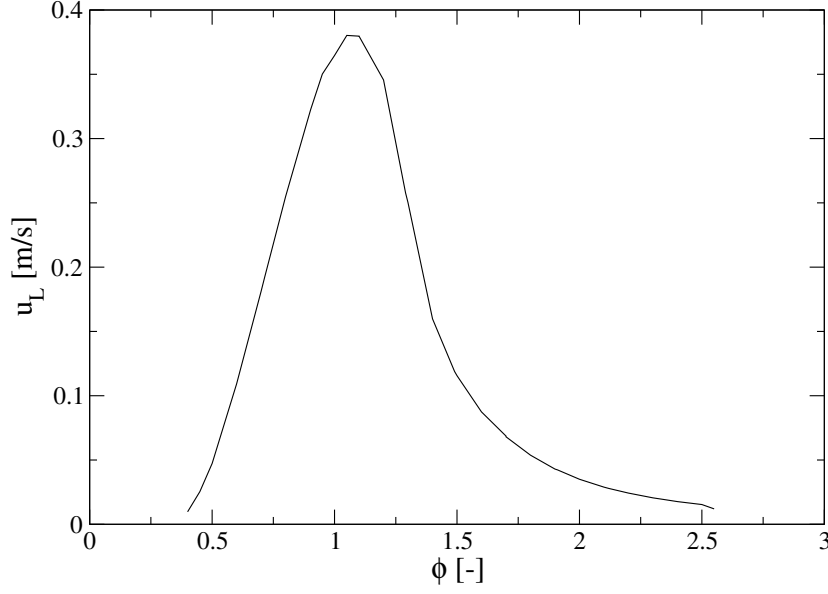


Figure 4.3: The laminar burning velocity as a function of equivalence ratio for CH_4 at 1 Atm and 298 K (—) [102].

and the entrainment of air results in a gradual decrease of the reaction rate and the burning velocity and limits the extent of the reaction zone. Furthermore, if reaction can be considered fast compared to mixing it may be assumed that the random variables ξ and c are independent and the joint PDF may be written as the product of the marginal PDFs [140]

$$\tilde{f}(\xi, c) = \tilde{f}(\xi)\tilde{f}(c). \quad (4.24)$$

Eq. (4.21) may thus be written

$$\tilde{\phi} = \int_0^1 \int_0^1 \phi(\xi, c) \tilde{f}(\xi) \tilde{f}(c) dc d\xi \quad (4.25)$$

where $\tilde{f}(\xi)$ is given by Eq. (4.22) and $\tilde{f}(c)$ is given by Eq. (2.51). The dependence of composition and temperature on the mixture fraction may thus be obtained from laminar flame calculations. Consequently, the chemistry is decoupled from the turbulence. The presumed PDF approach can then be used to obtain mean values that relate to the reaction progress variable and the mixture fraction. In the current context, propagating laminar premixed flames ranging roughly from the lean to the

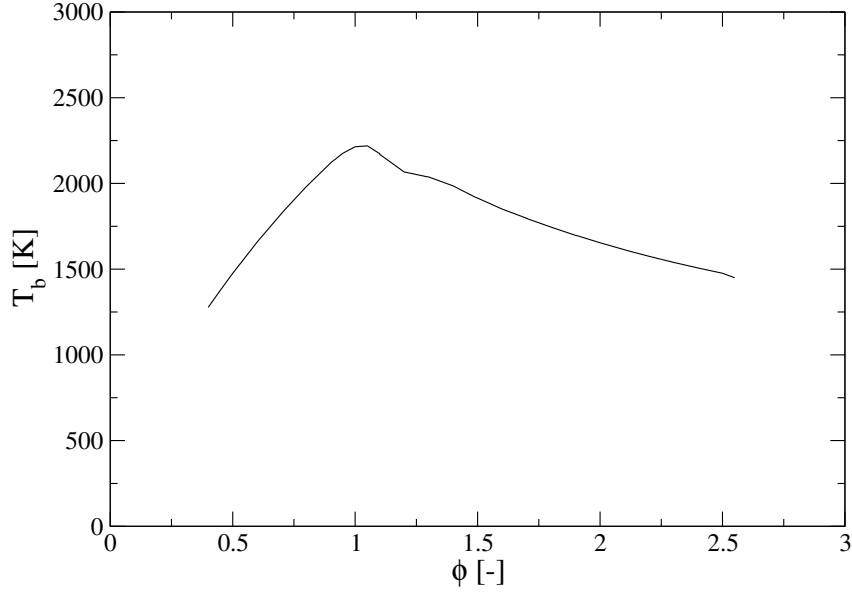


Figure 4.4: The adiabatic flame temperature as a function of equivalence ratio for CH_4 at 1 Atm and 298 K (—) [102].

rich limit ($0.40 \leq \phi \leq 2.55$), are computed to obtain primarily the laminar burning velocity (u_L), the temperature (T_b) and the viscosity (μ_b) of the burnt gases as a function of the mixture fraction. For these calculations the $C_1 - C_3$ mechanism of Leung & Lindstedt [102] was applied. In Figs. 4.3 and 4.4 the laminar burning velocity and adiabatic flame temperature can be seen as a function of equivalence ratio. The equivalence ratio is obtained from Eq. (4.10) with $\xi_{st} = 0.055$. The laminar flame properties are then tabulated and compiled as a pre-processing step.

4.3.2 Eulerian joint scalar PDF

In Chapter 3, a solution algorithm based on discrete particles in a Lagrangian framework is described. In all Lagrangian methods, convection is treated without reference to a grid [140] and the problem of numerical diffusion is avoided. The latter approach is the method of choice in simple geometries that can be discretised by structured meshes. In more complex configurations where unstructured meshes are required for the proper discretisation of the geometry, particle descriptions usually feature correction algorithms [182]. The correction algorithms are included to main-

tain consistency between the Lagrangian PDF solver and the Eulerian FV (finite volume) solver. Such algorithms increase the complexity and the already high computational demands. Therefore, an alternative approach is considered here — an Eulerian particle description. In the Eulerian description, all particles have equal weight and are associated with the cell center [49]. The fractional processes corresponding to convection and diffusion in scalar space are treated in the same way as in the Lagrangian approach, while transport in physical space differs due to the discrete representation of particle locations using cell centres.

4.3.2.1 Transport in physical space

In the Eulerian approach, transport in physical space is simulated by random jumps of particles between grid cells. Considering a general transport equation solved by the FV code

$$\frac{\partial \phi}{\partial t} + u_i \frac{\partial \phi}{\partial x_i} = \frac{\partial}{\partial x_i} \left[\Gamma \frac{\partial \phi}{\partial x_i} \right] \quad (4.26)$$

where only the spatial transport terms have been kept for simplicity. Integration over the grid cell volume ($\mathcal{V}$) followed by a first order FV discretisation allow Eq. (4.26) to be expressed as [49]

$$\mathcal{V}_l \frac{d\phi}{dt} = (Q\phi)^N + (Q\phi)^S + (Q\phi)^E + (Q\phi)^W - (Q_l^N + Q_l^S + Q_l^E + Q_l^W)\phi_l \quad (4.27)$$

where Q^k and Q_l^k ($k = N, S, E, W$) represent the effective volumetric flow rates in and out from adjacent cells to the l th cell, respectively. These flow rates are functions of the mean velocity, diffusivities and grid-cell geometry supplied by the FV code. The number of particles that jumps into the l th from neighboring cells are then given by [49]

$$N_l^k = \frac{Q^k \Delta t N_l}{\mathcal{V}_l} \quad (4.28)$$

where N_l^k represent an integer value. The particles are randomly selected with replacement so that the same particle can be selected more than once. The numerical treatment of the latter fractional step and the restriction to first order accuracy [49] is

the major disadvantage of Eulerian PDF codes since it will always lead to numerical diffusion. The only way of reducing numerical diffusion is to refine the grid if a sufficient number of particles is used.

4.3.2.2 Diffusion in scalar space

The molecular mixing term in the transport equation of the joint scalar PDF is closed by Modified Curl's model described in Section 3.3.3.1. During a small time increment Δt , N_{pq} pairs of particles out of N are selected without replacement and N_{pq} is given by Eq. (3.37) where $\beta_\phi = 3.0$ to ensure the correct decay rate of the scalar variance. The scalar dissipation rate (τ_ϕ^{-1}) is given by Eq. (3.41) and the standard value of 2.0 is maintained for C_ϕ .

4.3.2.3 Convection in scalar space

In the current computations, the global reaction scheme of Jones & Lindstedt [81, 82] is applied to compute the chemical source term (R_α) given by Eq. (3.42). This particular global scheme may be applied to model hydrocarbon combustion up to butane and include two competing fuel breakdown reactions. All radical species are eliminated and the rates are described by simple algebraic expressions. In the analysis of Jones & Lindstedt [81, 82] it is assumed that the flame structure comprises two reaction zones — the primary and the secondary reaction zones. In the primary zone, the fuel is converted to CO and H_2 and in the secondary zone, the combustion products are formed. The global four-step reaction mechanism is given in Table 4.1.

In the general case, the concentration dependence is not equal to the stoichiometric coefficient and the modified form of the forward kinetic rate expressions are given [81, 82]

$$r_i^{f*} = k_i^f(T)[C_x H_{2x+2}]^{\frac{1}{2}}[O_2]^{\frac{5}{4}} \quad (4.29)$$

$$r_{ii}^{f*} = k_{ii}^f(T)[C_x H_{2x+2}][H_2O] \quad (4.30)$$

$$r_{iii}^{f*} = k_{iii}^f(T)[H_2]^{\frac{1}{2}}[O_2]^{\frac{9}{4}}[H_2O]^{-1} \quad (4.31)$$

$$r_{iv}^f = k_{iv}^f(T)[CO][H_2O] \quad (4.32)$$

where the * indicates that the concentration dependences are not the same as those obtained from the stoichiometric coefficients. In the rate expressions above the equality $k^{f*}(T) \equiv k^f(T)$ has been used. The latter expression holds by definition in the case of global schemes. For the reversible reactions the reverse rates needs to be obtained. A change in the forward rate forces a change in the reverse rate constant which will now also be a function of species concentration. At equilibrium the forward and reverse rates are equal

$$r^f = r^r \quad \text{and} \quad r^{f*} = r^{r*} \quad \Rightarrow \quad \frac{r^{f*}}{r^{r*}} = \frac{r^f}{r^r} \quad (4.33)$$

which allows the modified reverse rate constant for reaction (iii) to be determined

$$\frac{k_{iii}^f [H_2]^{\frac{1}{2}} [O_2]^{\frac{9}{4}} [H_2O]^{-1}}{k_{iii}^{r*} [H_2O]} = \frac{k_{iii}^f [H_2] [O_2]^{\frac{1}{2}}}{k_{iii}^r [H_2O]} \Rightarrow k_{iii}^{r*} = \frac{[O_2]^{\frac{7}{4}}}{[H_2O][H_2]^{\frac{1}{2}}} k_{iii}^r \quad (4.34)$$

where

$$\frac{k_{iii}^r}{k_{iii}^f} = \frac{[H_2][O_2]^{\frac{1}{2}}}{[H_2O]} = K_{iii}^{-1} \quad (4.35)$$

where K_{iii} is the equilibrium constant.

Table 4.1: Global hydrocarbon mechanism

No	Reaction	x	A $m^3 kmol^{-1} s^{-1}$	b	E $J mol^{-1}$
(i)	$C_x H_{2x+2} + \frac{x}{2} O_2 \rightarrow x CO + (x+1) H_2$	1	0.440E+12	0	0.1255E+06
		2	0.420E+12	0	0.1255E+06
		3	0.400E+12	0	0.1255E+06
		4	0.380E+12	0	0.1255E+06
(ii)	$C_x H_{2x+2} + x H_2 O \rightarrow x CO + (2x+1) H_2$	1-4	0.300E+09	0	0.1255E+06
(iii)	$H_2 + \frac{1}{2} O_2 \rightleftharpoons H_2 O$	1	0.250E+17	-1	0.1674E+06
		2	0.350E+17	-1	0.1674E+06
		3	0.300E+17	-1	0.1674E+06
		4	0.280E+17	-1	0.1674E+06
(iv)	$CO + H_2 O \rightleftharpoons CO_2 + H_2$	1-4	0.275E+10	0	0.8368E+05

The modified reverse rate expression is then given by

$$r_{iii}^{r*} = k_{iii}^{r*}[H_2O] = \frac{[O_2]^{\frac{7}{4}}}{[H_2]^{\frac{1}{2}}} k_{iii}^r. \quad (4.36)$$

The forward and reverse rate expressions of reaction (iii) contain a negative concentration dependence of H_2O and H_2 , respectively. Small concentration levels may lead to numerical difficulties and eventually division by zero. A possible way forward is to derive modified rate expressions valid below some threshold value [105]. The current technique amounts to switching to a linear rate expression. Switching to a linear rate expression will necessarily lead to a change in the computation of the forward and reverse rates. To minimise such changes it is appropriate to introduce constraints. The first constraint is

$$r^{f*}(T, \phi_k)|_{\phi_k=c_{lim}} = r^{f**}(T, \phi_k)|_{\phi_k=c_{lim}} \quad (4.37)$$

where c_{lim} is the threshold value. The latter change must also be reflected in the reverse rates which is handled through the second constraint given by

$$\frac{r^{f*}}{r^{r*}} = \frac{r^{f**}}{r^{r**}}. \quad (4.38)$$

In the current situation, there are three possible scenarios: $[H_2] \rightarrow 0$, $[H_2O] \rightarrow 0$ and $[H_2], [H_2O] \rightarrow 0$. The rates are given by Eqs. (4.31), (4.36) and

$$r_{iii}^{f**} = k_{iii}^{f**}[H_2][O_2]^{\frac{1}{2}} \quad (4.39)$$

and

$$r_{iii}^{r**} = k_{iii}^{r**}[H_2O]. \quad (4.40)$$

Modified forward and reverse rates when $[H_2] \rightarrow 0 \Rightarrow [H_2] = c_{lim}$

$$\begin{aligned} r_{iii}^{f*} = r_{iii}^{f**} &\Rightarrow k_{iii}^{f**} = \frac{[O_2]^{\frac{7}{4}} k_{iii}^f}{[H_2O] \sqrt{c_{lim}}} \Rightarrow r_{iii}^{f**} = \frac{[O_2]^{\frac{9}{4}} [H_2] k_{iii}^f}{[H_2O] \sqrt{c_{lim}}} \\ \frac{r_{iii}^{f*}}{r_{iii}^{r*}} = \frac{r_{iii}^{f**}}{r_{iii}^{r**}} &\Rightarrow k_{iii}^{r**} = \frac{[O_2]^{\frac{7}{4}} k_{iii}^r}{[H_2O] \sqrt{c_{lim}}} \Rightarrow r_{iii}^{r**} = [O_2]^{\frac{7}{4}} \frac{k_{iii}^r}{\sqrt{c_{lim}}}. \end{aligned} \quad (4.41)$$

Modified forward and reverse rates when $[H_2O] \rightarrow 0 \Rightarrow [H_2O] = c_{lim}$

$$\begin{aligned} r_{iii}^{f*} = r_{iii}^{f**} &\Rightarrow k_{iii}^{f**} = \frac{[O_2]^{\frac{7}{4}} k_{iii}^f}{[H_2]^{\frac{1}{2}} c_{lim}} \Rightarrow r_{iii}^{f**} = [O_2]^{\frac{9}{4}} [H_2]^{\frac{1}{2}} \frac{k_{iii}^f}{c_{lim}} \\ \frac{r_{iii}^{f*}}{r_{iii}^{r*}} = \frac{r_{iii}^{f**}}{r_{iii}^{r**}} &\Rightarrow k_{iii}^{r**} = \frac{[O_2]^{\frac{7}{4}} k_{iii}^r}{[H_2]^{\frac{1}{2}} c_{lim}} \Rightarrow r_{iii}^{r**} = \frac{[O_2]^{\frac{7}{4}} [H_2O] k_{iii}^r}{[H_2]^{\frac{1}{2}} c_{lim}}. \end{aligned} \quad (4.42)$$

Modified forward and reverse rates when $[H_2], [H_2O] \rightarrow 0 \Rightarrow [H_2], [H_2O] = c_{lim}$

$$\begin{aligned} r_{iii}^{f*} = r_{iii}^{f**} &\Rightarrow k_{iii}^{f**} = [O_2]^{\frac{7}{4}} \frac{k_{iii}^f}{(\sqrt{c_{lim}})^3} \Rightarrow r_{iii}^{f**} = [O_2]^{\frac{9}{4}} [H_2] \frac{k_{iii}^f}{(\sqrt{c_{lim}})^3} \\ \frac{r_{iii}^{f*}}{r_{iii}^{r*}} = \frac{r_{iii}^{f**}}{r_{iii}^{r**}} &\Rightarrow k_{iii}^{r**} = [O_2]^{\frac{7}{4}} \frac{k_{iii}^r}{(\sqrt{c_{lim}})^3} \Rightarrow r_{iii}^{r**} = [O_2]^{\frac{7}{4}} [H_2O] \frac{k_{iii}^r}{(\sqrt{c_{lim}})^3} \end{aligned} \quad (4.43)$$

where $c_{lim} = 10^{-3}$. For reaction (iv) the reverse rate simply follows from the equilibrium condition

$$r_{iv}^r = k_{iv}^r [CO_2] [H_2] = k_{iv}^f [CO] [H_2O] = r_{iv}^f. \quad (4.44)$$

4.4 Numerical procedure

The physical domain is represented by a 90° sector of one of the nozzles. The physical domain is discretised in control volumes by means of an unstructured mesh featuring 3.5×10^5 non-uniform hexahedral cells with a maximum cell skewness of 0.5 and local refinement towards the stagnation point. The cell sizes approaching the stagnation point are below 0.25 mm in the axial direction, which is of the order of the Kolmogorov scale (l_K) as estimated by Geipel [52]. The grid was prepared using ANSYS Gambit and may be viewed in Fig. 4.5. The inlet boundary is prescribed

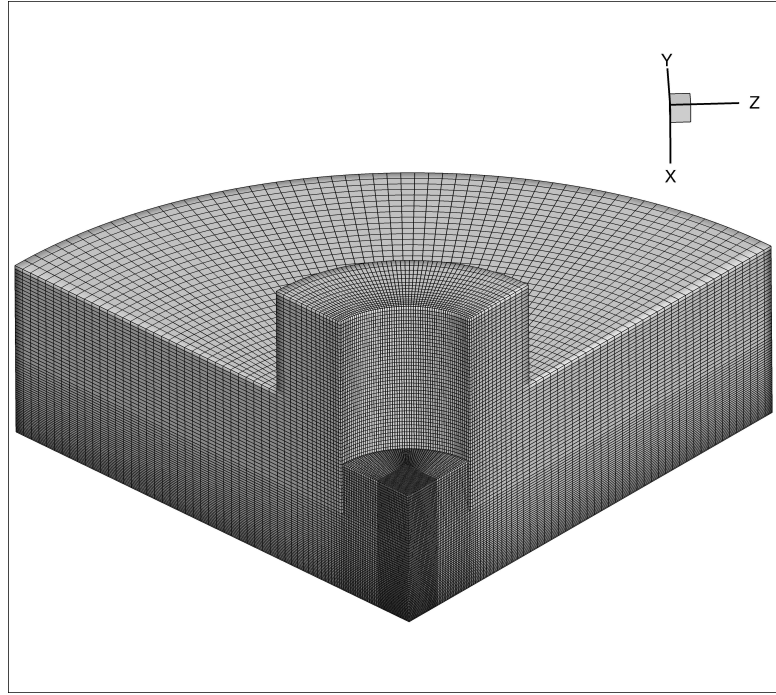


Figure 4.5: The unstructured mesh featuring 3.5×10^5 non-uniform hexahedral cells.

10 mm upstream of the nozzle exit while the outlet boundary is located three nozzle diameters from the stagnation point, see Fig. 4.1. Symmetry boundaries have been used where appropriate and standard wall functions are applied on the nozzle and coflow-nozzle walls.

4.4.1 The presumed PDF approach

The velocity-pressure coupling is handled via a PISO [73] algorithm allowing a free number of correctors. Spatial numerical diffusion is minimised through a blending scheme with the blending factor set to 0.5 for momentum and scalars and 0.2 for the turbulence equations. The scheme blends a first order upwind with central differencing, see Section 4.4.1.1. Temporal discretisation is approximated by Euler expressions and the time step is limited to a local Courant number of 0.2 and at least ten time steps per minimum turbulent time scale. The solution procedure is block structured featuring a momentum/scalar block and a turbulence block and the solver was forced to do a minimum of three to five iterations within each equation

block depending on the turbulence model. Furthermore, the numerical procedure features convergence adaptive time step control including step splitting on error. Convergence check is handled through four monitors, one for pressure, one for each block and one overall. All convergence monitors allow a maximum error of 10^{-3} except pressure (10^{-6}) within each time step. In the case of reacting opposed flows, the mean reaction rate is closed by the expression given by Eq. (1.57) and a reaction rate constant (C_R) of 2.6 [108] has been used unless otherwise stated.

4.4.1.1 Spatial discretisation of convective terms

All the governing transport equations are represented by a convection-diffusion type equation. Interpolation of nodal values to cell faces of the diffusion terms are traditionally done using second order accurate schemes like central differencing. The diffusion process affects the distribution of the transported quantity gradient in all directions, while the convective terms are dominated by the direction of the flow. The relative strength between convection and diffusion sets an upper limit of the cell size for non-oscillating convection-diffusion calculations. With central differencing, cells larger than the upper limit may produce oscillating solutions. The oscillations depend on the local Peclet (Pe) number defined as

$$Pe = \frac{\rho u \Delta x}{\Gamma} \quad (4.45)$$

where Δx represent a 1-dimensional cell size and Γ is the diffusion coefficient. It can be shown that no oscillations occur if $Pe \leq 2$ [48]. This constraint may, in practice, require cell sizes that gives very large grids (number of computational cells). One alternative, that is unconditionally stable, is to use a first order accurate scheme like an upwind scheme. The latter type of schemes are, however, known to produce numerical diffusion and a reduction in accuracy is inevitable.

In the present work a blending scheme is used for the convective cell face fluxes (M_f^C). The current scheme blends upwind differencing (UDS) with central differ-

encing (CDS)

$$M_f^C = M_f^{C,CDS} - (1 - \Upsilon) \left[M_f^{C,CDS} - M_f^{C,UDS} \right] \quad (4.46)$$

and the blending factor (Υ) takes on values between zero and unity where zero represents a pure upwind scheme and unity pure central differencing. In the present work, the blending factor is set to 0.5 for the momentum and scalar equations while a value of 0.2 is used for all turbulence equations.

4.4.2 The transported PDF approach

To ensure a good starting point for the PDF solver, the flow field is initialised using the presumed PDF approach. Each computational cell is allocated with 100 particles and particle values are initialised assuming a bimodal distribution followed by ten virtual PDF solver steps to smooth the first initial guess. After the ten virtual PDF solver steps, the PDF solver stops, and the field is initialised. The solution procedure is here structured so that the finite volume (FV) and the PDF solvers are decoupled with the ambition to obtain a solution close to steady state. This is achieved by letting the FV solver perform 250 iterations and then let the PDF solver to do 25 iterations. As a result, the FV and PDF solvers are not synchronised in time. The settings for the FV solver are maintained from the presumed PDF approach while the time step for the PDF solver is limited by requiring a turbulent time scale resolution of 0.03. The particle values are ensemble averaged during eight PDF solver time steps and the moments are under-relaxed to ensure numerical stability. The under-relaxation factor was set to 0.3.

4.4.3 Boundary conditions

For the isothermal flow, Geipel [52] replaced one of the steel nozzles with a glass nozzle of equal dimensions in order to enable measurements of the in-nozzle flow field. Measurements of this type are of significant importance for computational studies as boundary conditions are easily extracted. The in-nozzle data covers mean axial velocity, axial and radial Reynolds stress components at different locations from

the fractal grid. Unfortunately, turbulence is not fully characterised as information about the turbulent integral length scale is missing inside the nozzle. It is, however, possible to get some guidance through the measured turbulent integral length scale at the nozzle exit [53] which is of the order of 3.1 ± 0.1 mm. In studies featuring perforated plates for turbulence generation, a value of the order of 70% of the hole diameter of the perforated plates is often used [149]. The latter estimate agrees reasonably well with the values obtained by Cho et al. [30] (2 mm for 3.2 mm hole diameter) and Geipel [52] (2.6 mm for 4.0 mm hole diameter).

Along the centreline, the effect (blockage) on the mean axial velocity of the largest fractal cross prevails all the way to the nozzle outlet. The effect of this is discussed further in Section 4.5.1. At a location of 10 mm from the nozzle outlet the axial and radial Reynolds stress components are of the same order — turbulence is close to isotropic. This location was therefore considered as an appropriate choice for the inlet boundary condition.

The inlet boundary condition for the nozzle is located 10 mm upstream of the nozzle exit. The current case correspond to a nozzle separation of one diameter and bulk velocity (u_b) of 4 m/s. The in-nozzle measurement [52] is used as a basis for the mean axial velocity, axial and radial turbulence intensities in the isothermal case. The mean axial velocity profile is extracted from the in-nozzle measurement due to the influence of the largest fractal cross while top-hat profiles were set for the turbulence intensities. In the case of a $k - \epsilon$ model isotropic turbulence is assumed. For the Reynolds stress computations an anisotropy of the order of 15% in turbulence intensities is introduced. This level correspond to the uncertainty in the measurements [52] and was found to be beneficial in terms of predictions close to the first measuring point. The turbulent integral length scale was adjusted until a value of 3.1 ± 0.1 mm was obtained at the nozzle exit. The latter value was found to correspond to a value of 2.6 mm 10 mm upstream of the nozzle exit. In the annular coflow channel surrounding each nozzle, top-hat profiles of mean velocity and turbulence parameters are prescribed. The velocity of the coflow corresponds to 30% of the nozzle bulk velocity. Furthermore, a turbulence intensity of 5% and

turbulent integral length scale of 2.6 mm was assumed for the coflow. The outlet boundary condition is located three nozzle diameters from the nominal stagnation point and a (far-field) pressure of 101325 Pa is assumed.

For the reacting case, a perfectly premixed mixture of methane and air at an equivalence ratio of 0.9 and temperature 298 K was prescribed at the nozzle inlet. A comparison between the experimentally derived turbulence levels in the isothermal and the reacting cases reveals a difference of the order of 25% at the first measuring point. In the PIV-measurements of Geipel [52], different seedings were used in the isothermal and reactive cases. In the former case, the velocity field was obtained using silicon oil droplets with an average diameter of 1 micrometer while in the latter case aluminium-oxide particles with sizes of 3 microns were applied. The change in seeding particles required a change of the section upstream of the turbulence generation plates. This led to an increase in the turbulence intensities and needed to be taken into account [51]. The turbulence levels were therefore adjusted accordingly at the nozzle inlet boundary condition. The turbulent integral length scale was maintained at 2.6 mm.

4.5 Results

In the next two Sections the computed isothermal and reacting opposed flows are presented. The predictions are compared with the measurements performed by Geipel [52] and Geipel et al. [53]. Experimental data in opposed flows typically include [52, 90, 91, 121, 125] data points along the burner centreline between the nozzles and along the stagnation plane. The stagnation plane [18] is the plane that is perpendicular to the approaching flow, located midway between the nozzles. The point where the centreline crosses the stagnation plane is defined as the stagnation point. The flow is usually axi-symmetrical [18] and data points on the stagnation plane may be represented by a single line. For both the isothermal and reacting cases, the mean velocities and turbulence levels are measured and, in addition, the reaction progress variable and its variance were measured for the reacting case.

From the two-dimensional data, values were extracted along the burner centreline, the stagnation plane and additional velocity and turbulence profiles were extracted 1.5 mm downstream of the nozzle exit in the isothermal case. In cases where the $k-\epsilon$ model is applied, the measured axial and radial velocity fluctuations are compared with an isotropic velocity fluctuation ($u' = v' = w' = q'$) defined as

$$k = \frac{3}{2}q'^2 \quad \Rightarrow \quad q' = \sqrt{\frac{2k}{3}} \quad (4.47)$$

as no anisotropic information can be extracted from k alone.

For flows with significant variable density effects, such as the current reacting case, Favre averages are usually applied to the governing equations. The experimentally determined values are arguably conventionally averaged and differences might be expected in the reaction zone. As a consequence, either the computed or the experimentally determined values need to be transformed. It is, however, rather difficult to obtain accurate measurements of the turbulence scalar flux terms used in the transformation formula. The current computational results have therefore been transformed into conventional averages in the manner of Lindstedt et al. [116] using relations from the BML [14] theory valid in the flamelet regime of combustion. Geipel [52] estimated the Da and the Ka numbers to 10.3 and 0.46, respectively, for the current opposed jet configuration. In view of the Borghi diagram given in Fig. 1.1, the flamelet regime is in the region where $Da > 1$ and $Ka < 1$. The conventionally averaged mean velocity is given by (cf. Eq. (2.56))

$$\langle u_i \rangle = \tilde{u}_i + \langle u_i'' \rangle \cong \tilde{u}_i + \frac{\mathcal{T} \widetilde{u_i'' c''}}{1 + \mathcal{T} \tilde{c}} \quad (4.48)$$

and the Reynolds stresses [14, 116]

$$\langle u_i' u_j' \rangle \cong \widetilde{u_i'' u_j''} - \frac{\widetilde{u_i'' c''} \widetilde{u_j'' c''}}{\tilde{c}(1 - \tilde{c})}. \quad (4.49)$$

At the reaction progress variable scalar bounds ($c = [0, 1]$), Eq. (4.49) breaks down and a cut-off (ϵ) is therefore introduced. The equation is defined for $c = [\epsilon, 1 - \epsilon]$

where $\varepsilon = 10^{-3}$ and outside this range it assumed that $\langle u'_i u'_j \rangle \cong \widetilde{u''_i u''_j}$. On the other hand, as c approaches the scalar bounds $\widetilde{u''_i c''} \rightarrow 0$ and $\langle u'_i u'_j \rangle = \widetilde{u''_i u''_j}$. The conventionally averaged reaction progress variable is given by (cf. Eqs. (2.57)-(2.58))

$$\langle c \rangle = \tilde{c} + \langle c'' \rangle \cong \tilde{c} + \frac{\mathcal{T}\tilde{c}(1 - \tilde{c})}{1 + \mathcal{T}\tilde{c}} = \frac{(1 + \mathcal{T})\tilde{c}}{1 + \mathcal{T}\tilde{c}} \quad (4.50)$$

and the variance [89]

$$\langle c'^2 \rangle \cong \langle c \rangle (1 - \langle c \rangle). \quad (4.51)$$

It should be noted that only the last two equations are used in the case of a gradient diffusion closure. Calculated vales are presented for two nozzles while the solution domain only covers a 90° sector of one of the nozzles. All calculated values are therefore reflected and in some cases, depending on the flow direction, the values are multiplied by -1 . All results are time averaged.

4.5.1 Isothermal opposed flow

The standard $k - \epsilon$ model agrees well with the experimental data, both along the centreline and stagnation plane. In Fig. 4.6 the predictions along the centreline are shown. The mean axial velocity component (u) agrees comparatively well with experimental data. A small asymmetry can be seen in the experimental data whereas the computations suggest a more narrow turbulence peak than the experimental data. This may be a result of low frequency instabilities observed in previous studies (e.g. [91]). The peak value, at the stagnation point, of the turbulent kinetic energy (k) is reasonably well predicted in contrast to previous studies (cf. [112, 121]) where the turbulence peak was significantly over-predicted. Inspection of the individual velocity fluctuation components reveal, however, that the axial (u') is under-predicted and the radial (v') component is over-predicted.

In Fig. 4.7, a comparison between fractal-generated turbulence and turbulence generated by traditional perforated plates is made. The cases correspond to a bulk velocity of 4 m/s with fractal-generated turbulence and 3.4 m/s with the perforated plates. The predictions and the experimental data have been normalised with the

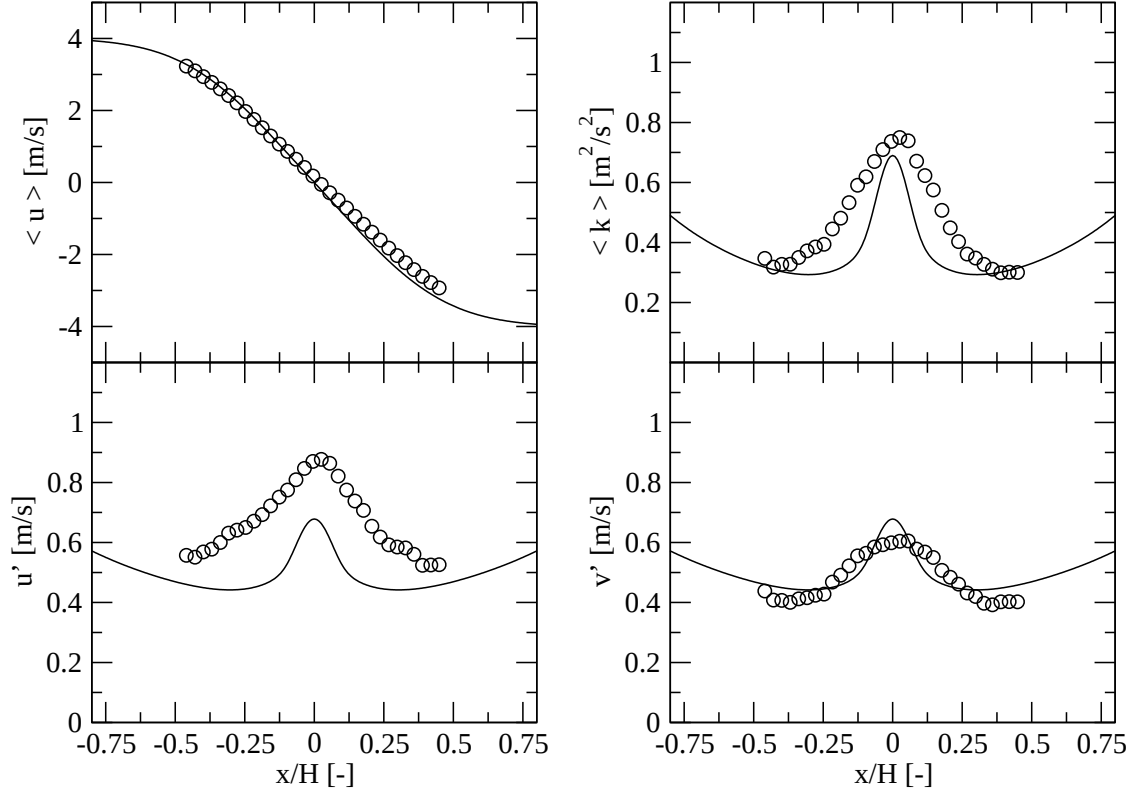


Figure 4.6: Predictions using the $k - \epsilon$ model along the centreline. Top left (TL): Mean axial velocity component, top right (TR): Turbulent kinetic energy, bottom left (BL): Axial velocity fluctuation and bottom right (BR): Radial velocity fluctuation. Predictions (—) and experimental data (o).

corresponding bulk velocity to make the comparison possible. First, the fractal plates lead to a reduction in mean axial velocity along the burner centreline due to the largest fractal cross [52]. As a consequence, turbulence production by axial strain along the centreline in the numerical simulation is significantly reduced leading to a lower relative increase at the stagnation point compared to the case with the perforated plates. The absolute peak value at the stagnation point is, of course, higher with the fractal-generated turbulence as Re_T is higher at the nozzle exit. Secondly, the turbulence models applied in this work are applicable for high Re_T number flows and as shown by Lindstedt et al. [112], Reynolds stress predictions are improved with increasing Reynolds number. Predictions along the stagnation plane using the $k - \epsilon$ model are shown in Fig. 4.8. Again, the predictions agree well with the experimental data for the mean radial velocity (v) component and

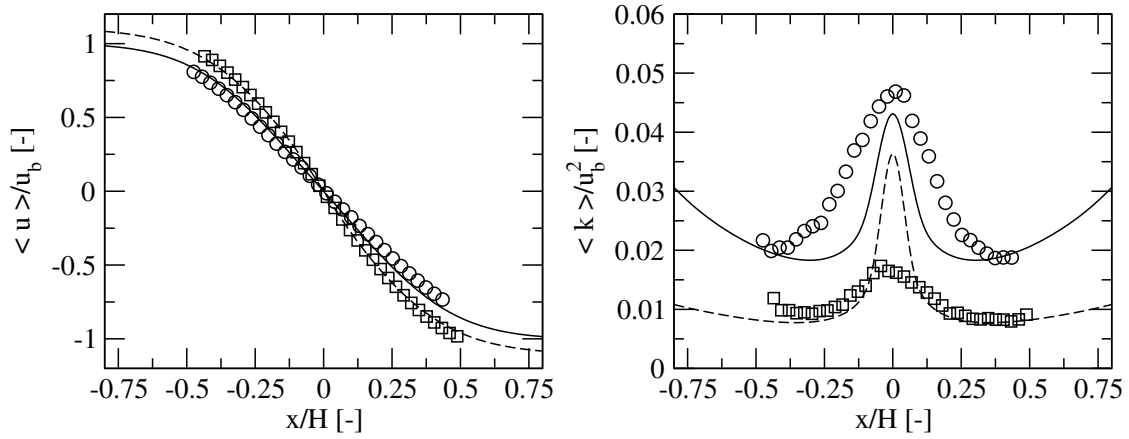


Figure 4.7: Predictions using the $k - \epsilon$ model along the centreline. Left: Mean axial velocity component normalised by u_b . Right: Turbulent kinetic energy normalised by u_b^2 . Fractal generated turbulence, $u_b = 4.0$ m/s, predictions (—) and experimental data ($\circ$). Perforated plates, $u_b = 3.4$ m/s, predictions (- - -) and experimental data ($\square$).

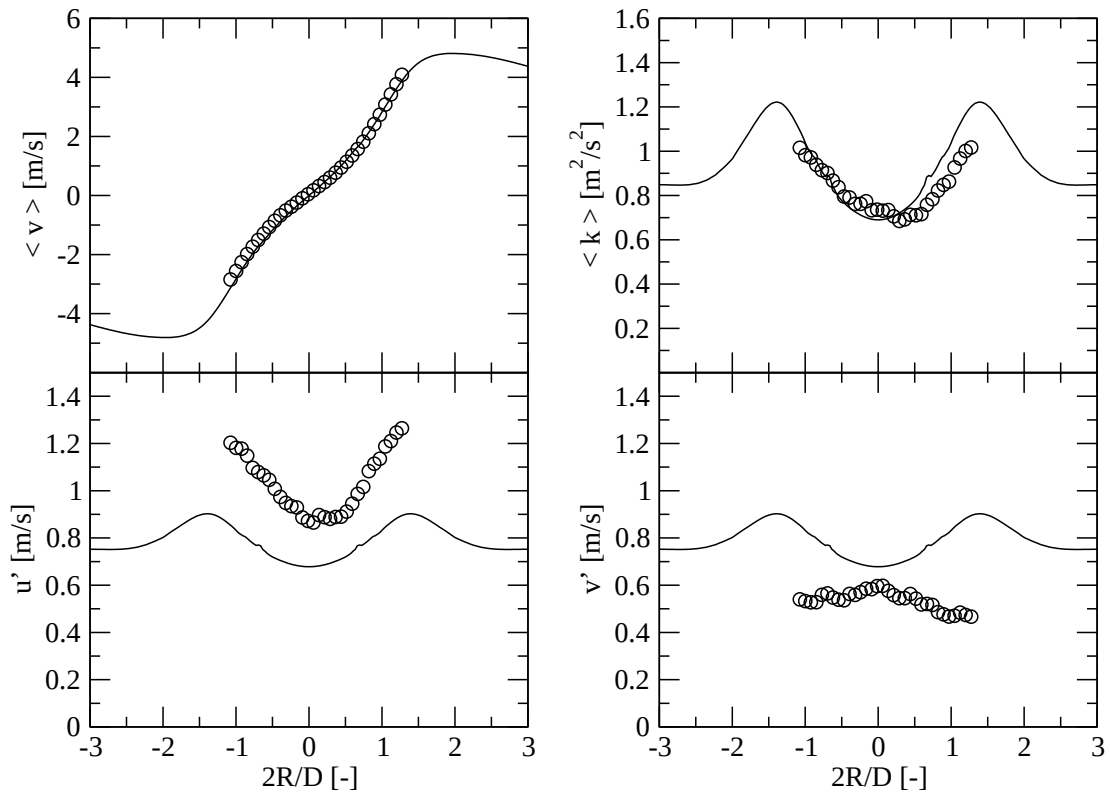


Figure 4.8: Predictions using the $k - \epsilon$ model along the stagnation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions (—) and experimental data ($\circ$).

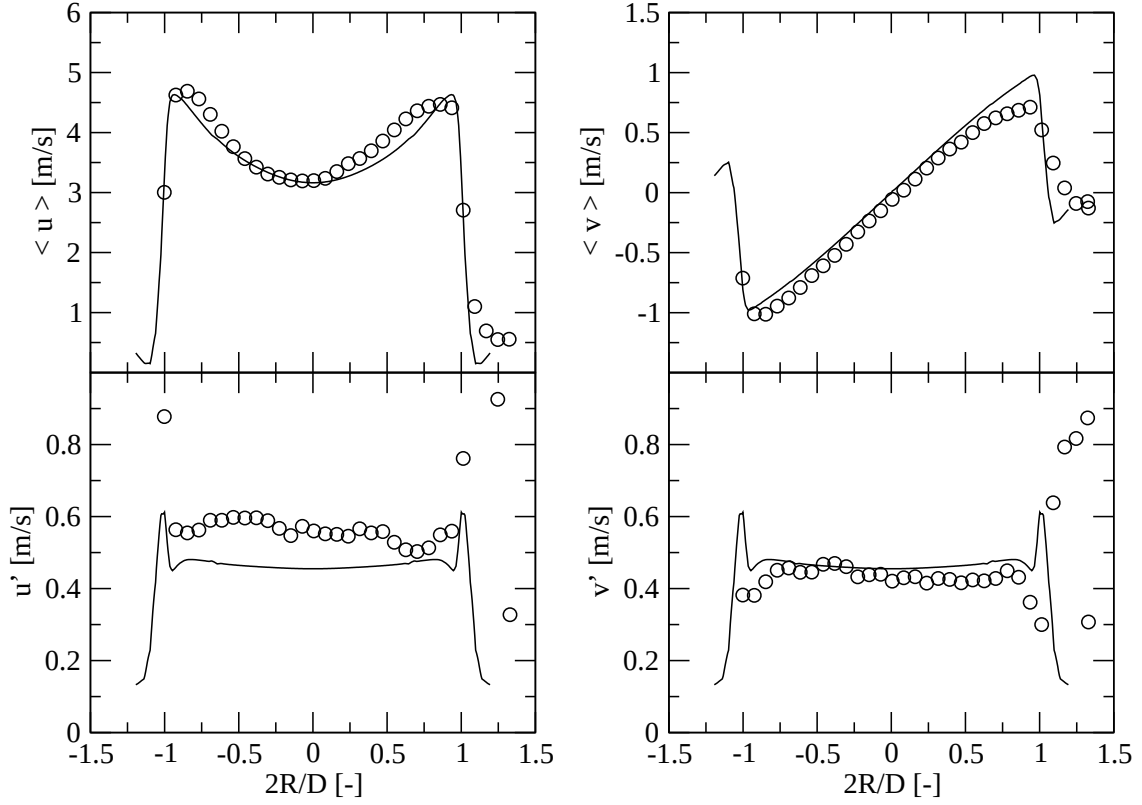


Figure 4.9: Predictions using the $k - \epsilon$ model 1.5 mm downstream of the nozzle exit. TL: Mean axial velocity component, TR: Mean radial velocity component, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions (—) and experimental data ($\circ$).

the turbulence kinetic energy while deviations can be seen for the axial and radial velocity fluctuations. The measured axial velocity fluctuation suggests an increase in turbulence levels beyond a radial distance of one half burner diameter. The increase is a result of the shear layer formed between the flow and the surrounding air [52, 112] and is captured to some degree by the $k - \epsilon$ model. The same increase can be seen in the computed radial velocity fluctuation while the measured values remain constant. In Fig. 4.9, predictions 1.5 mm downstream of the nozzle exit are shown. The mean axial and radial velocities are well reproduced while some deviations can be seen for the turbulence intensity profiles where the experimental data suggests a degree of anisotropy. The radial turbulence intensity profile is reasonably well captured.

Fig. 4.10 shows predictions along the centreline using two different Reynolds

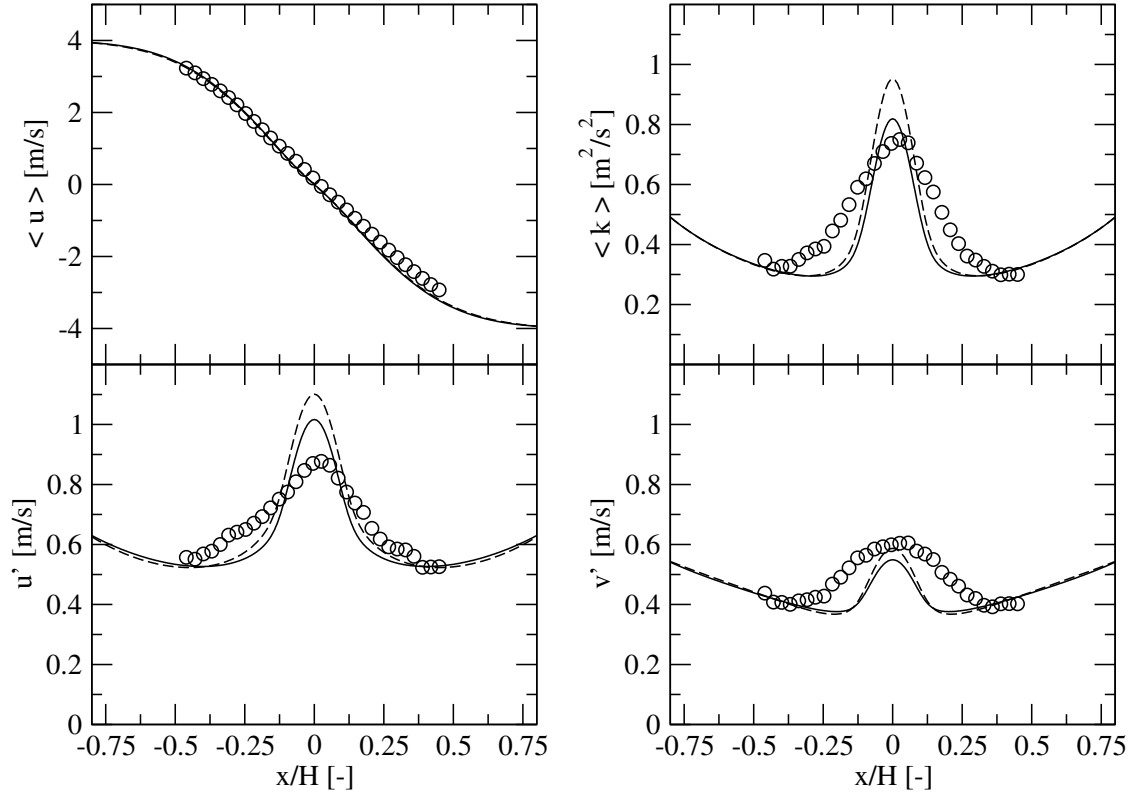


Figure 4.10: Predictions using Reynolds stress models along the centreline. TL: Mean axial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions using the model of Haworth & Pope (—), Jones & Musonge (- - -) and experimental data (o).

stress turbulence models, the models of Jones & Musonge [83] (JM) and Haworth & Pope [66, 67] (HP). The models are described in detail in Section 2.3.2. The mean axial velocity is well predicted with very small differences between the two transport equation based Reynolds stress closures. Both model predictions suggest a more narrow peak than the experimentally derived values. Geipel et al. [53] showed that the stagnation point moves in both the axial and radial directions and this movement results in a wider turbulence peak. The JM model predicts both a higher and a wider turbulent kinetic energy peak as the stagnation point is approached compared to the HP model. Both models over-predict the peak value at the nominal stagnation point. The HP model over-predicts the axial turbulence intensity component while the radial component is slightly low. The JM model, on the other hand, predicts the radial component reasonably well while the axial

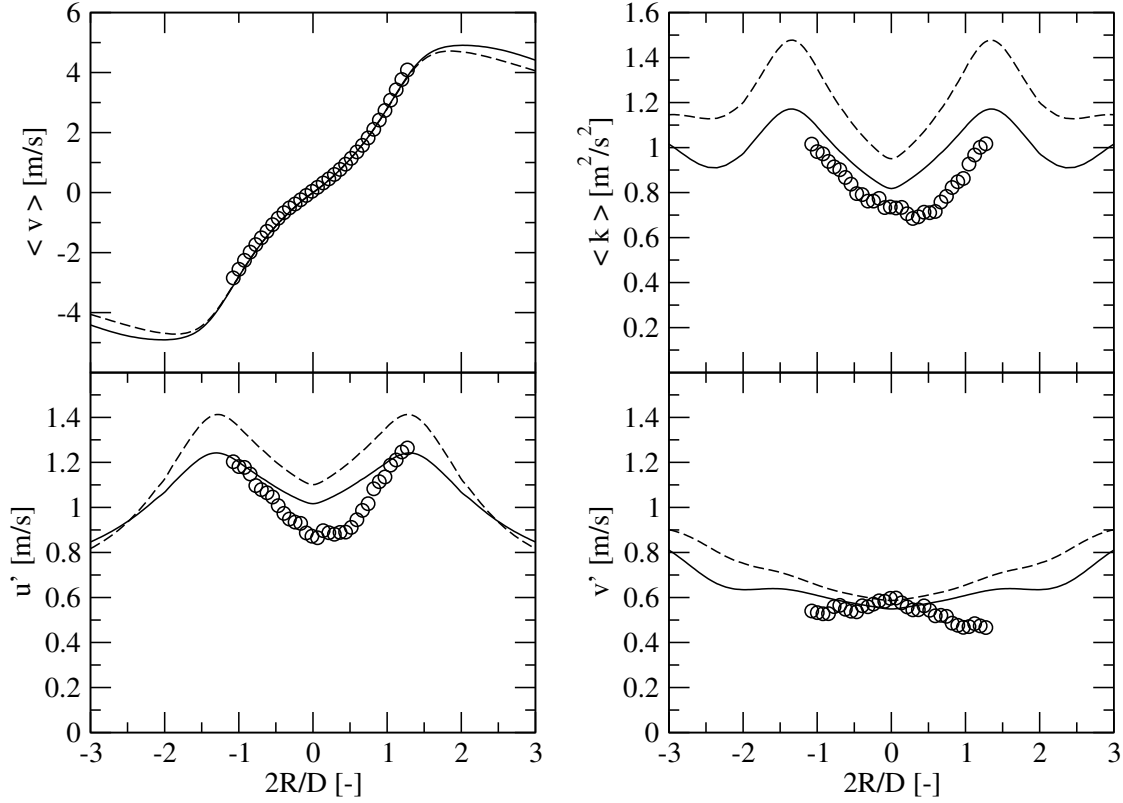


Figure 4.11: Predictions using Reynolds stress models along the stagnation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions using the model of Haworth & Pope (—), Jones & Musonge (- - -) and experimental data (o).

peak is even higher than the predictions of the HP model — consistent with the turbulence kinetic energy predictions. The difference between the JM and the HP models is a result of the different formulations of the redistributive part of the pressure strain tensors. At the stagnation plane, shown in Fig. 4.11, the mean radial velocity component is well predicted by both models. Some difference may be noted beyond a radial distance of two nozzle diameters. The turbulent kinetic energy along the stagnation plane is significantly higher than the experimental data suggests with the JM model while the HP model shows a reasonable agreement with a slight over-prediction. The axial turbulence intensity component is responsible for the over-predictions while both models agree comparatively well for the radial component. The predicted nozzle exit profiles using the Reynolds stress models,

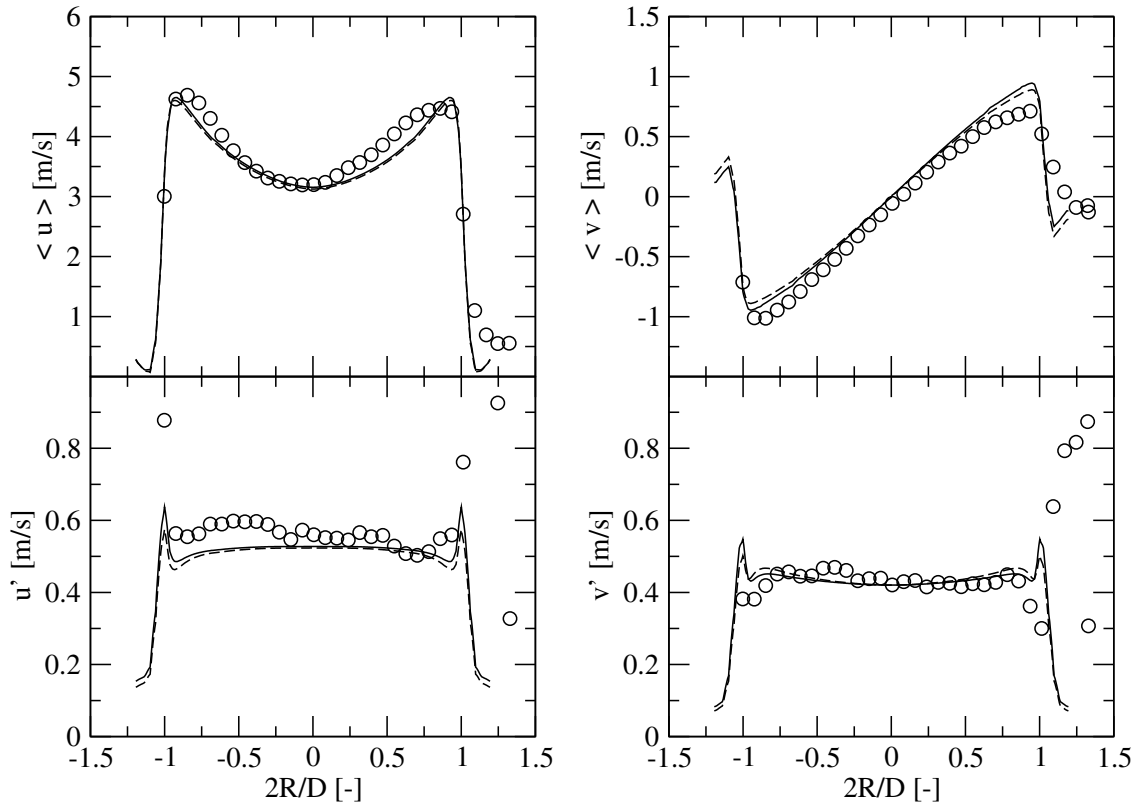


Figure 4.12: Predictions using Reynolds stress models 1.5 mm downstream of the nozzle exit. TL: Mean axial velocity component, TR: Mean radial velocity component, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions using the model of Haworth & Pope (—), Jones & Musonge (---) and experimental data ($\circ$).

shown in Fig. 4.12, show an improved behaviour compared to the $k - \epsilon$ model. Mean axial and radial components agree well with the experimental data as well as the radial turbulence intensity profile while the axial turbulence intensity is slightly low for both Reynolds stress models.

For the current opposed flow configuration, the standard $k - \epsilon$ model performs well in contrast to earlier studies where second moment closures typically outperformed eddy viscosity based closures. The predictions of the Reynolds stress models agree reasonably well with the experimental data. In general, predictions using the HP model are closer to the measured values and the JM model will therefore not be considered for the reacting opposed case.

4.5.2 Reacting opposed flow

4.5.2.1 The presumed PDF approach

The standard $k-\epsilon$ model, combined with a gradient diffusion model for scalar fluxes, fails to predict the peak of the axial velocity fluctuation, and the level at the first measuring point is too low as shown in Fig. 4.13. Furthermore, the width of the turbulence peak is too narrow compared to the experimental data. The model fails to predict the radial velocity fluctuation and therefore also the turbulent kinetic energy as the radial peak is taken into account twice in $\tilde{k}$. On the other hand, it is a bit surprising to see that the experimental data suggests that the axial velocity fluctuation is lower than the radial peak as the flow is purely axial along the burner centreline and turbulence is produced due to strain in this direction and redistributed to the radial component. One possible explanation is stagnation point movement [53] in the radial direction in the experiments and this movement is not captured in the simulations as the position of the stagnation point is dictated by the symmetry boundary conditions. The experimental data of the mean axial velocity suggests a local reduction in strain due to the presence of the flame. The $k-\epsilon$ model correctly predicts this local reduction, but at the wrong position as the model fails to predict the turbulent flame thickness as shown in Fig. 4.14. The Favre average reaction progress variable variance is also shown in the figure. In Fig. 4.15, predictions along the stagnation plane are shown. The mean radial velocity is in excellent agreement while the axial and radial velocity fluctuation levels, and therefore, also the turbulent kinetic energy are too low.

The HP model combined with a gradient diffusion model does not improve the situation significantly as shown in Fig. 4.16. The radial turbulence peak and the turbulent kinetic energy is even lower than the predictions using the $k-\epsilon$ model. Again, the peak of the axial turbulence intensity at the stagnation point is reasonably well reproduced. The anisotropy introduced in the boundary condition allow the correct level to be set of the axial turbulence intensity at the first measured point. The HP model correctly predicts a local increase in the axial turbulence intensity

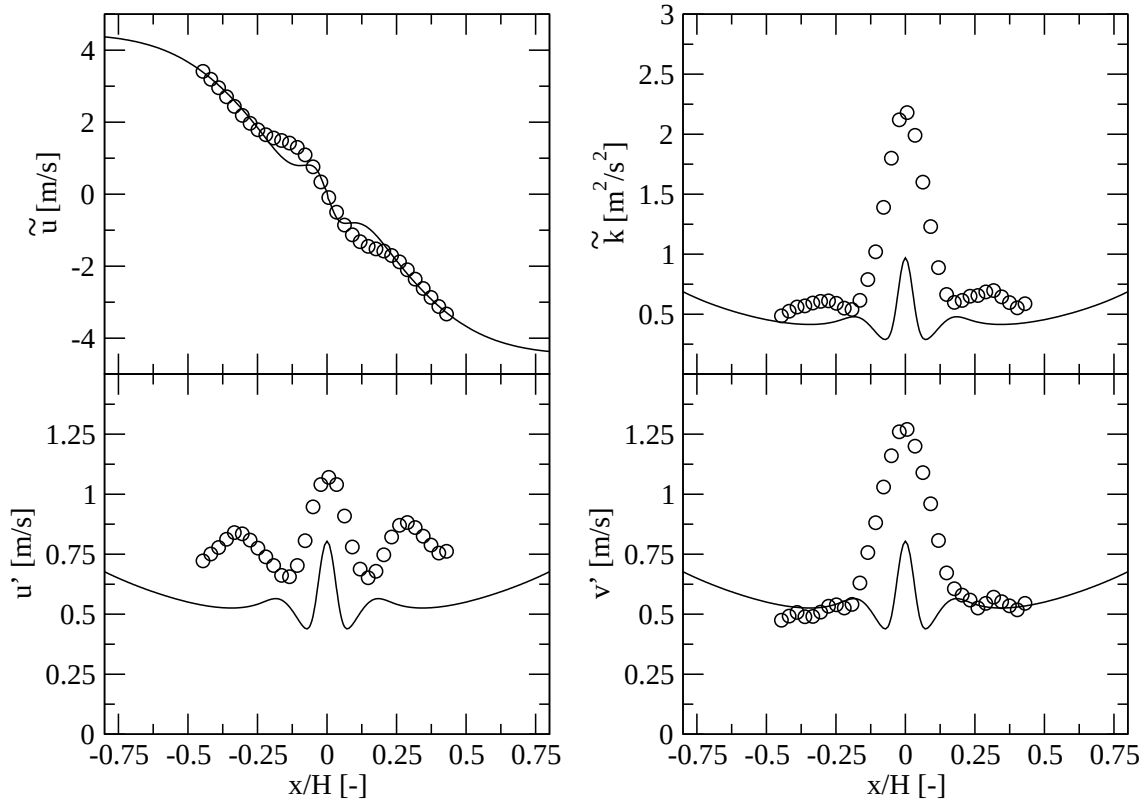


Figure 4.13: Predictions using $k - \epsilon$ /gradient diffusion models along the centreline. TL: Mean axial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions (—) and experimental data ($\circ$).

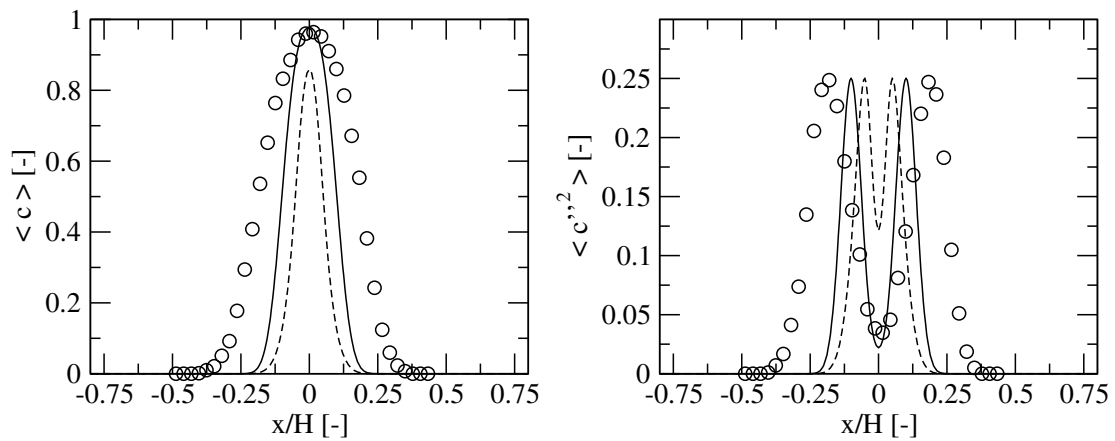


Figure 4.14: Predictions using $k - \epsilon$ /gradient diffusion models along the centreline. Left: Mean reaction progress variable profile. Right: Mean reaction progress variable variance. Conventional averages (—), Favre averages (---) and experimental data ($\circ$).

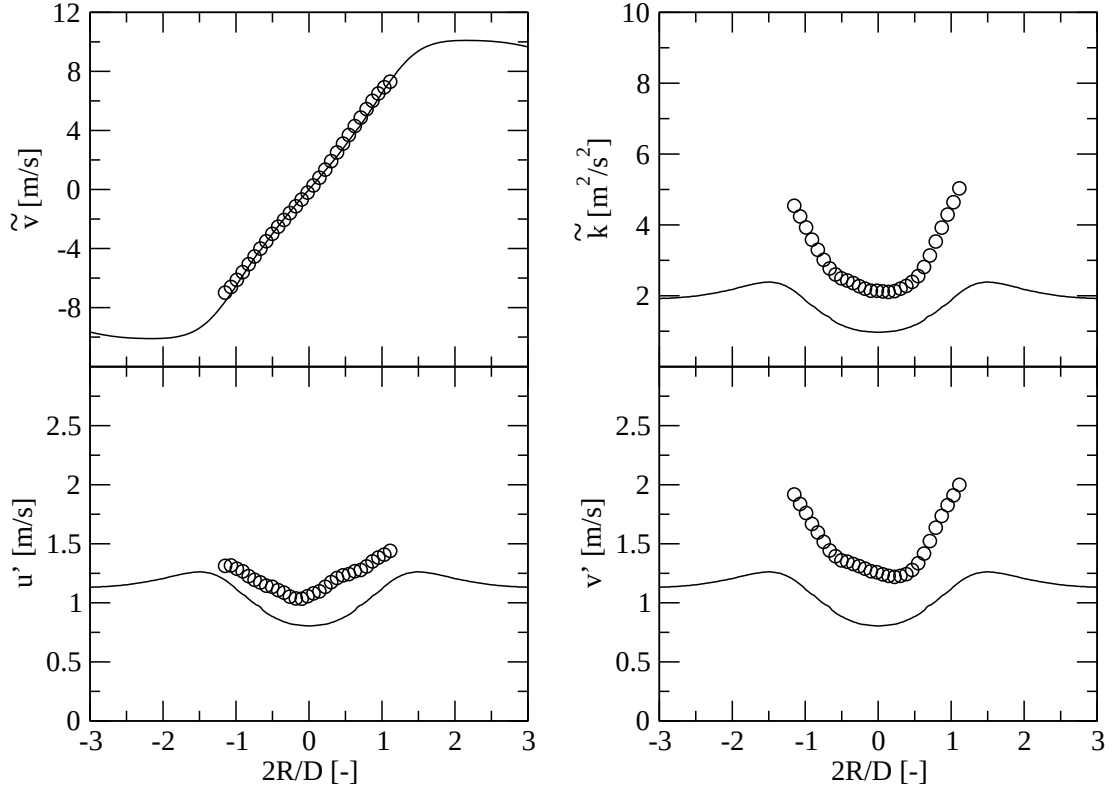


Figure 4.15: Predictions using $k - \epsilon$ /gradient diffusion models along the stagnation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions (—) and experimental data (o).

as the flame is approached but at the wrong position. The latter is also reflected in the mean axial velocity prediction and is a consequence of the gradient diffusion model that fails to predict the turbulent flame thickness and the reaction progress variable variance, as shown in Fig. 4.17. This finding is consistent with the study by Lindstedt & Város [108]. The mean radial and the axial turbulence intensity along the stagnation plane agrees well with the experimental data as shown in Fig. 4.18. The radial turbulence intensity and the turbulence kinetic energy are under-predicted as a consequence of the predicted peak level along the centreline. The application of transport equation based closures for the turbulent scalar fluxes results in a significant improvement in general. The radial turbulence intensity and the turbulent kinetic energy are still low but improved as shown in Fig. 4.19. The predicted axial turbulence intensity and the mean axial velocity are much closer to

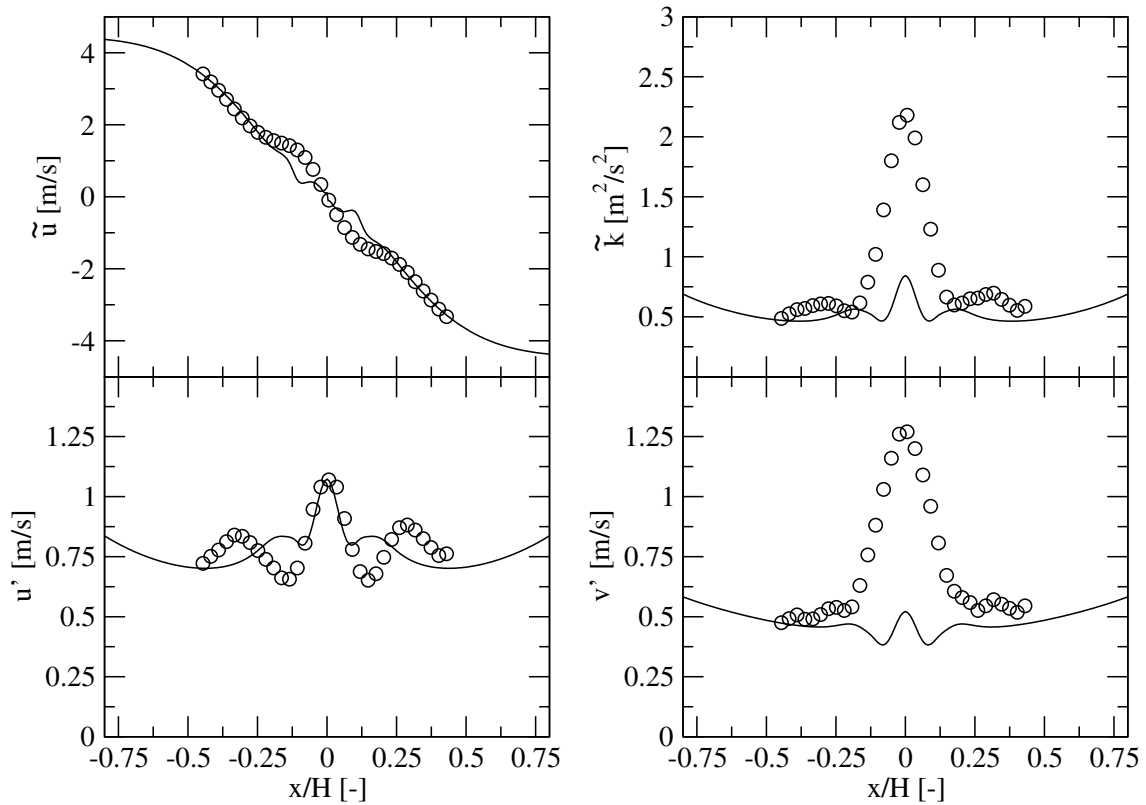


Figure 4.16: Predictions using HP/gradient diffusion models along the centreline. TL: Mean axial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions (—) and experimental data ($\circ$).

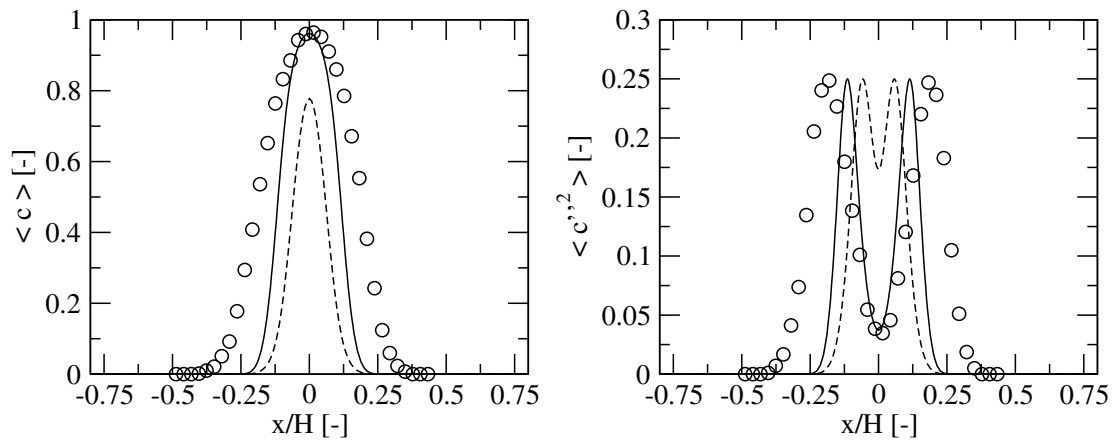


Figure 4.17: Predictions using HP/gradient diffusion models along the centreline. Left: Mean reaction progress variable profile. Right: Mean reaction progress variable variance. Conventional averages (—), Favre averages (---) and experimental data ($\circ$).

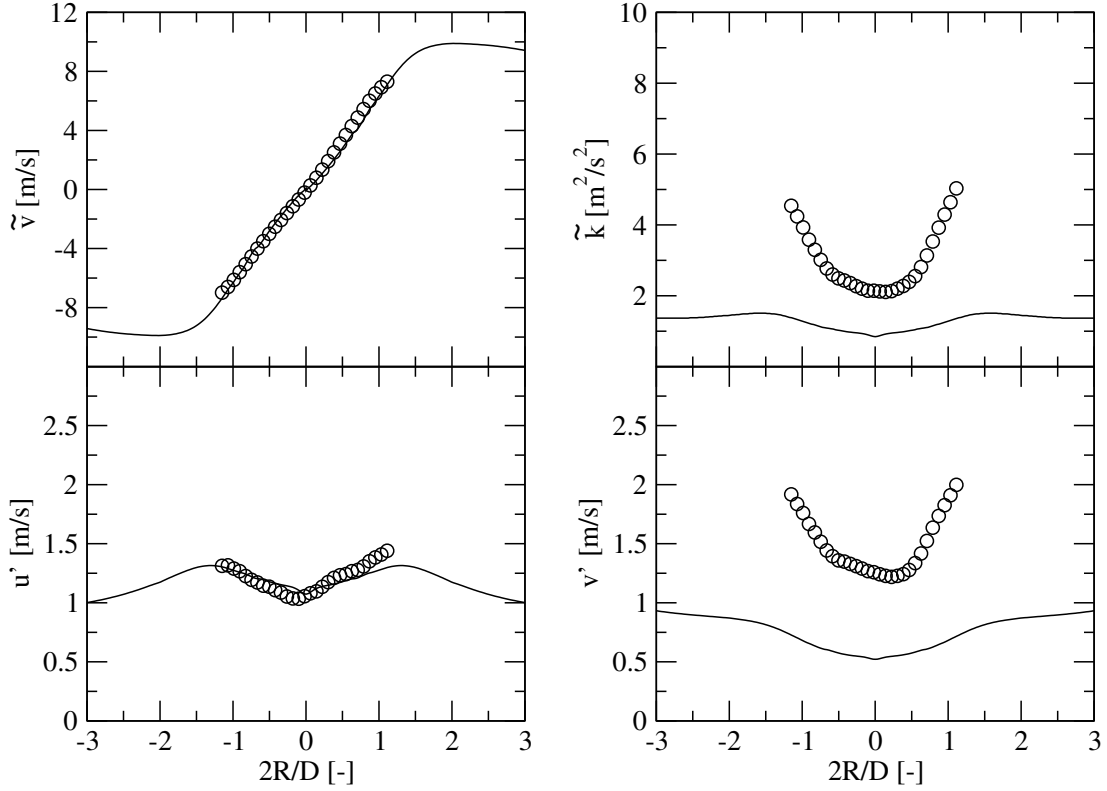


Figure 4.18: Predictions using HP/gradient diffusion models along the stagnation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions (—) and experimental data (o).

the experimentally derived values compared to results obtained using the gradient diffusion model. The axial turbulence intensity peak at the stagnation point is slightly too high. The computed reaction progress variable and its variance agrees very well with the experimental data as shown in Fig. 4.20. The dominating term responsible for this improvement is the turbulence-reaction rate correlation in the transport equation for the reaction progress variable turbulent scalar fluxes. The predictions along the stagnation plane are comparable to the predictions using the gradient diffusion model. In Fig. 4.21, the mean radial velocity component and the axial turbulence intensity agrees well with the experiments while similar deviations as before can be seen for the radial turbulence intensity and the turbulent kinetic energy. The same closure is also extended to include the variable density correction terms of Lindstedt & Város [108]. In Fig. 4.22, predictions along the burner centreline

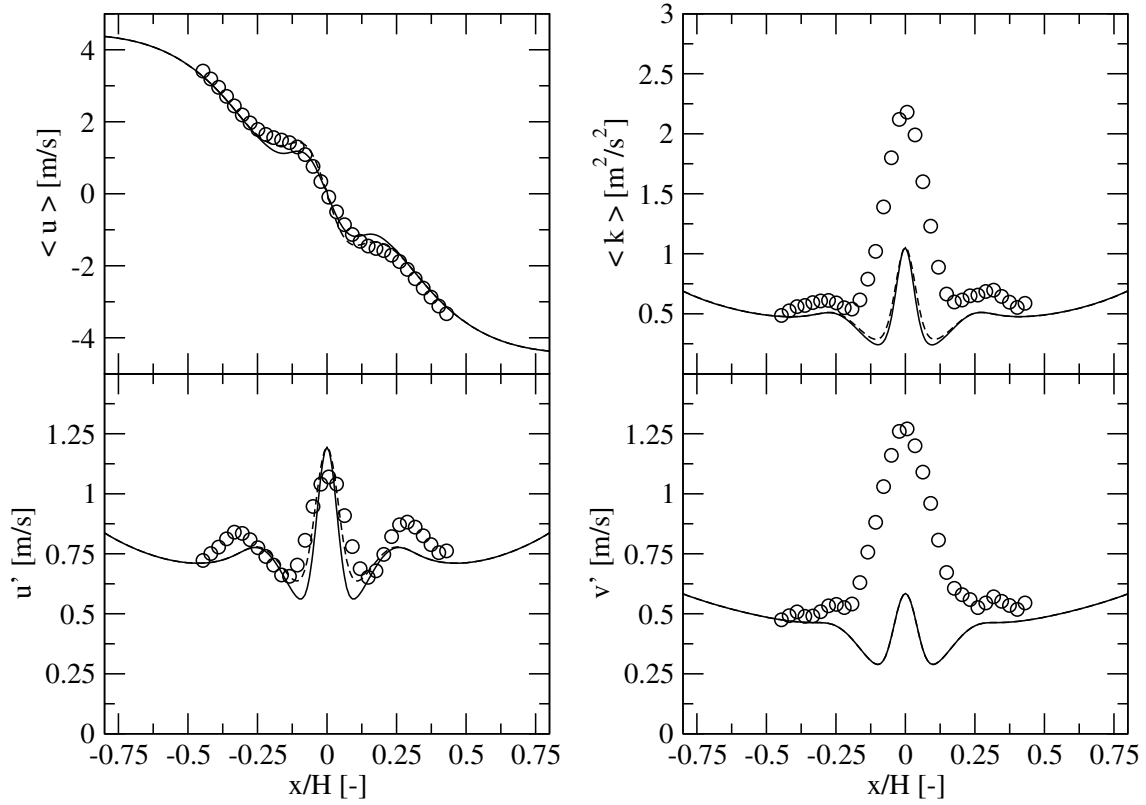


Figure 4.19: Predictions using HP/scalar flux models along the centreline. TL: Mean axial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Conventional averages (—), Favre averages (---) and experimental data ($\circ$).

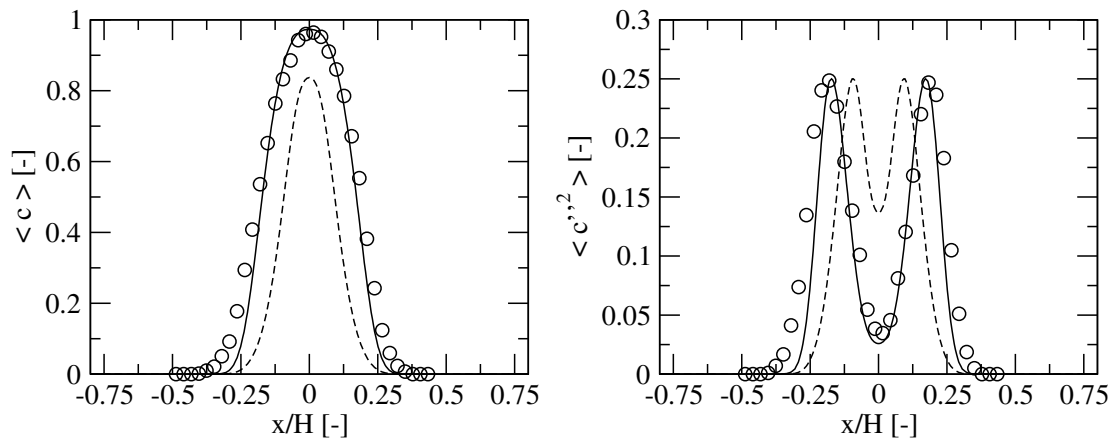


Figure 4.20: Predictions using HP/scalar flux models along the centreline. Left: Mean reaction progress variable profile. Right: Mean reaction progress variable variance. Conventional averages (—), Favre averages (---) and experimental data ($\circ$).

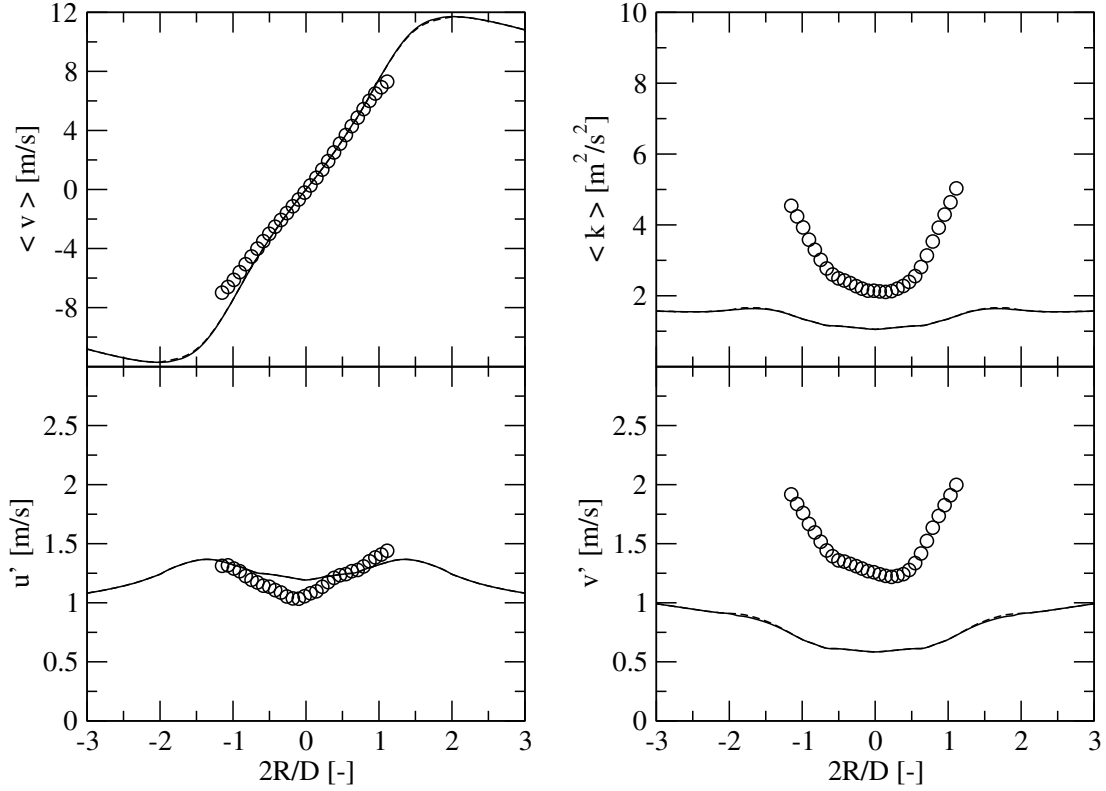


Figure 4.21: Predictions using HP/scalar flux models along the stagnation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Conventional averages (—), Favre averages (---) and experimental data ($\circ$).

are shown and the mean axial velocity is very well reproduced. This model is the only one that is approaching the measured turbulent kinetic energy, but inspection of the individual Reynolds stress components reveals that the axial velocity fluctuation is over-predicted and the radial, consistent with all other models, is under-predicted. The scalar field shown in Fig. 4.23 is again well reproduced. Small differences in the computed turbulent flame thickness can be observed between the extended and the standard closures (cf. Fig. 4.20). The extended model predicts a slightly thicker reaction zone than the experimentally derived values while the turbulent flame thickness obtained with the standard closure is slightly too thin. On the other hand, these observations are just details as both transport equation based scalar flux models are out-performing the eddy viscosity closure. Predictions along the stagnation plane are shown in Fig. 4.24 and the mean radial velocity is in

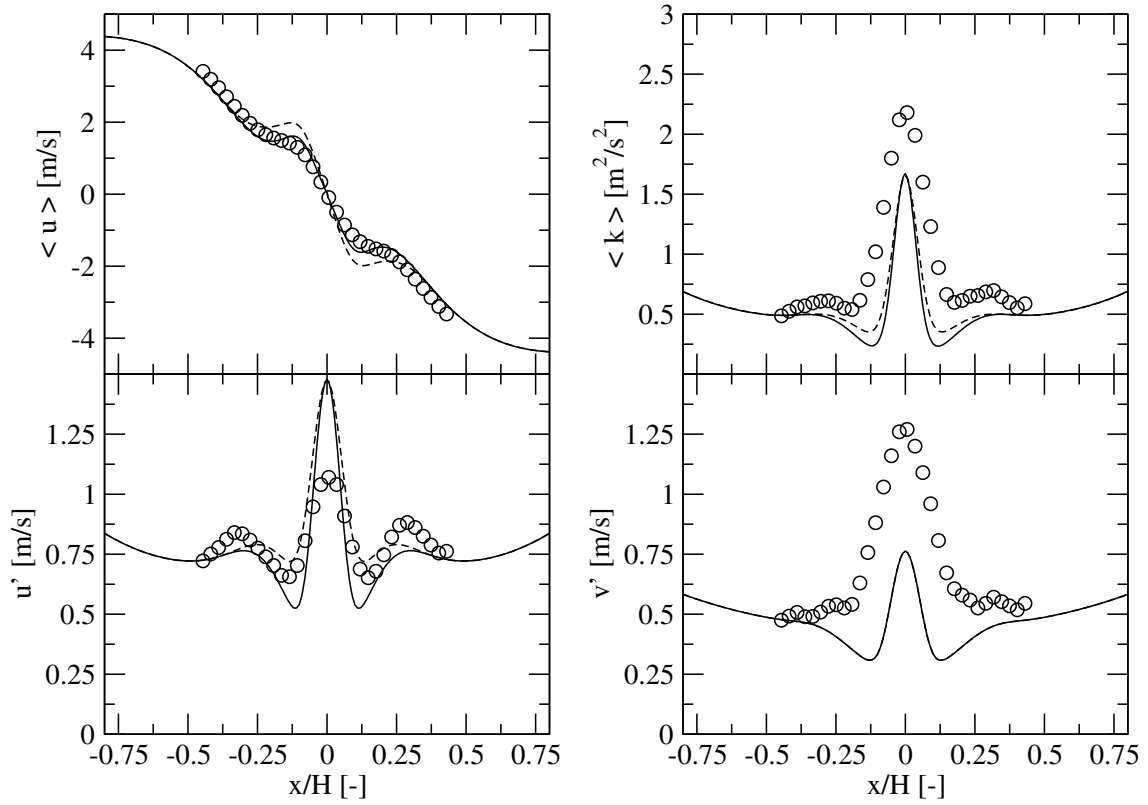


Figure 4.22: Predictions using HP/extended scalar flux models along the centreline. TL: Mean axial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Conventional averages (—), Favre averages (---) and experimental data ($\circ$).

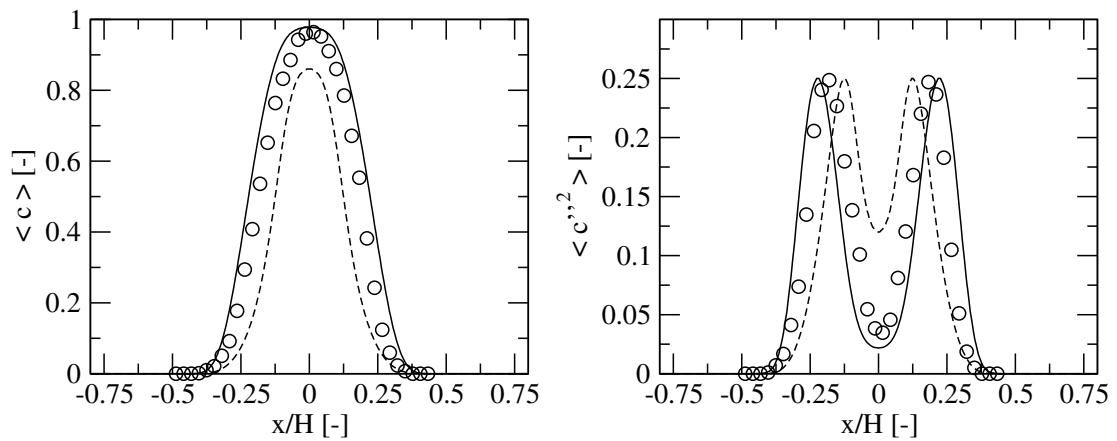


Figure 4.23: Predictions using HP/extended scalar flux models along the centreline. Left: Mean reaction progress variable profile. Right: Mean reaction progress variable variance. Conventional averages (—), Favre averages (---) and experimental data ($\circ$).

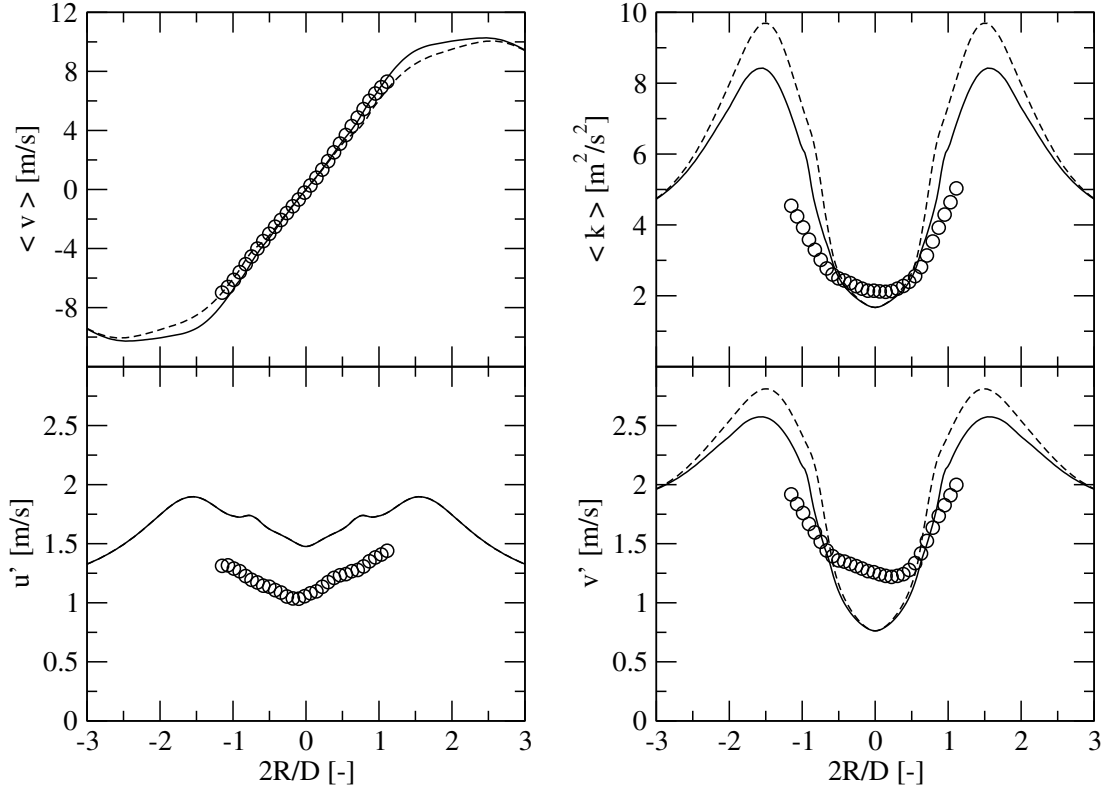


Figure 4.24: Predictions using HP/extended scalar flux models along the stagnation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Conventional averages (—), Favre averages (---) and experimental data ($\circ$).

excellent agreement with the experimental data. The turbulent kinetic energy is also well reproduced while some deviations can be observed for the axial and radial velocity fluctuations. Furthermore, the difference between the computed Favre and the transformed conventional averages in comparison to the standard closure (cf. Fig. 4.21) is indicating a significant change in the scalar flux distribution as a result of the extended closure.

4.5.2.2 The transported PDF approach

The node-based joint scalar transported PDF approach coupled with the HP model for the velocity field is here applied to simulate the reacting opposed flow. The current closure level corresponds to a gradient diffusion assumption and the results obtained should therefore primarily be compared to the predictions given in

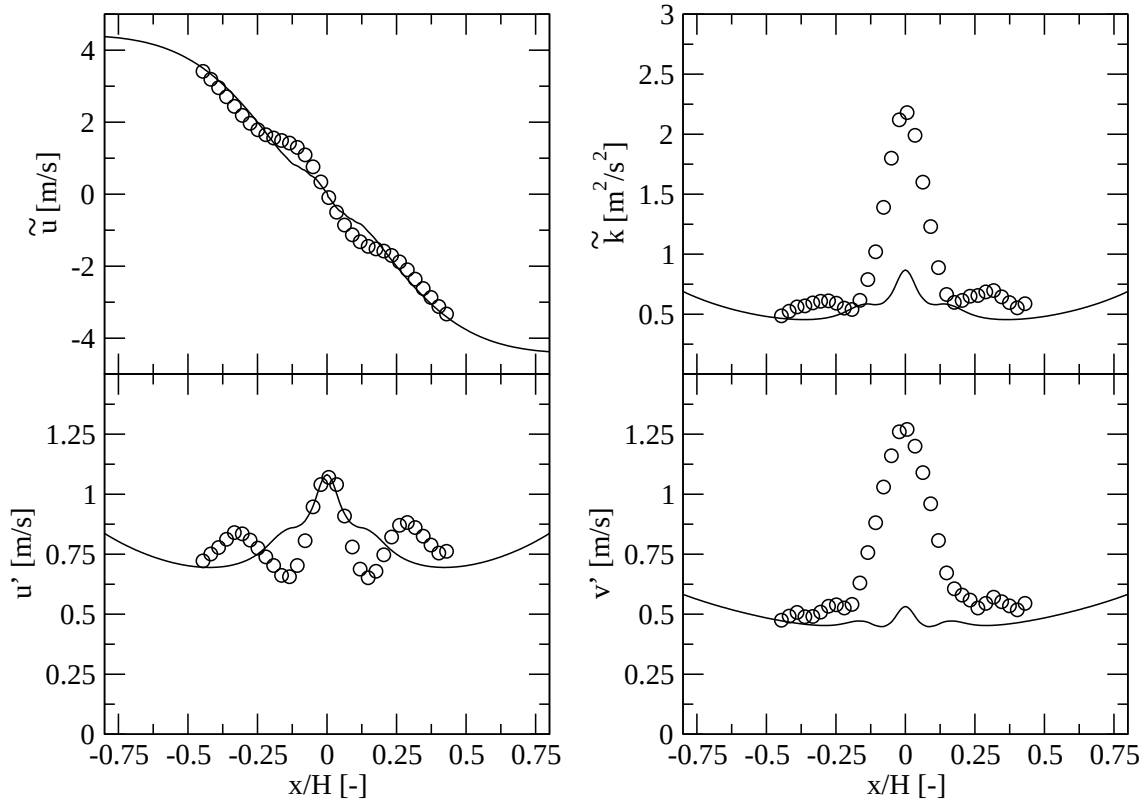


Figure 4.25: Predictions using HP/transported PDF along the centreline. TL: Mean axial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions (—) and experimental data (○).

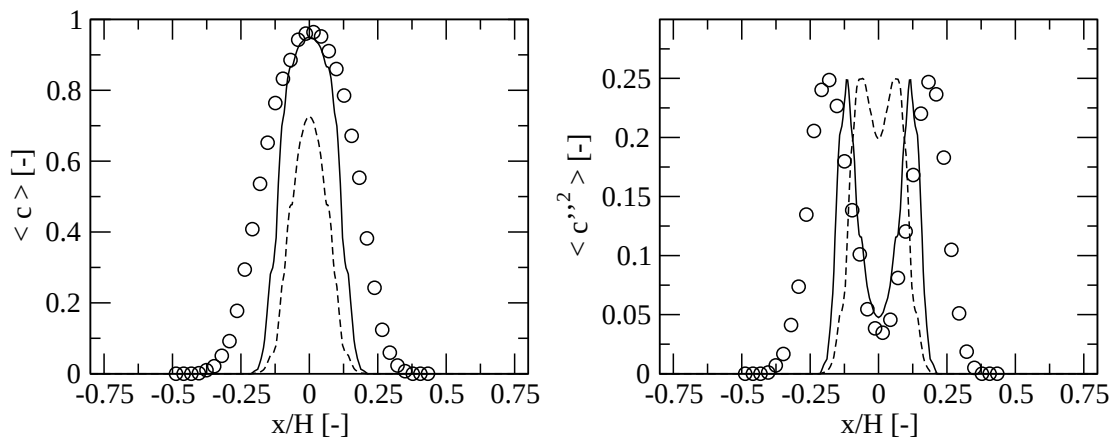


Figure 4.26: Predictions using HP/transported PDF along the centreline. Left: Mean reaction progress variable profile. Right: Mean reaction progress variable variance. Conventional averages (—), Favre averages (---) and experimental data (○).

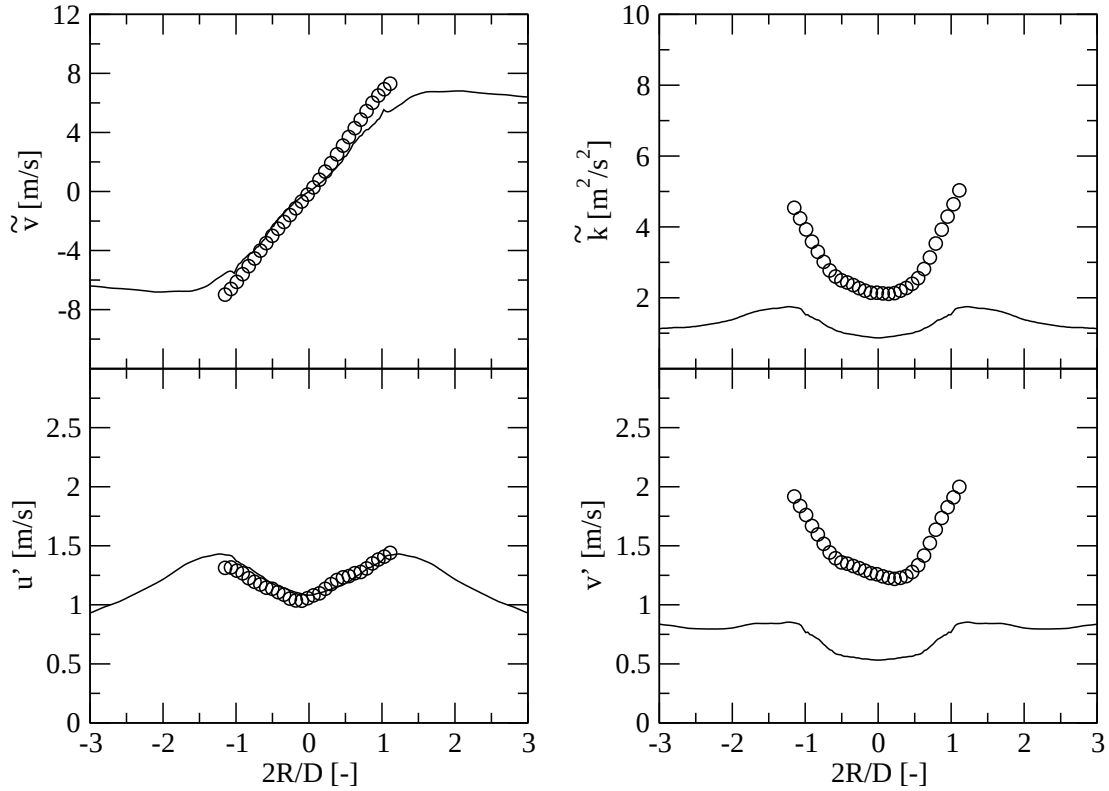


Figure 4.27: Predictions using HP/transported PDF along the stagnation plane. TL: Mean radial velocity component, TR: Turbulent kinetic energy, BL: Axial velocity fluctuation and BR: Radial velocity fluctuation. Predictions (—) and experimental data ($\circ$).

Figs. 4.16-4.18. The current computation is interesting in the sense that it will give an indication of how the transported PDF approach performs for premixed flames in the flamelet regime of combustion using multiple scalars. The scalar field is still presented in terms of the reaction progress variable, which is not a solved scalar. The reaction progress variable is, however, easily obtained as a post-processing step from the definition using fuel mass fractions given by Eq. (1.29).

In Figs. 4.25 and 4.26 the predicted velocity and scalar fields along the burner centreline are shown. The computed velocity field is similar to the HP/gradient diffusion closure with a low turbulent kinetic energy peak at the stagnation point as a result of the low radial turbulence intensity. The axial turbulence intensity is reasonably well predicted at the stagnation point. The model fails to predict the mean axial velocity and the axial turbulence intensity distributions as a result of

an under-predicted flame thickness. This finding is not surprising as the current closure level corresponds to a gradient diffusion assumption. The predicted peak value of the reaction progress variable is slightly lower than both the experimental data and the predictions using the fractal flame surface density closure. In the latter case, a reaction rate constant of 2.6 is used throughout. This is a rather low value in combination with gradient diffusion closures (cf. [108]) but still approaching the correct reaction progress variable value towards the stagnation point. The predicted c -profile is therefore an indication that the turbulent burning velocity is under-predicted with the current transported PDF closure level. Support for the latter is given in Fig. 4.27 where the mean radial velocity is too low as a result of the low heat release. Turbulent burning velocity predictions using the transported PDF approach are therefore investigated in detail in Chapter 5. The radial turbulence intensity and the turbulent kinetic energy levels are too low along the stagnation plane while the axial turbulence intensity is well reproduced. However, it appears that a closure at the current level remains insufficient.

4.6 Summary

Computations of isothermal and reacting opposed flows featuring fractal-generated turbulence have been performed. The computational domain is represented by a 90° sector of one of the nozzles and the geometry is discretised using an unstructured hexahedral mesh featuring 3.5×10^5 computational cells. Different classes of models, ranging from eddy viscosity based closures to full second moment closures, have been applied in both the isothermal and reacting cases. The reacting case is in the flamelet regime of combustion and a two-scalar joint β -bimodal presumed PDF approach or the node-based joint scalar transported PDF approach are applied for scalar statistics. The predictions are compared with the experimental data of Geipel [52] and Geipel et al. [53]. In the isothermal case the standard $k - \epsilon$ model performs very well in contrast to previous studies. One major difference compared to previous studies is the significant increase in Re_T . Two Reynolds stress models,

the models of Haworth & Pope (HP) and Jones & Musonge (JM), are evaluated in the isothermal case. The HP model performs better in general, compared to the JM model, and is the only Reynolds stress model considered for the reacting case. In the case of a presumed PDF approach, closure for the mean reaction rate is obtained using the fractal model of Lindstedt & Váos [108] and a reaction rate constant of 2.6 is used throughout. In the case of a transported PDF approach, closure for the molecular mixing term is obtained using Modified Curl's model and the chemistry is represented by a four-step global reaction scheme featuring seven solved species. The experimental data in the reacting case is arguably conventionally averaged while the solved quantities are represented by Favre averages. The latter are therefore transformed into conventional averages using relations from the BML theory. Consistent with previous studies is that the closure for the turbulence scalar flux term is crucial in stagnating flows and the transport equation based closures are outperforming gradient diffusion models, especially in the scalar field predictions. The addition of the acceleration/redistribution model to the redistribution and scrambling terms results in an over-prediction of the axial velocity fluctuation at the stagnation point while it is the only model approaching the measured turbulent kinetic energy. None of the models are able to predict the experimentally determined radial velocity fluctuation. It is, however, possible that the height of the radial peak is due to stagnation point movement which this simple approach can not capture. Predictions using the transported PDF approach indicates that the turbulent burning velocity is under-predicted resulting in a low burning rate around the stagnation point. Turbulent burning velocity predictions using the joint scalar transported PDF approach are therefore explored in detail in Chapter 5.

Chapter 5

Burning velocity predictions using transported PDF methods

5.1 Introduction

The ability of the transported PDF approach to predict turbulent burning velocities across a wide range of Re numbers is of great importance in the development of practical devices as the propagation speed will dictate the flame stabilisation point. In PDF methods, the chemical source term appears in closed form [140] and the inclusion of finite chemistry allows emissions and extinction/re-ignition phenomena to be predicted. Further details are provided in the review by Haworth [68]. One of the major closure challenges concerns transport in composition space. Furthermore, the application of the approach typically features non-premixed flames and the number of studies with premixed reactants is much more limited. Previous efforts predominantly feature single scalar formulations coupled with simplified chemical source terms. Anand & Pope [4, 139] used a joint velocity-reaction progress variable transported PDF approach to calculate steady premixed flames in the flamelet regime of combustion. Hůlek & Lindstedt [69] used a closure at the joint velocity-scalar level and computed transient premixed flames. Roekaerts [147, 148] used a joint scalar transported PDF approach to simulate an axi-symmetric premixed jet stirred reactor. Lindstedt & Város [115] studied the influence of alternative closures

for the mixing time scale expression on turbulent burning velocities using a reaction progress variable transported PDF approach. Two piloted turbulent premixed flames at different Damköhler numbers were also computed using comprehensive finite rate chemistry. The extended multi-scale mixing time scale closure [115] was also applied by Lindstedt et al. [117] in the context of partially premixed flames. The standard time scale expression had a tendency to produce an excessive amount of extinction while the extended closure improved the temperature predictions. Correa [32] simulated a partially stirred reactor with a CO/H_2 premixed mixture and made a qualitative comparison between different mixing models and that the differences are smaller at higher frequencies.

The joint PDF closure as implemented in the context of LES/filtered density function (FDF) methods is also starting to be explored in the context of turbulent premixed flames. Yilmaz et al. [180] applied a closure at the joint scalar level to compute a turbulent premixed flame stabilised on a Bunsen burner with encouraging results. Furthermore, McDermott and Pope [126] analysed the role of molecular transport in physical space alongside transport in composition space and showed that it is possible to produce FDF models that reduce to the DNS limit with vanishing filter width. The approach has the interesting feature of effectively combining the solution of a reactive diffusive formulation in physical space with a mixing model for transport in composition space. By contrast, the traditional PDF approach tends to treat the impact exclusively through the model for transport in composition space (e.g. [26, 115, 146]) or implicitly through the application of flamelet type source terms [4, 69, 115]. The interactions between the mixing model and the reaction source term is mainly confined to a region close to the “cold” boundary and the width is inversely proportional to the Da number [70]. The role of the mixing model is to induce transport of the discrete PDF in composition space so that chemical reactions become effective. Predictions of the turbulent burning velocity will depend on the structure of the model for turbulent transport in composition space, the magnitude of the mixing time scale and molecular transport in physical space. The impact of the latter can be expected to be reduced at high turbulence levels.

5.1.1 The present contribution

The current work explores the ability of the transported PDF approach to predict turbulent burning velocities with results compared against the experimental data of Abdel-Gayed et al. [1] for lean ($\phi = 0.88$) and stoichiometric CH_4 , stoichiometric C_2H_6 as well as the fuel rich ($\phi = 1.6$) H_2 flames. The matter is of great importance in the development of practical devices as the propagation speed will dictate where the turbulent premixed flame will stabilise in space. The present effort extends past work in several aspects. Turbulent burning velocities are computed for (i) a wide range of Damköhler numbers as indicated in Fig. 1.1 and for (ii) different fuels using detailed or systematically reduced chemistry. (iii) The impact of molecular transport on the turbulent burning velocity is explored and analysed in terms of the Zeldovich (β) number through the inclusion of an explicit analytical formulation. (iv) The multi-scale scalar dissipation rate closure proposed by Lindstedt & Város [115] that accounts for the influence of the Da number is extended in a simple manner to include Le number effects in order to explore the sensitivity of predictions.

5.2 Analytical work on burning velocities

Nearly all combustion related calculations today are performed using numerical methods since the complexity of combustion physics does, in general, not allow any analytical solutions. Valuable information can however be extracted by considering simplified forms of the conservation equations. Zeldovich & Frank-Kamenetskii [175] investigated analytically laminar premixed flame propagation. The starting point of the analysis is the transport equation for species mass fractions, Eq. (1.14). The time derivative is eliminated through the assumption of a steady state solution. The chemical kinetics are described by a one-step global reaction where fuel and oxidiser reacts into products of combustion through a first order Arrhenius reaction rate expression. The thermal conductivity, the specific heat capacity and the product of density and the diffusion coefficient are all assumed to be constant. Furthermore, the Le number is assumed to be unity. The latter assumption implies that the

transport equations for mass fraction and temperature have the same general form

$$v \frac{dc}{dx} = D \frac{d^2c}{dx^2} - cAT^b \exp\left(-\frac{E_a}{RT}\right). \quad (5.1)$$

Solving Eq. (5.1) analytically is complicated and only possible for a limited region of the flame. It can, however, be shown [175] that a solution only exists if v has the eigenvalue

$$v = \left[DAT^b \exp\left(-\frac{E_a}{RT}\right) \right]^{1/2} \quad (5.2)$$

showing that laminar premixed flame propagation essentially amounts to diffusive transport and chemical reaction.

Another example is the Kolmogorov-Petrovski-Piskunov (KPP) analysis [136, 170] to investigate basic model trends of some turbulent reaction rate models. The analysis is based on a steady one-dimensional flame propagating in a uniform mixture and a frozen turbulence field. The latter can be described by the following balance equation for the reaction progress variable

$$\rho_u u_T \frac{d\tilde{c}}{dx} = -\frac{d \langle \rho \rangle \widetilde{u''c''}}{dx} + \langle \rho \rangle \tilde{S}_c \quad (5.3)$$

where ρ_u denotes density of the unburnt gases and u_T the turbulent burning velocity. The reaction progress variable takes on values between 0 and 1. Catlin & Lindstedt [28] have shown that the numerical integration of Eq. (5.3) presents difficulties in general. For cases with significant density variations, the flame may exhibit unlimited increase in thickness and burning velocity. The latter issues may however be avoided through the introduction of a mean reaction rate cut-off in reaction progress variable space [28]. In Eq. (5.3) the terms on the RHS are unclosed and need to be modelled. The terms represent turbulent scalar fluxes and the mean rate of reaction. The turbulent scalar flux term is closed by, for illustrative purposes, a gradient diffusion type model

$$\widetilde{u''c''} = -\frac{\nu_T}{\sigma_T} \frac{d\tilde{c}}{dx} \quad (5.4)$$

and the mean reaction rate might be closed by for example an EBU model

$$\langle \rho \rangle \tilde{S}_c = C_{EBU} \langle \rho \rangle \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{c}(1 - \tilde{c}) \quad (5.5)$$

where C_{EBU} is a reaction rate parameter to be tuned. The KPP theorem basically states that the propagation speed of a turbulent premixed flame is dictated by the turbulence characteristics at the leading edge of the flame. Since turbulence is frozen, $\tilde{\epsilon}/\tilde{k}$ and $\langle \rho \rangle \nu_T$ are constant. The transport equation at the leading edge ($\tilde{c} \rightarrow 0$) becomes

$$\rho_u u_T \frac{d\tilde{c}}{dx} = \rho_u \frac{\nu_T}{\sigma_T} \frac{d^2 \tilde{c}}{dx^2} + C_{EBU} \rho_u \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{c}. \quad (5.6)$$

It can be shown [136], based on the KPP analysis (Eq. (5.6)), that the lowest turbulent burning velocity is given by

$$u_T = 2 \sqrt{\nu_T \frac{C_{EBU}}{\sigma_T} \frac{\tilde{\epsilon}}{\tilde{k}}}. \quad (5.7)$$

Note the similarity between Eqs. (5.2) and (5.7). The latter result is of help in terms of tuning the reaction rate constant C_{EBU} . Catlin & Lindstedt [28] points out that the KPP analysis predicts only a minimum and not necessarily a unique burning velocity.

5.3 Closure considerations

In the joint scalar transported PDF approach, conditional expectations appear that require modelling. The unclosed terms represent molecular mixing and transport of the PDF in physical space. Transport in physical space is closed by the commonly used gradient diffusion type closure given by Eq. (3.27) while the molecular mixing term is closed by modified Curl's [41] model. During a small time increment Δt , N_{pq} pairs of particles out of N are selected without replacement to interact (mix). N_{pq} is given by Eq. (3.37) in Section 3.3.3.1. Models for the characteristic mixing time scale τ_ϕ^{-1} are extensively discussed below.

The applied thermochemistry features a systematically reduced mechanism with 142 reactions, 15 solved (H_2 , O_2 , H_2O , H , O , OH , HO_2 , CO , CO_2 , CH_4 , CH_3 , C_2H_2 , C_2H_4 , C_2H_6 , N_2) and 14 steady state (C , C_2 , CH , 1CH_2 , CH_2 , C_2H , C_2H_3 , C_2H_5 , CHO , CH_2O , CH_3O , CH_2OH , C_2HO , C_2H_2O) species for the CH_4 and C_2H_6 flames [115]. A detailed H/O subset featuring 21 reactions and 9 solved (H_2 , O_2 , H_2O , H , O , OH , HO_2 , H_2O_2 , N_2) species was used for the H_2 flames. Details about the mechanisms can be found in Appendix A.

5.3.1 The scalar dissipation rate

In the context of premixed turbulent flames in the laminar flamelet regime of combustion, Bray [12] established that the closure for the mean reaction rate essentially corresponds to a closure for the scalar dissipation rate. Hence, assuming a bimodal PDF, the decay time scale of scalar fluctuations of Eq. (3.41) is equivalent to an EBU model, Eq. (1.59), in the laminar flamelet regime of combustion where C_ϕ represents the reaction rate parameter

$$\begin{aligned} \langle \rho \rangle \tilde{S} &\propto \langle \rho \rangle \tilde{\epsilon}_c = \langle \rho \rangle \tau_\phi^{-1} \widetilde{c''^2} = \langle \rho \rangle \frac{1}{2} C_\phi \tau^{-1} \widetilde{c''^2} \\ &= C_{EBU} \langle \rho \rangle \frac{\tilde{\epsilon}}{\tilde{k}} (1 - \tilde{c}). \end{aligned} \quad (5.8)$$

Váos [170] performed turbulent burning velocity calculations using a single scalar (reaction progress variable) joint scalar transported PDF approach. Application of the standard time scale closure presented above reproduced the 'standard' scaling behaviour ($u_T/u' = \text{constant}$) of turbulent burning velocities, in contrast to the experimental data of Abdel-Gayed et al. [1]. Lindstedt & Váos [108] assumed the flamelet geometry to be fractal and derived an alternative closure for the mean reaction rate given by Eq. (1.57). Recently, Aluri et al. [2] investigated the effect of the Le number of mean reaction rate closures. A large number of turbulent methane, ethylene and propane bunsen flames at atmospheric pressure were used for comparison. Based on their calculations, a modified form of the fractal model,

including a linear scaling of the Le number, was proposed

$$\langle \rho \rangle \tilde{S} = \frac{C_R}{Le} \rho_u \frac{u_L^0}{V_K} \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{c} (1 - \tilde{c}). \quad (5.9)$$

Aluri et al. [3] extended their study to cover a wide range of stoichiometries, fuels (Le number effects) and elevated pressure effects. During this study, the fractal model was the only mean reaction rate closure considered and the outcome was an alternative Le number scaling and a high pressure scaling

$$\langle \rho \rangle \tilde{S} = C_R C_{P,Le} \rho_u \frac{u_L^0}{V_K} \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{c} (1 - \tilde{c}) \quad (5.10)$$

where

$$C_{P,Le} = \sqrt{\frac{p}{p_0}} \left(\frac{1}{e^{Le-1}} \right). \quad (5.11)$$

Furthermore, the scalar dissipation rate analysis by Váos [170] and Lindstedt & Váos [115] shows that the standard time scale expression of Eq. (3.41) is based on non-reacting flows with passive scalars. For flows with reactive scalars such as the reaction progress variable, the scalar dissipation rate transport equation features additional reaction specific correlations. Accordingly, Lindstedt & Váos [115] proposed an alternative scaling to include the desired scaling behaviour of the fractal model of the mixing time scale

$$\tau_\phi^{-1} = \frac{\tilde{\epsilon}_c}{\widetilde{\mathcal{D}}'^2} \propto \frac{\rho_u}{\langle \rho \rangle} \frac{u_L}{V_K} \frac{\tilde{\epsilon}}{\tilde{k}}. \quad (5.12)$$

A major disadvantage of the proposed mixing time scale expression is that it is limited to reactive scalars only, since for passive scalars $u_L = 0$ m/s and $\tau_\phi^{-1} = 0$ s⁻¹. To keep the generality of the model Lindstedt & Váos [115] suggested a combination of the standard mixing time scale expression and the fractal time scale expression

$$\tau_\phi^{-1} = \frac{\tilde{\epsilon}_c}{\widetilde{\mathcal{D}}'^2} = \frac{1}{2} \left[C_\phi + C_\phi^* \frac{\rho_u}{\langle \rho \rangle} \frac{u_L}{V_K} \right] \frac{\tilde{\epsilon}}{\tilde{k}} \quad (5.13)$$

where C_ϕ and C_ϕ^* have the standard values 2.0 and 2.4 [170]¹, respectively. In the current effort a broad range of fuels have been studied, consequently the Le number scaling suggested by Aluri et al. [2, 3] have been included in the fractal part of the mixing time scale expression

$$\tau_\phi^{-1} = \frac{\tilde{\epsilon}_c}{\widetilde{c''^2}} = \frac{1}{2} \left[C_\phi + C_\phi^* \frac{1}{Le_\alpha} \frac{\rho_u}{\rho} \frac{u_L}{V_K} \right] \frac{\tilde{\epsilon}}{\widetilde{k}} \quad (5.14)$$

or alternatively

$$\tau_\phi^{-1} = \frac{\tilde{\epsilon}_c}{\widetilde{c''^2}} = \frac{1}{2} \left[C_\phi + C_\phi^* \frac{1}{e^{Le_\alpha-1}} \frac{\rho_u}{\rho} \frac{u_L}{V_K} \right] \frac{\tilde{\epsilon}}{\widetilde{k}}. \quad (5.15)$$

Alternative closures for the scalar dissipation rate have been discussed by Swaminathan & Bray [167] and Kolla et al. [88] among others.

The Le numbers for the deficient reactant (Le_α) and the laminar burning velocities are precomputed using detailed chemistry. The Le_α number is defined as

$$Le_\alpha = \frac{\lambda}{c_p \rho D_\alpha} \quad (5.16)$$

and represents the ratio of the diffusion speeds of heat and species α . A summary of the precomputed Le_α numbers and laminar burning velocities can be found in Table 5.1.

Table 5.1: Summary of precomputed parameters at atmospheric conditions and 328 K

Fuel	ϕ	Species α	Le_α	u_L^0 [m/s]
CH_4	1.00	CH_4	0.960	0.451
CH_4	0.88	CH_4	0.961	0.386
C_2H_6	1.00	C_2H_6	1.40	0.541
H_2	1.60	O_2	2.15	3.90

¹Váos [170] excluded the $\frac{1}{2}$ in front of the expression and used the standard values $C_\phi = 1.0$ and $C_\phi^* = 1.2$.

5.3.2 The impact of closures for molecular transport and chemical reaction

One of the major motivations of the current work is the inclusion of finite chemistry effects in premixed flame propagation problems. The ability to predict turbulent burning velocities is of great importance in the development of practical devices. The propagation speed will dictate where the premixed turbulent flame will stabilise in space. Furthermore, finite rate chemistry allows emissions and extinction/re-ignition phenomena to be predicted [68].

The recent study by Lindstedt & Város [115] showed that application of the extended mixing time scale closure together with a chemical source term extracted from laminar detailed chemistry calculations gives excellent results in terms of the scaling of the turbulent burning velocity. Early calculations in the initial phase of the present work reveals, however, that the turbulent reaction rate reduces too rapidly towards the leading edge of the flame resulting in too low values of the turbulent burning velocity. There might be several possible explanations for this. First, transport in physical space is closed by a gradient diffusion type closure. Lindstedt & Város [110] have shown that this level of closure tends to lead to reduced turbulent burning velocities (e.g. $u_T/u' \simeq 1.32$ as obtained with the modified Curl's model) as compared to higher order approximations ($u_T/u' \simeq 1.65$). On the other hand, a gradient diffusion closure was used in the aforementioned study by Lindstedt & Város [115]. However, multi-scalar extensions remain to be evaluated and the gradient closure has been retained for reasons of simplicity. Secondly, differences between the reduced and the detailed chemical mechanism is a possibility. A pseudo-laminar flame was simulated to calculate the laminar burning velocity and to test the reduced chemical mechanism (e.g. overall numerical accuracy). The laminar flame was solved using stoichiometric CH_4 at 328 K and assuming the following conditions

$$\tau_\phi^{-1} = 1.5 \times 10^5 \text{ s}^{-1} \quad u' = 10^{-3} \text{ m/s} \quad l_T = 10^{-5} \text{ m.} \quad (5.17)$$

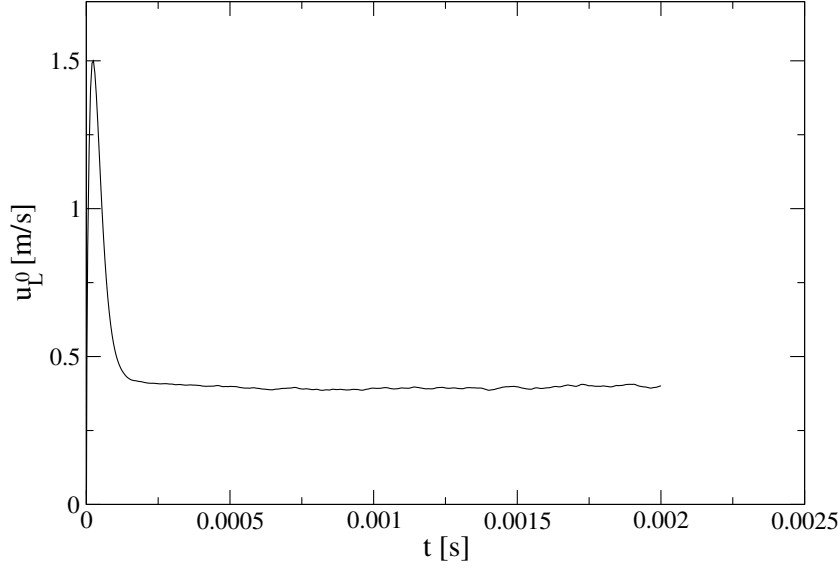


Figure 5.1: Evolution of the laminar burning velocity for a stoichiometric CH_4 flame.

The value of τ_ϕ was determined by setting some (lower) value and then increase it until $\widetilde{c''^2} \rightarrow 0$ and no change in the predicted laminar burning velocity could be seen. The obtained laminar burning velocity shown in Fig. 5.1, was 0.42 m/s, slightly lower than the value obtained using the detailed mechanism but well within experimental uncertainties. A third possibility is an inadequate account of molecular diffusion at the leading edge of the flame. The terms responsible for reaction and diffusion may be expressed in the customary form [118],

$$\frac{\partial}{\partial \Psi_\alpha} \left[\left\langle -\rho(\Psi) S_\alpha(\Psi) + \frac{\partial J_i^\alpha}{\partial x_i} \middle| \underline{\Psi} \right\rangle f_\phi \right] = \frac{\partial}{\partial \Psi_\alpha} \left[\omega_\alpha(\Psi) f_\phi \right] \quad (5.18)$$

where the quantity $\omega_\alpha(\Psi)$ appears in closed form for laminar flamelets. Fox [49] argues that, in premixed turbulent flames one would expect a strong dependence between the joint scalar dissipation rate $\langle \epsilon_\phi | \underline{\Psi} \rangle$ and the chemical source term and that the majority of all mixing models are missing this important feature. In general, two different aspects needs to be considered in the modelling of the conditional expectation of the molecular scalar flux term given in Eq. (5.18). The first is transport in physical space and the second is transport in composition space [68, 126]. McDermott and Pope [126], in the context of the FDF approach, closed the trans-

port in composition space through the IEM model [40], while the modified Curl's model [41, 77] is applied here. In the context of PDF methods, the former closure has been shown to result in significantly ($\leq 300\%$) lower turbulent burning velocities as compared to the modified Curl's or binomial Langevin models [110]. It can further be argued that mixing models that enforce locality in composition space [166, 173] are better suited to handling combustion in the high Da number regime [68]. However, the modified Curl's model has been retained here for reasons of simplicity and computational cost. At high Re numbers and for Sc and σ numbers of order unity, the term describing transport in physical space is typically small. The implicit coupling present in the laminar flamelet assumption will weaken at lower Da numbers and can be expected to breakdown in the well stirred reactor regime. However, for premixed combustion at high Da numbers the term can be important and the effect may be included via the addition of a random walk term in the equation for the particle position in physical space [68]. The approach provides a correction for the mean scalar composition at the expense of a spurious production term in the scalar variance equation [172]. An alternative approach, which does not lead to such difficulties [68, 126], is to add an explicit deterministic approximation of the molecular transport term at the leading edge of the flame in the manner implied by Eq. (5.18). The approach has been analysed by McDermott and Pope [126] in the context of FDF methods and the impact is explored below in the context of PDF methods.

5.3.2.1 Laminar reaction rates

As a first logical step, and as a continuation of the work of Lindstedt & Város [115], a reaction rate modification is proposed. The extracted chemical source term used in the study of Lindstedt & Város [115] *does* implicitly contain effects of molecular diffusion [81, 82]. The molecular diffusion term is not explicitly included in the manner of Anand & Pope [4, 139], but the chemical source carries traces since all the different processes are interconnected. In the present work the effect is initially explored using a modification of the reaction rate via the introduction of a simple

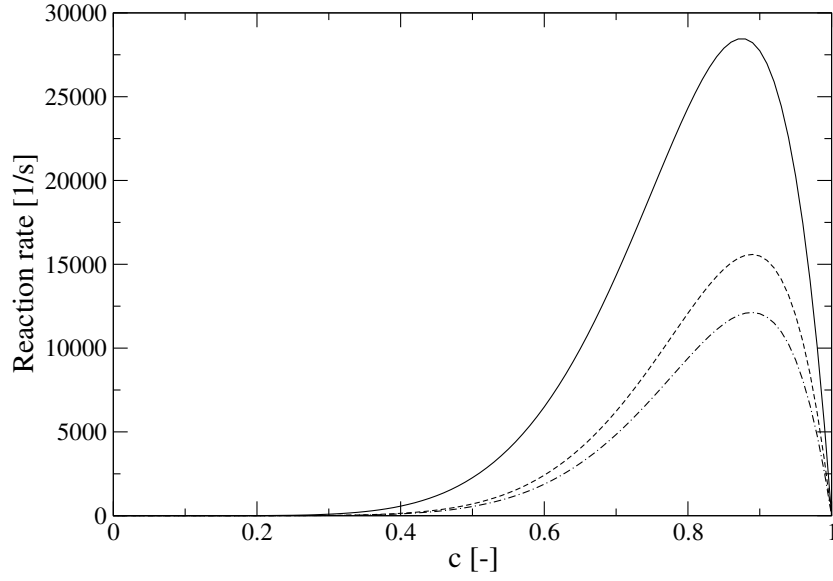


Figure 5.2: Flamelet reaction rates at 328 K in reaction progress variable space for the hydrocarbon fuels. Stoichiometric C_2H_6 (—), stoichiometric CH_4 (- - -) and $\phi = 0.88$ CH_4 (- · -).

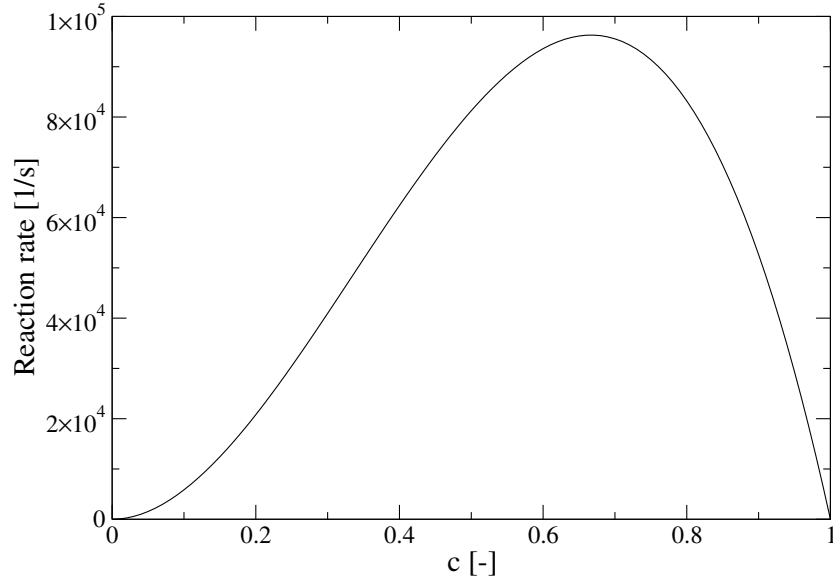


Figure 5.3: Flamelet reaction rate at 328 K in reaction progress variable space for hydrogen. $\phi = 1.6$ H_2 (—).

coupling function

$$\rho S_\alpha = R_\alpha M_\alpha = (1 - c)R_\alpha^{flamelet} M_\alpha + cR_\alpha^{chemical} M_\alpha \quad (5.19)$$

that accounts approximately for the impact of molecular diffusion effects at the cold front of the flame. A coupling function of this kind have been used by Darbyshire et al. [37] in the context of scalar dissipation rate closures for stratified combustion. The flamelet reaction rates for the various fuels and stoichiometries can be viewed in Figs. 5.2 and 5.3 and c represents the reaction progress variable

$$c = 1 - \frac{Y_\alpha}{Y_{\alpha,u}} \quad (5.20)$$

defined in terms of fuel mass fractions for lean and stoichiometric mixtures and in terms of the oxygen mass fractions for rich conditions. For the flamelet source term in Eq. (5.19), it is assumed that the formation and consumption of species follows a global reaction step. The reaction rate for all the species within the global reaction step are identical to that of the fuel and adjusted to ensure mass conservation according to a global step. The global reaction step valid for hydrocarbon fuels is given by Eq. (1.1) and the corresponding reaction rates are

$$\begin{aligned} \frac{d[C_x H_y]}{dt} &= -R_{C_x H_y}^{flamelet} \\ \frac{d[O_2]}{dt} &= -\left(x + \frac{y}{4}\right) R_{C_x H_y}^{flamelet} \\ \frac{d[CO_2]}{dt} &= x R_{C_x H_y}^{flamelet} \\ \frac{d[H_2O]}{dt} &= \frac{y}{2} R_{C_x H_y}^{flamelet}. \end{aligned} \quad (5.21)$$

Furthermore, it is assumed that the global reaction step is valid for all stoichiometries.

5.3.2.2 Mixture reactivity

Inspection of Figs. 5.2 and 5.3 indicates that hydrogen is more active at the flame front compared to the hydrocarbon fuels. In Fig. 5.4, the normalised laminar reaction rates, assuming equal diffusivities, of the rich H_2 and the stoichiometric CH_4 and C_2H_6 mixtures are shown. Again, hydrogen indicates significantly higher flame front activity as compared to the hydrocarbon fuels. To further investigate and characterise the fuels, the Zeldovich number [36]

$$\beta = \frac{E_a(T_b - T_u)}{RT_b^2} \quad (5.22)$$

that represent a normalised global activation energy is introduced. Global activation energies are given by Abdel-Gayed et al. [1] for all their measured flames. Shepherd [158] give a lower value for hydrogen, while Dryer & Glassman [43] give a slightly higher value for methane. Egolfopoulos & Law [44] estimates global activation energies using

$$E_a = -2R \left\{ \frac{\partial[\ln(m^0)]}{\partial[1/T_b]} \right\}_p \quad (5.23)$$

where $m^0 = \rho_u u_L^0$ and $p = \text{constant}$. Thus with a given set of experimental or numerical data, the global activation energy may be computed. It should, however, be noted that the use of Eq. (5.23) is limited because of the simultaneous influence of equivalence ratio (ϕ) and adiabatic flame temperature T_b on m^0 . Egolfopoulos & Law [44] overcame the latter issue by fixing the equivalence ratio at stoichiometry and altering the flame temperature through variation of the nitrogen concentration. The value obtained, based on their experimental data, for stoichiometric methane is slightly higher than the value of Dryer & Glassman [43]. A similar estimate may be performed for hydrogen close to stoichiometry. Egolfopoulos & Law [45] fixed the stoichiometry at $\phi = 1.058$ and diluted the mixture with nitrogen to vary the flame temperature. At a flame temperature of $T_b = 2100$ K a laminar burning velocity $u_L^0 = 1.44$ m/s is obtained and at $T_b = 1700$ K $u_L^0 = 0.62$ m/s giving a global activation energy of $E_a = 125$ kJ/mol assuming $\rho_u = \text{constant}$, slightly lower

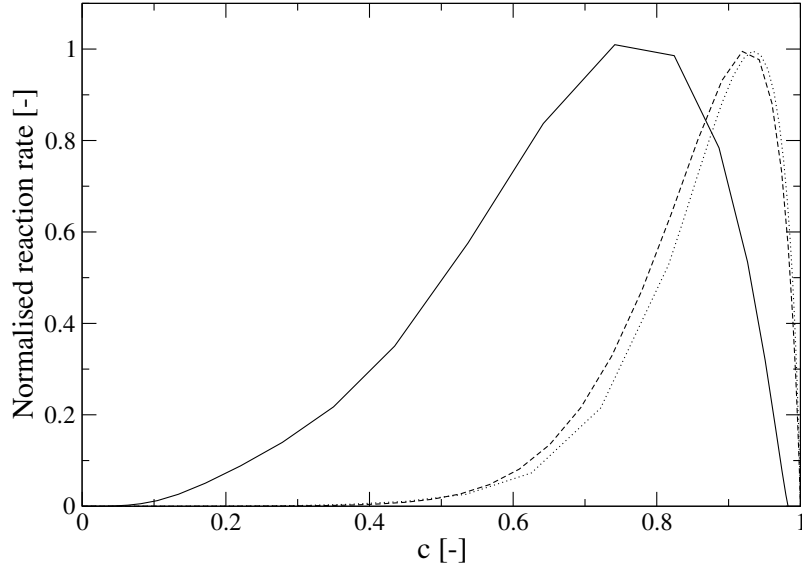


Figure 5.4: Flamelet reaction rates at 328 K in reaction progress variable space for the rich ($\phi = 1.6$) H_2 (—), stoichiometric CH_4 (- - -) and C_2H_6 (- · -) assuming equal diffusivities.

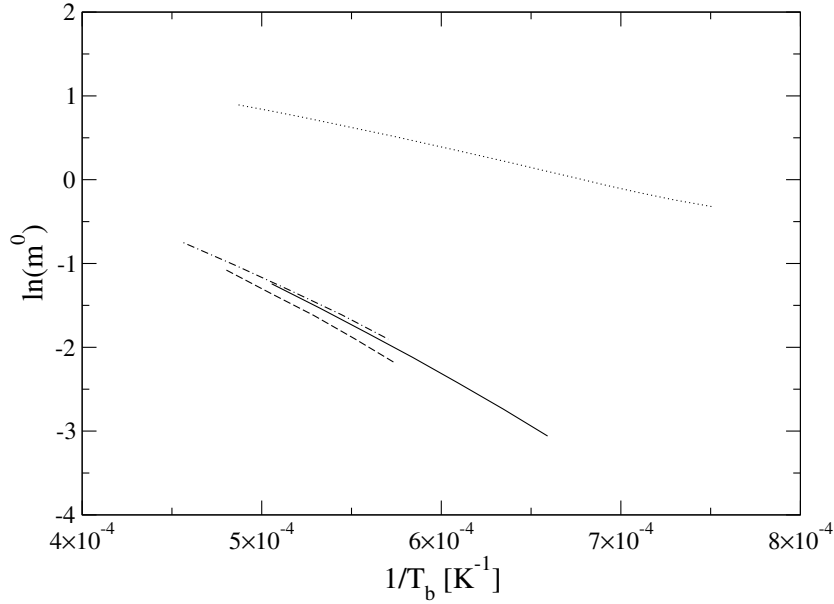


Figure 5.5: Arrhenius plot of the computed laminar burning rate of the diluted lean ($\phi = 0.88$) methane-oxygen-nitrogen flames (—), stoichiometric methane-oxygen-nitrogen flames (- - -), stoichiometric ethane-oxygen-nitrogen flames (- · -) and rich ($\phi = 1.6$) hydrogen-oxygen-nitrogen flames ($\cdots$).

than the value of Shepherd [158]. A summary of the range of global activation energies and Zeldovich numbers may be found in Table 5.2 where temperatures are from the data of Abdel-Gayed et al. [1]. A comparison between the fuels reveal that the Zeldovich number is lower for hydrogen compared to methane. Ethane, on the other hand, has the lowest value. The latter finding is somewhat surprising — one would expect hydrogen to have the lowest β -value. To further investigate the fuel-air mixtures, the global activation energies and the Zeldovich numbers were also computed using detailed chemistry. The approach follows the methodology of Egolfopoulos & Law [44], described above, the stoichiometries are fixed and the flame temperatures varied through different levels of nitrogen dilution. The conditions and fuel-oxygen-nitrogen mixtures are given in Appendix B and the result in Fig. 5.5 and in Table 5.3. As suspected, the β -value of hydrogen is significantly lower than the value of ethane.

Table 5.2: Global activation energies and Zeldovich numbers from literature

Fuel	T_u [K]	T_b [K]	E_a [kJ/mol]	β	ref
CH_4	328	2223	188	8.67	[1]
	328	2223	200	9.22	[43]
	328	2223	215	9.92	[44]
C_2H_6	328	2257	117	5.33	[1]
H_2	328	2211	160	7.41	[1]
	328	2211	134	6.21	[158]
	328	2211	125	5.79	[45]

Table 5.3: Computed global activation energies and Zeldovich numbers as predicted in the current work.

Fuel	ϕ	T_u [K]	T_b [K]	E_a [kJ/mol]	β
CH_4	0.88	328	2091	197	9.55
CH_4	1.00	328	2194	196	9.14
C_2H_6	1.00	328	2253	168	7.66
H_2	1.60	328	2130	77	3.68

5.3.2.3 Molecular transport terms

As discussed above, at high Re numbers the molecular transport terms tend to be small and the equal diffusivity approximation is invoked here in order to explore the magnitude of their overall contribution. Laminar diffusion terms may be included as an explicit correction at the leading edge of the flame. Consider the transport equation of species mass fractions

$$\rho \frac{\partial Y_\alpha}{\partial t} + \rho u \frac{\partial Y_\alpha}{\partial x} = \frac{\partial}{\partial x} \left(\frac{\mu}{Sc} \frac{\partial Y_\alpha}{\partial x} \right) + R_\alpha M_\alpha. \quad (5.24)$$

Solving this equation for a flat laminar propagating premixed flame allows the diffusion term Γ_{Y_α} to be extracted as a function of x

$$\Gamma_{Y_\alpha}(x) = \frac{\partial}{\partial x} \left(\frac{\mu}{Sc} \frac{\partial Y_\alpha}{\partial x} \right). \quad (5.25)$$

Since $Y_\alpha(x)$ is a monotonic function of x , the diffusion term can be expressed as a function of x , as shown in Eq. (5.25), or transformed into c through Eq. (5.20)

$$\Gamma_{Y_\alpha}(x) \quad \Rightarrow \quad \Gamma_{Y_\alpha}(c). \quad (5.26)$$

The extracted diffusion terms in reaction progress variable space, assuming equal diffusivities, for all the solved species can be viewed in Figs. 5.6 - 5.9. A way to reduce the complexity of explicitly including effects of molecular transport for all the solved species is to include the diffusion terms for the global step only. A convenient feature of this simplified approach is that conservation of mass is ensured for the additional terms. The diffusion terms for the global step may be viewed in Fig. 5.10. The laminar diffusion terms are included as source terms

$$\omega_\alpha = [H(c) - H(c - \xi_c)] \Gamma_{Y_\alpha}(c) + R_\alpha M_\alpha \quad (5.27)$$

where $H(c)$ is the Heaviside step function and ξ_c is a cut-off in reaction progress variable space. The value of ξ_c is chosen to be the point where the flux changes

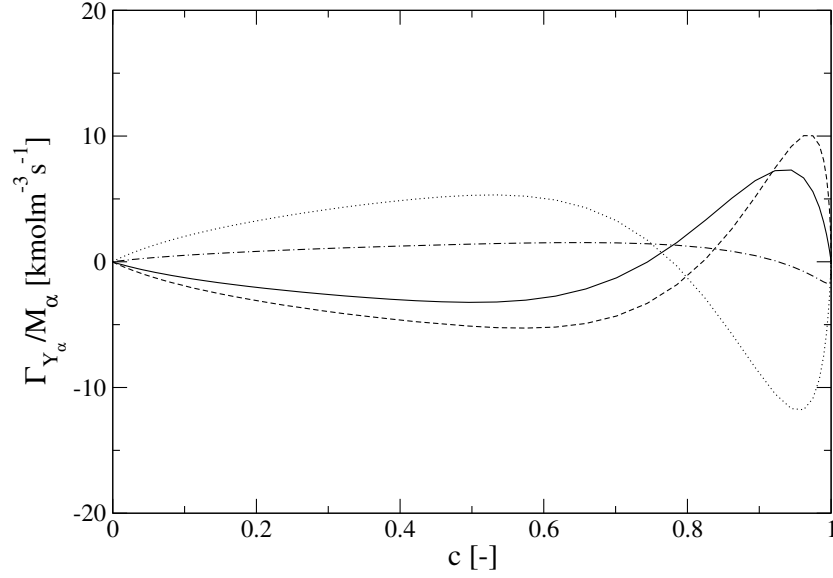


Figure 5.6: Laminar diffusion terms at 328 K in reaction progress variable space for a stoichiometric CH_4 flame. CH_4 (—), O_2 (- - -), CO_2 (- · -) and H_2O (···).

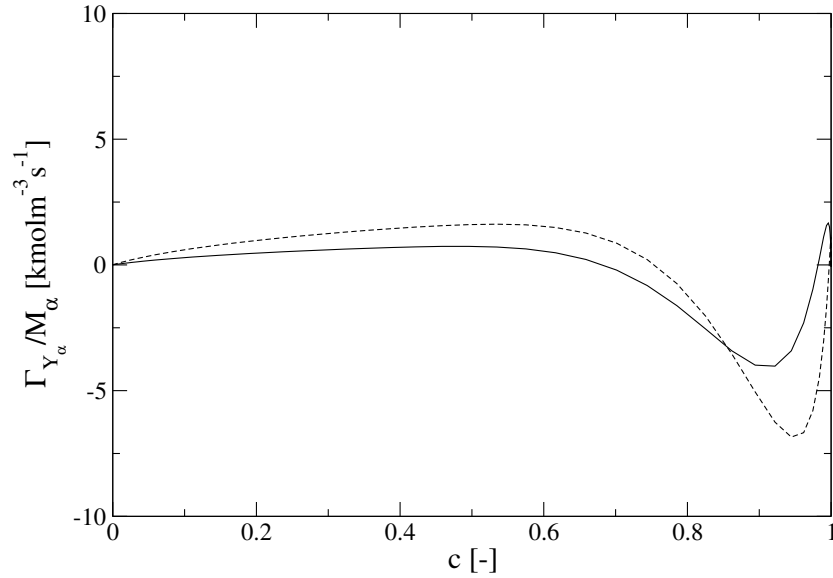


Figure 5.7: Laminar diffusion terms at 328 K in reaction progress variable space for a stoichiometric CH_4 flame. H_2 (—) and CO (- - -).

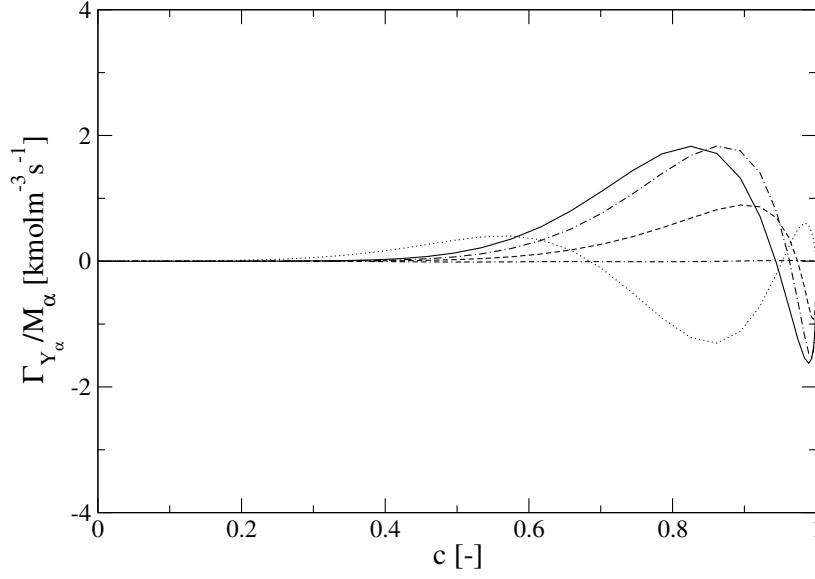


Figure 5.8: Laminar diffusion terms at 328 K in reaction progress variable space for a stoichiometric CH_4 flame. H (—), O (---), OH (- · -), HO_2 (· - - ·) and CH_3 (...).

sign. Beyond this point it is assumed that the inner reaction layer of the flame has been reached and that chemical reaction dominates. Before this point, the function ω_α is used in place of the actual chemical source term $R_\alpha M_\alpha$. The extracted diffusion terms for the global step are evaluated in the same manner as the flamelet reaction rates given by Eq. (5.21) and hence following the global reaction step of Eq. (1.1) to ensure conservation of mass. Consider Eq. (5.24) rewritten in terms of the reaction progress variable, c , and the introduction of a normalised coordinate $\eta = x/\delta_L \Rightarrow \delta_L d\eta = dx$

$$\rho \frac{Dc}{Dt} = \frac{1}{\delta_L} \frac{\partial}{\partial \eta} \left(\frac{\mu}{Sc} \frac{1}{\delta_L} \frac{\partial c}{\partial \eta} \right) + \rho S_c \quad (5.28)$$

where δ_L is the laminar flame thickness. The definition of the laminar flame thickness is to some extent arbitrary, here it is evaluated for the full reaction progress variable profile (i.e. for $0 \leq c \leq 1$). The dynamic viscosity, μ , is independent of pressure and is proportional to $T^{1/2}$ [175]. An approximation for the diffusion coefficient of

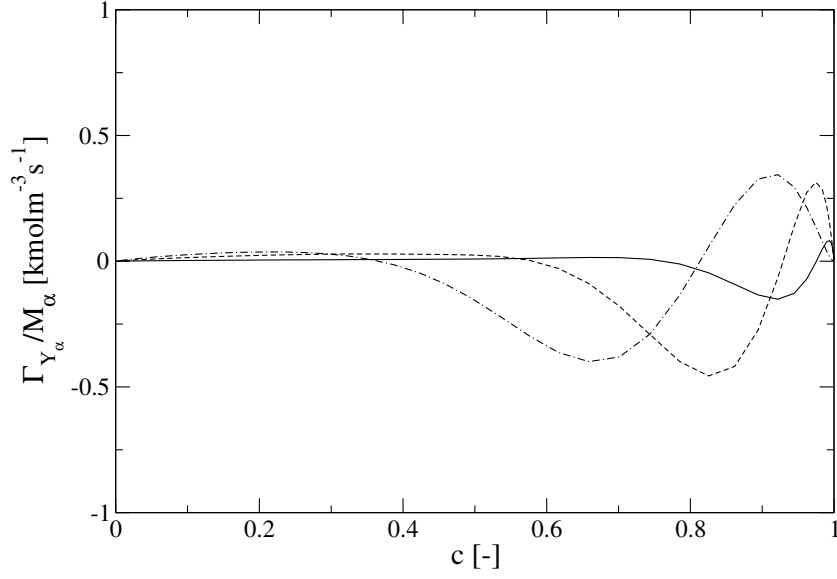


Figure 5.9: Laminar diffusion terms at 328 K in reaction progress variable space for a stoichiometric CH_4 flame. C_2H_2 (—), C_2H_4 (- - -) and C_2H_6 (- · -).

Eq. (5.28) may thus be introduced

$$\frac{\mu}{Sc} \sim A_\mu \mu_u (1 + \sqrt{T}c) \quad (5.29)$$

where A_μ is a constant of the order of unity, μ_u is the viscosity of the fresh gases and τ is given by Eq. (1.31). Eqs. (5.28) and (5.29) give

$$\rho \frac{Dc}{Dt} = \frac{A_\mu \mu_u}{\delta_L^2} \frac{\partial}{\partial \eta} \left((1 + \sqrt{T}c) \frac{\partial c}{\partial \eta} \right) + \rho S_c. \quad (5.30)$$

Furthermore, if it is assumed that the solution to Eq. (5.30) is self-similar for a range of fuels and conditions c may be represented in a functional form, $c = f(\eta)$. Several authors have approximated the turbulent reaction progress variable profile using an error function [20, 119]. An alternative function (Eq. 5.31), closely related to the error function [20], is chosen here because the inverse function may easily be expressed analytically.

$$c = f(\eta) = \frac{1}{1 + e^{-A_c \eta}} \quad \Leftrightarrow \quad \eta = f^{-1}(c) = \frac{1}{A_c} \ln \left(\frac{c}{1 - c} \right) \quad (5.31)$$

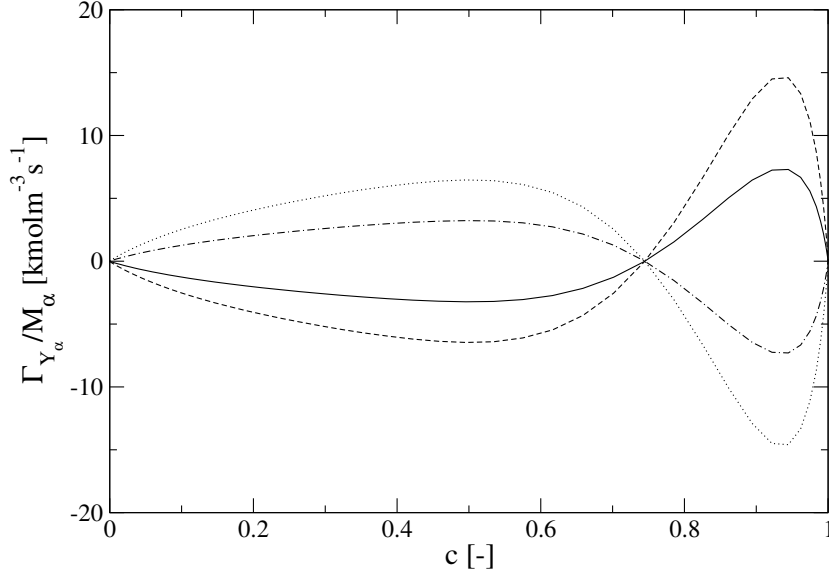


Figure 5.10: Laminar diffusion terms at 328 K in reaction progress variable space for a stoichiometric CH_4 flame assuming a global reaction step. CH_4 (—), O_2 (- -), CO_2 (- · -) and H_2O (···).

In the above expression, it may be noted that η is not defined at the scalar bounds, $c = [0, 1]$. In the computational procedure a cut-off value is introduced

$$\eta = \frac{1}{A_c} \ln \left(\frac{c^*}{1 - c^*} \right) \quad (5.32)$$

where $\varepsilon \leq c^* \leq 1 - \varepsilon$ and $\varepsilon = 1 \times 10^{-6}$. A plot of Eq. (5.31) may be viewed in Fig. 5.11 together with the normalised computed laminar profile of a stoichiometric CH_4 flame. Eq. (5.31) allows an analytical expression to be derived for the diffusion term of Eq. (5.30)

$$\Gamma_c(\eta) = \frac{A_\mu \mu_u}{\delta_L^2} \frac{A_c^2 e^{-A_c \eta}}{(1 + e^{-A_c \eta})^4} \left[-1 + e^{-2A_c \eta} + \frac{\sqrt{T}(-1 + 3e^{-2A_c \eta} + 2e^{-3A_c \eta})}{(1 + e^{-A_c \eta})^2} \right] \quad (5.33)$$

where

$$\Gamma_c(\eta) = \frac{A_\mu \mu_u}{\delta_L^2} \frac{\partial}{\partial \eta} \left((1 + \sqrt{T}c) \frac{\partial c}{\partial \eta} \right). \quad (5.34)$$

The behaviour of Eq. (5.33), which contains approximate spatial information through the flame thickness parameter (δ_L), can be seen in Fig. 5.12. The parameters A_c ,

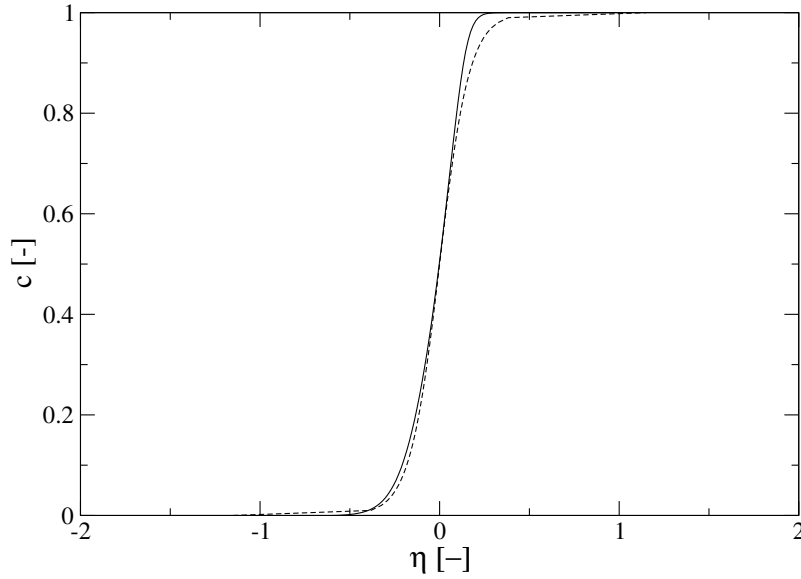


Figure 5.11: Reaction progress variable profiles in η -space at 328 K. Computed profile using detailed chemistry and equal diffusivities, spatial coordinate normalised by $\delta_L = 1$ mm (—), functional form of Eq. (5.31) with $A = 12$ (- - -).

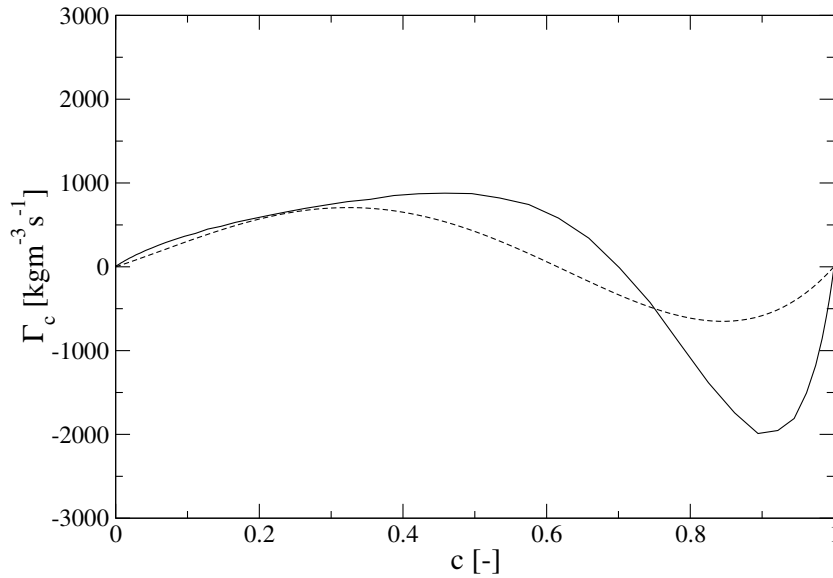


Figure 5.12: Laminar diffusion terms in reaction progress variable space at 328 K. Computed profile using detailed chemistry and equal diffusivities (—), diffusion term model of equations (5.30) - (5.33) (- - -) with $A = 12$, $A_\mu = 1.0$, $\tau = 6.0$, $\delta_L = 1$ mm and $\mu_u = 1.9 \times 10^{-5}$ kgm $^{-1}$ s $^{-1}$.

A_μ and δ_L were obtained from laminar flame solutions and not used as fitting parameters. A comparison with the numerical solution reveals a close match at the cold edge of the flame and acceptable agreement up to $c \approx 0.4$. The latter value corresponds to a temperature of ≥ 1000 K and hence to the region of the onset of high temperature chemistry. The tipping point is slightly shifted towards lower values in c -space for the curve represented by the above functional form due to the discrepancies shown in Fig. 5.11. In order to transform Eq. (5.30) back to mass fractions use is made of the definition of the reaction progress variable, (Eq. (5.20)).

$$\rho \frac{DY_F}{Dt} = \rho \frac{D}{Dt} \left(Y_{F,u}(1-c) \right) = -Y_{F,u} \rho \frac{Dc}{Dt} = -Y_{F,u} \Gamma_c(\eta) - Y_{F,u} \rho S_c. \quad (5.35)$$

The impact of the modelled diffusion term was evaluated by assuming an interchange of major reactants and products in order to ensure conservation of mass. More complete specifications of the composition vector are, of course, possible. However, the simple functional form given in Eq. (5.36) was viewed as sufficient for evaluation purposes. For each particle, the reaction progress variable is computed according to Eq. (5.20) during the third fractional step. The computed c -value is then transformed into an η -value through Eq. (5.32) that determines the magnitude of the diffusion term in c -space via Eq. (5.33). The diffusion term is then transformed back into fuel mass fractions according to Eq. (5.35) and then added to the reaction rate. Consider the global reaction step given by Eq. (1.1) then the source terms take the following form

$$\begin{aligned} \omega_{C_x H_y} &= \left[-[H(c) - H(c - \xi_c)] \frac{Y_{C_x H_y, u}}{M_{C_x H_y}} \Gamma_c(\eta) + R_{C_x H_y} \right] M_{C_x H_y} \\ \omega_{O_2} &= \left[-\left(x + \frac{y}{4} \right) [H(c) - H(c - \xi_c)] \frac{Y_{C_x H_y, u}}{M_{C_x H_y}} \Gamma_c(\eta) + R_{O_2} \right] M_{O_2} \\ \omega_{CO_2} &= \left[x [H(c) - H(c - \xi_c)] \frac{Y_{C_x H_y, u}}{M_{C_x H_y}} \Gamma_c(\eta) + R_{CO_2} \right] M_{CO_2} \\ \omega_{H_2O} &= \left[\frac{y}{2} [H(c) - H(c - \xi_c)] \frac{Y_{C_x H_y, u}}{M_{C_x H_y}} \Gamma_c(\eta) + R_{H_2O} \right] M_{H_2O} \end{aligned} \quad (5.36)$$

to ensure mass conservation. In all cases the rates of reaction (R_α) were evaluated from the full chemistry solution. The current methodology thus includes the effect of molecular transport and the scaling provided by the mixing model. The former accounts for the laminar contribution while the mixing model provides the turbulent counterpart. The approach is similar to the single scalar reaction progress variable joint PDF calculations performed by Anand & Pope [4, 139]. In the latter approach, however, the entire function ω_α was prescribed while the above procedure only amounts to an explicit correction to account for molecular transport towards the cold edge of the flame.

5.4 Numerical procedure

In the current effort, turbulent burning velocities are calculated for a wide range of fuels, stoichiometries and turbulence levels using a joint scalar transported PDF method including finite rate chemistry effects. The approach is similar to that of Hůlek and Lindstedt [69] and is based on the KPP theorem [136] — a steady one-dimensional flat flame propagating in a uniform premixed mixture and a frozen turbulence field. The turbulence field is characterised by a fluctuating velocity component (u') and the turbulent integral length scale (l_T), see Fig. 5.13. The current approach is regarded to be sufficient for the present purposes. It should, however, be noted that the detailed structure (flame thickness, turbulence levels etc.) of the turbulent flames will be different compared to more sophisticated joint velocity scalar approaches where turbulence production effects across the reaction zone are included. On the other hand, solving for turbulence across the flame without letting it decay requires special treatment; an additional source term is usually added in the manner of Anand & Pope [4]. This additional source term balances exactly the turbulence energy loss due to viscous dissipation.

The numerical procedure is based on a time dependent version of the parabolic *GENMIX* [163] code extended to include a *Monte Carlo* part for the solution of the joint scalar PDF. The governing equations have been transformed into one dimension

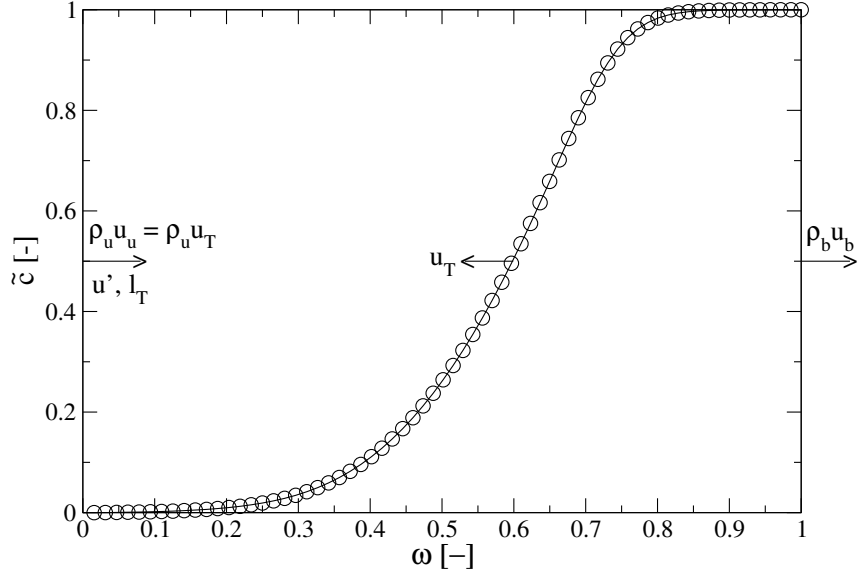


Figure 5.13: 1D simulations schematically shown in the solved ω -space as given in Appendix C.

in space and time, see Appendix C for details.

The equations are then discretised and solved numerically using the finite volume technique [171]. The starting point is the integration of the governing equations over a control volume that surrounds the nodal point. An attractive feature of the finite volume method is that the discretised equation has a clear physical meaning — it constitutes a balance equation for the solved variable over the control volume. Scalar values are stored at the nodal point while velocities are stored midway between the nodes. Storing at the same location may lead to convergence issues and oscillations [48] in the velocity and pressure fields. To evaluate fluxes and gradients at the cell (control volume) faces, the nodal values (scalar and velocity nodes) are then linearly interpolated (central differencing scheme) to the cell faces. The resulting system of linear algebraic equations are then solved using the tri-diagonal matrix algorithm (TDMA) [171] to obtain the distribution of the solved variable at the nodal points. The TDMA features forward elimination and back substitution.

The domain is discretised by means of 80 initially equi-distant cells with an expected average of 200, 800 or 1600 particles per cell (ppc). The time step was varied between $1.0 \times 10^{-7} \leq \Delta t \leq 2.5 \times 10^{-6}$ s as burning velocities increase exponen-

tially for $\Delta t > 1.0 \times 10^{-5}$ s [115]. The turbulence integral length scale was fixed to 40 mm [1] for all flames considered unless otherwise stated. In past work featuring hydrocarbon flames [69], the length scale was varied between 10 and 40 mm and only a weak dependence was observed in accordance with the theoretical analysis that suggests $u_T \propto l_T^{1/8}$ [170]. Nevertheless, a length scale of 20 mm was also used for H_2 flames to further investigate the sensitivity.

5.5 Experimental data

The computed turbulent burning velocities are compared with the measured values of Abdel-Gayed et al. [1]. The experimentally determined turbulent burning velocities are obtained from a cylindrical cast steel explosion bomb of 305 mm diameter and 305 mm length. In each end plate, a 150 mm diameter concentric window of 25.4 mm thickness was fitted allowing the whole of the flame to be photographed. The uniform and isotropic turbulence field was obtained using four identical eight-bladed fans equispaced around the central circumference. Turbulent velocity fluctuations were varied through changes in the fan speed between 50 and 167 Hz. The turbulent burning velocities were determined through the double kernel method. That is, the closing velocity of two propagating flame fronts of separate kernels was measured. Flame propagation was recorded with a high speed camera at a maximum rate of 10000 frames/s. A 10 mW helium-neon laser was used to define the flame front using the schlieren technique. The helium-neon laser light was focused firstly by a microscope lens and secondly by a larger lens. The larger lens created a 100 mm diameter beam of light that was reflected from a mirror and dichroic filter, through the concentric windows of the explosion bomb. The turbulent velocity fluctuations were determined under isothermal conditions by a forward scattering laser doppler counting system. For this, a 2 W argon ion laser rated at 100 mW, was used.

In the sections below the computed turbulent burning velocities are compared with the measured values of Abdel-Gayed et al. [1] marked as (o). The experimental data points correspond to a least square fit. The measured value from the explosion

bomb differs from the turbulent burning velocity of a flame stabilised in a burner due to an initial reduction of the eddy diffusivity and thereby a reduction of the turbulent transport processes. The measured value is therefore lower than the fully developed turbulent burning velocity. With the passage of time the developing turbulent burning velocity will reach the value as if obtained from a burner. The measured turbulent burning velocity is therefore corrected using a simple formula [1]

$$u_T = u_T^*[1 - \exp(-\bar{t})]^{1/2} \quad (5.37)$$

where u_T^* represents the fully developed turbulent burning velocity and $\bar{t}$ is the elapsed time divided by the Lagrangian eddy life time, given as $0.44l_T/u'$. The corrected values are marked with ($\square$). Error bars are also included to give an estimate of the scatter in the experiments. In order to be consistent, the data was non-normalised using the values given by Abdel-Gayed et al. [1] and then normalised using the values given in Table 5.1. It should be pointed out that significant uncertainties in experimentally determined turbulent burning velocities remain (cf. [119, 120]) and, accordingly, caution is required when making quantitative comparisons. More recent investigations have been performed (e.g. [47, 101, 153]). However, data sets are typically limited to very low turbulence levels [101, 153] or feature not fully developed flames [47]. The mean turbulent reaction rate data are given by Cheng & Shepherd [29] and Lawn & Schefer [101].

5.6 Results

Calculation methods for turbulent premixed flames based on an integral scale mixing frequency (ϵ/k), such as the Eddy-Break-Up closure, can be expected to result in a linear relationship $u_T \propto u'$ [62]. It is hence natural to present result on this basis [4, 115] and the u_T/u' normalisation has the further benefit of emphasising deviations at high Da numbers. A KPP type analysis (see Section 5.2 for details) of a variant of the BML closure suggests a constant of proportionality $\simeq 1.5$ for lean and stoichiometric methane flames [62]. The result is in good agreement with

computations using transported PDF methods with the source term extracted from laminar flame solutions [110] using the conventional closure for the scalar dissipation rate ($C_\phi^* = 0.0$) as discussed in Section 5.3.2.

5.6.1 Standard closure for the scalar dissipation rate

Application of the standard closure for the scalar dissipation rate given by Eq. (3.41) with $C_\phi = 2.0$ for the rich hydrogen fuel mixture without the diffusion correction term reveals a linear scaling in terms of turbulence intensity variations and contrasts qualitatively with the experimental data of Abdel-Gayed *et al.* [1] as shown in Fig. 5.14. The linear scaling is qualitatively incorrect and consistent with the earlier findings of Lindstedt & Váos [115]. The solution at high Re numbers approaches the correct value as may be anticipated due to the reduced importance of molecular transport terms.

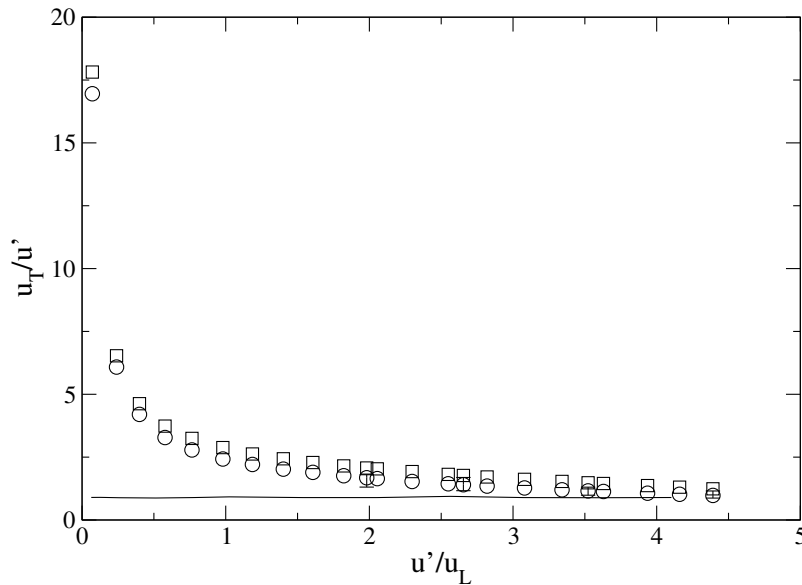


Figure 5.14: Predicted turbulent burning velocities for the rich ($\phi = 1.6$) hydrogen flames ($l_T = 40$ mm) using 1600 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed *et al.* [1]. Mixing time scale expression given by Eq. (3.41) with $C_\phi = 2.0$ (—).

5.6.2 Extended closure for the scalar dissipation rate

As shown by Lindstedt & Váos [115], the scaling of turbulent burning velocities can be improved with respect to turbulence intensity variations (Da number) through the application of the extended closure for the scalar dissipation rate given by Eq. (5.13). The latter closures introduces a scaling through the density and the Kolmogorov velocity variations across the flame. Furthermore, a Le number scaling of the unstrained laminar burning velocity is introduced to cover a range of fuel mixtures.

The computed turbulent burning velocities for the rich hydrogen flames using the aforementioned scalar dissipation rate closures, still without diffusion term correction, shows a significant qualitative improvement in terms of the scaling with respect to turbulence intensity variations as shown in Fig. 5.15. Two limiting cases are shown: (i) The use of Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ and (ii) Eq. (5.15) with $C_\phi = 0.0$ and $C_\phi^* = 2.4$. Predictions obtained using the extended scalar dissipation rate closure without Le number compensation are also shown. Arguably, the best overall quantitative and qualitative agreement is achieved using the exponential Le number scaling without the impact of the standard mixing time scale expression ($C_\phi = 0.0$). The impact of a reduction in l_T to 20 mm is very modest as also shown. For the stoichiometric methane flames the picture changes considerably, qualitatively the predictions are very good for $0 < u' < 16$ m/s but quantitatively, the computed turbulent burning velocities are grossly underpredicted as shown in Fig. 5.16. The predicted turbulent burning velocities of stoichiometric ethane are slightly low compared to the experimental data as shown in Fig. 5.17. Inspection of the normalised turbulent reaction rates for methane and ethane for one selected flame ($u' = 4$ m/s) in reaction progress variable space reveals a qualitatively incorrect behaviour. The actual reaction rate for methane, shown in Fig. 5.18, is very low at the cold edge of the flame, which explains the low turbulent burning velocities. Ethane on the other hand show slightly higher flame front activity. For illustrative purposes, the reaction rates are also compared with the normalised reaction progress variable variance, assuming a bimodal PDF ($\widetilde{c''^2} = \widetilde{c}(1 - \widetilde{c})$). There are apparently differences in the behaviour of the methane, ethane and hydrogen flames at the cold

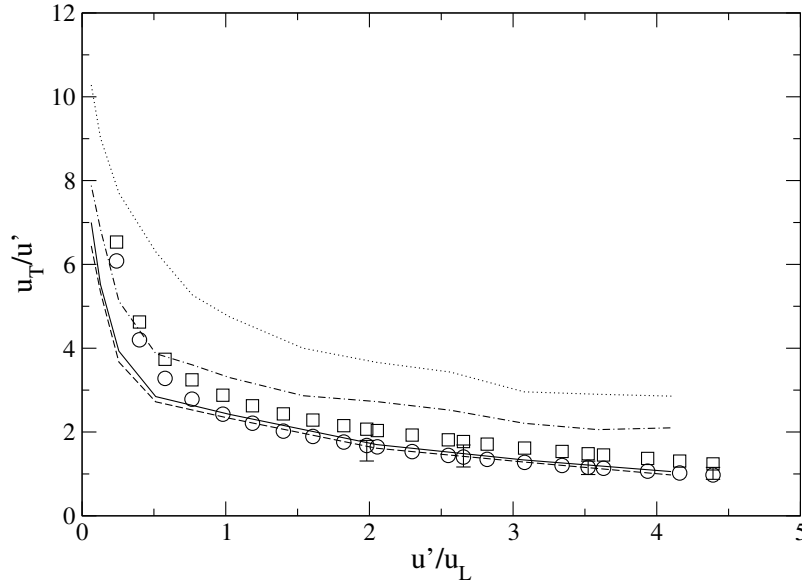


Figure 5.15: Predicted turbulent burning velocities for the rich ($\phi = 1.6$) hydrogen flames. Measured ($\circ$), corrected for fully developed flames ($\square$) [1]. $l_T = 40$ mm; τ_ϕ^{-1} via Eq. (5.13) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$, 1600 ppc ($\cdots$); τ_ϕ^{-1} via Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$, 800 ppc ($-\cdots-$); τ_ϕ^{-1} via Eq. (5.15); $C_\phi = 0.0$ and $C_\phi^* = 2.4$, 800 ppc ($-$); $l_T = 20$ mm; $C_\phi = 0.0$ and $C_\phi^* = 2.4$, 800 ppc ($- - -$).

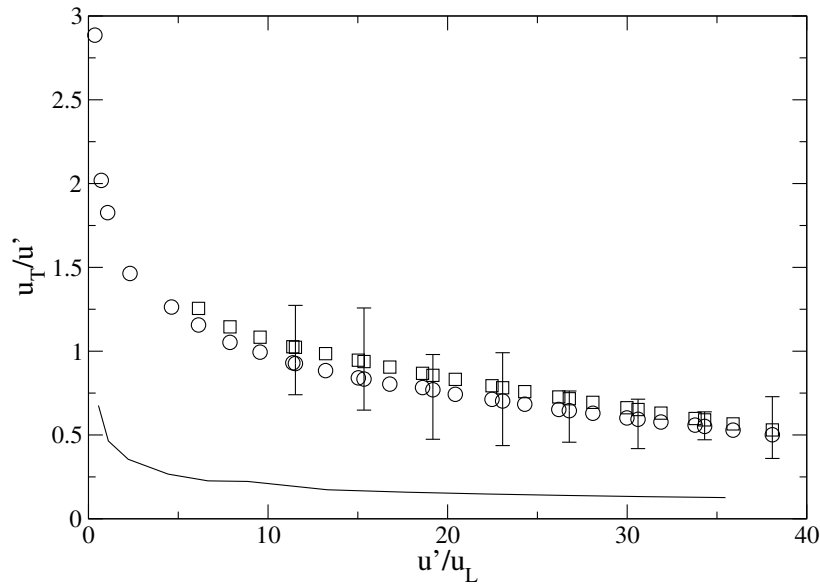


Figure 5.16: Predicted turbulent burning velocities for stoichiometric ($\phi = 1.0$) methane flames ($l_T = 40$ mm) using 1600 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed *et al.* [1]. τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ ($-$)

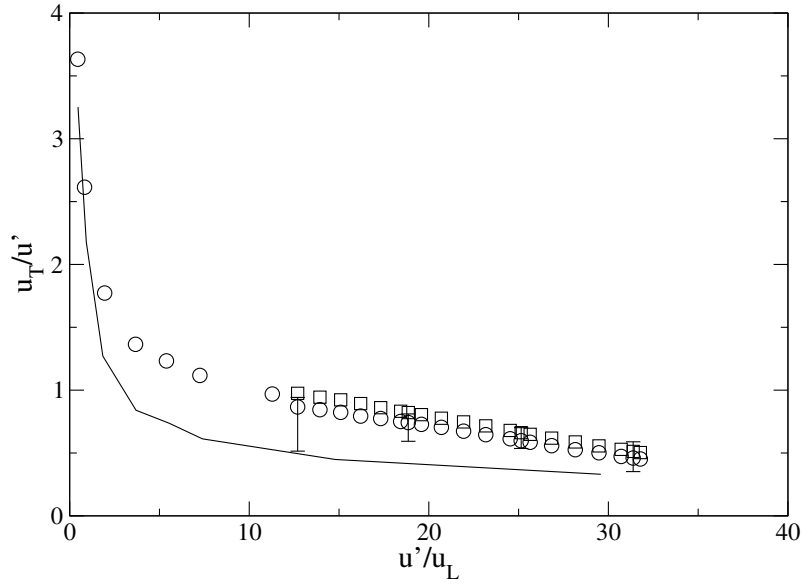


Figure 5.17: Predicted turbulent burning velocities for the stoichiometric ethane flames ($l_T = 40$ mm) using 1600 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed *et al.* [1]. τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (—).

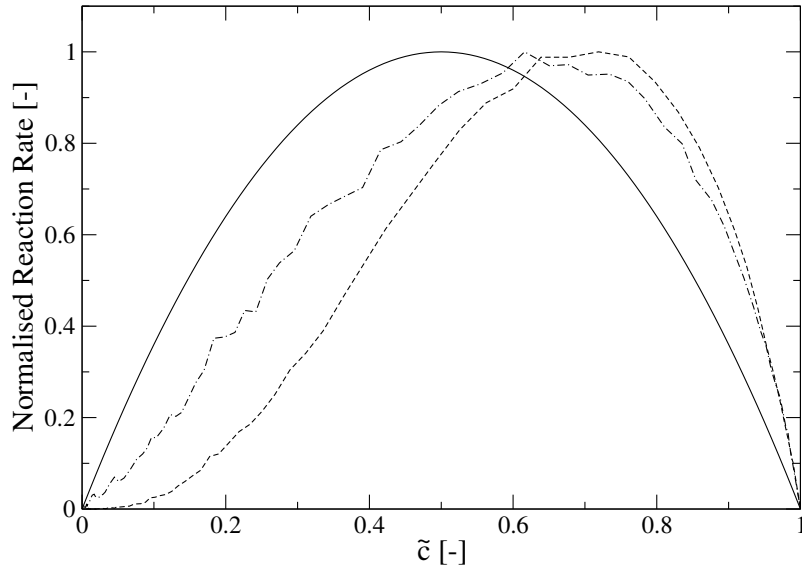


Figure 5.18: Predicted average normalised turbulent reaction rate for stoichiometric methane (---) and stoichiometric ethane (— · —) using 1600 ppc, $u' = 4$ m/s, $l_T = 40$ mm, τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$. Normalised progress variable variance, $\tilde{c}(1 - \tilde{c})$ (—).

edge of the flame. This observation is consistent with the earlier discussion regarding flame front activity and Zeldovich numbers of the different fuels in Section 5.3.2.1. As shown in Fig. 5.4, hydrogen is comparatively active at the flame front as indicated by the low Zeldovich number. Ethane has a higher flame front activity as indicated by the Zeldovich number as compared with methane. An interesting observation is that the recent study by Lindstedt & Város [115], where stoichiometric methane flames were computed under similar conditions using an extracted flamelet source term, indicate excellent agreement with measurements.

5.6.3 Implicit impact of molecular transport

Application of the combined flamelet and chemical source terms (see Fig. 5.2) given by Eq. (5.19) together with the extended mixing time scale closure including the Le number scaling yields a satisfactory agreement between predictions and experimental data for all hydrocarbon flames considered.

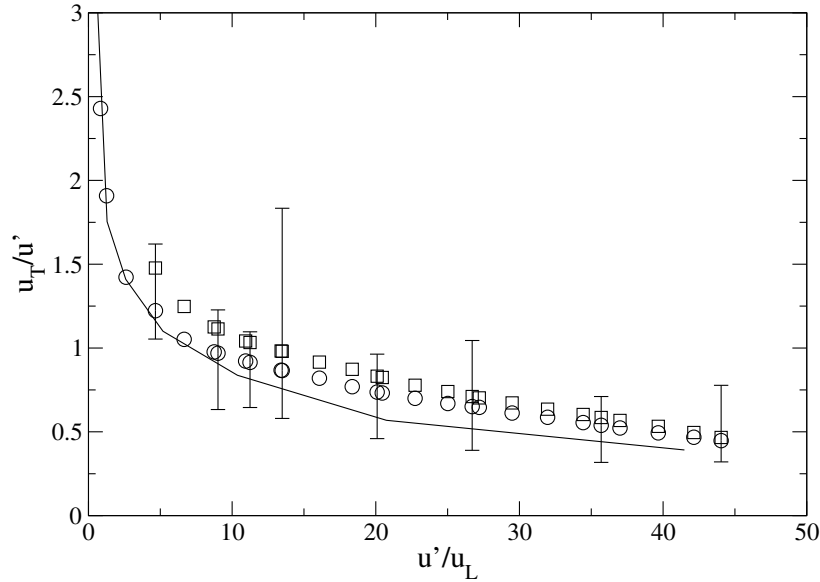


Figure 5.19: Predicted turbulent burning velocities for lean ($\phi = 0.88$) methane flames ($l_T = 40$ mm) using 200 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed *et al.* [1]. τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (—).

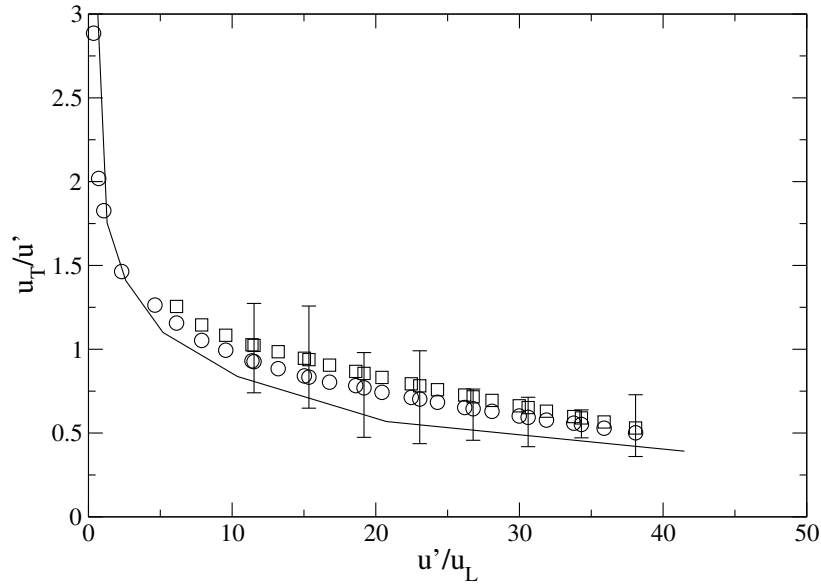


Figure 5.20: Predicted turbulent burning velocities for stoichiometric ($\phi = 1.0$) methane flames ($l_T = 40$ mm) using 200 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed *et al.* [1]. τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (—)

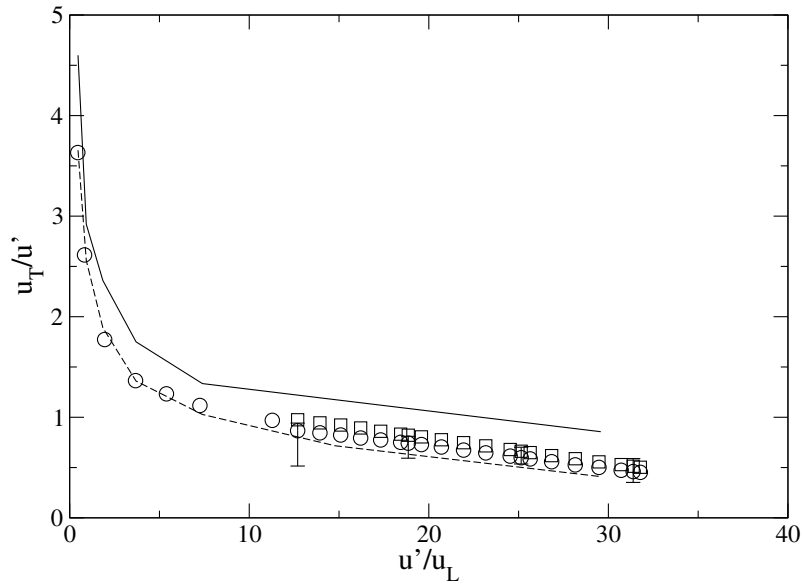


Figure 5.21: Predicted turbulent burning velocities for stoichiometric ($\phi = 1.0$) ethane flames ($l_T = 40$ mm) using 200 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed *et al.* [1]. τ_ϕ^{-1} given by: Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (—), Eq. (5.15) with $C_\phi = 0.0$ and $C_\phi^* = 2.4$ (- -).

The overall agreement for the slightly lean ($\phi = 0.88$) methane flames shown in Fig. 5.19 is general good and well within experimental uncertainties. For low u' , the predictions are in excellent agreement with the experimental data while for higher u' , the predicted value is slightly low. The same trend can be seen for the stoichiometric methane flames in Fig. 5.20. The latter finding may seem inconsistent with the recent calculations of Lindstedt & Város [115], but in their work the C_ϕ and C_ϕ^* constants were set to 4.0 and 4.8, respectively. As indicated by Eq. (5.7), an increase of the reaction rate constant by a factor of two theoretically increases the turbulent burning velocity by a factor of $\sqrt{2}$.

For the ethane flames shown in Fig. 5.21, the linear Le number scaling result in a slight over-prediction, especially for higher u' as compared to the experimental data. At low u' a reasonable agreement is achieved. The predictions using the exponential Le scaling with the fractal mixing time scale expression only ($C_\phi = 0.0$) improves the predictions overall. The latter finding is consistent with the hydrogen predictions presented above.

Although being attractive due to its simplicity, the major disadvantage with the current approach is the inability to predict extinction/re-light phenomena.

5.6.4 Explicit impact of molecular transport

The inclusion of the explicit laminar diffusion correction was initially explored using the extracted diffusion terms shown in Fig. 5.10. That is, the laminar diffusion terms are included according to Eq. (5.36) assuming equal diffusivities for the species involved in the global reaction step. Turbulent stoichiometric methane flames using 200 ppc were initially evaluated to see the effect. The characteristic mixing frequency is closed by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$. In Fig. 5.22, the predictions are shown and compared with the experimental data of Abdel-Gayed et al. [1]. The scaling in terms of u' variations is preserved but the actual level is slightly too high but within the experimental uncertainty. The result is encouraging and motivates the inclusion of the modelled correction term.

The inclusion of the explicit laminar diffusion correction derived above, was

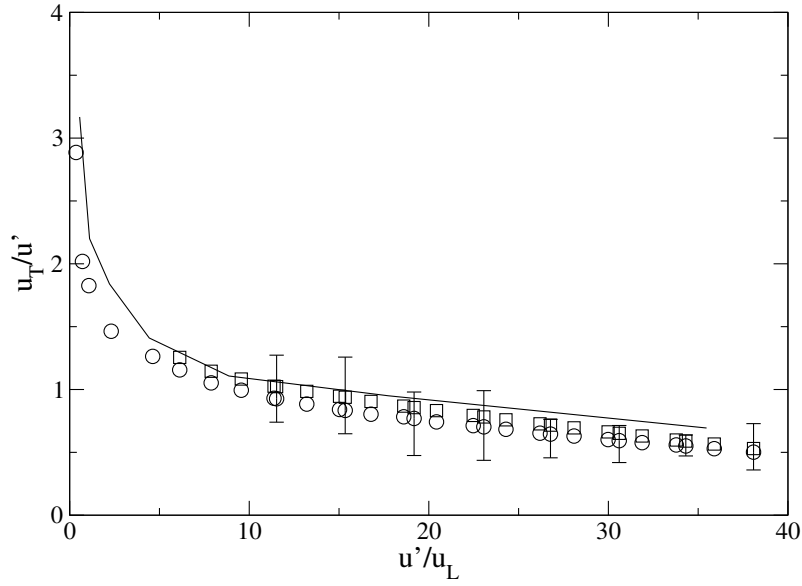


Figure 5.22: Predicted turbulent burning velocities for the stoichiometric methane flames ($l_T = 40$ mm) using extracted diffusion terms and 200 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed *et al.* [1]. τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (—).

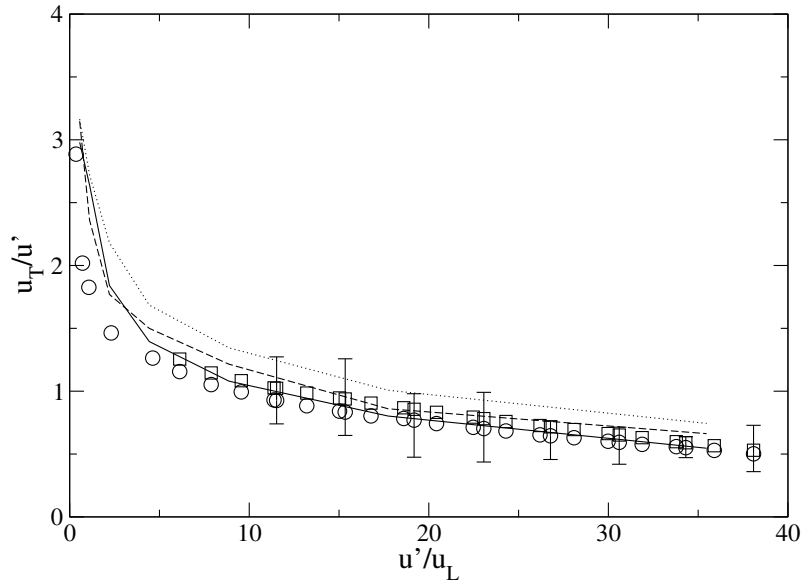


Figure 5.23: Predicted turbulent burning velocities for the stoichiometric methane flames ($l_T = 40$ mm) using 200 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed *et al.* [1]. Reaction rate expression given by Eq. (5.36) with $A_c = 12$ and $\delta_L = 1$ mm. τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$, $A_\mu = 1.0$ ($\cdots$), $A_\mu = 0.5$ (---). τ_ϕ^{-1} given by Eq. (5.15) with $C_\phi = 0.0$ and $C_\phi^* = 2.4$, $A_\mu = 1.0$ (—).

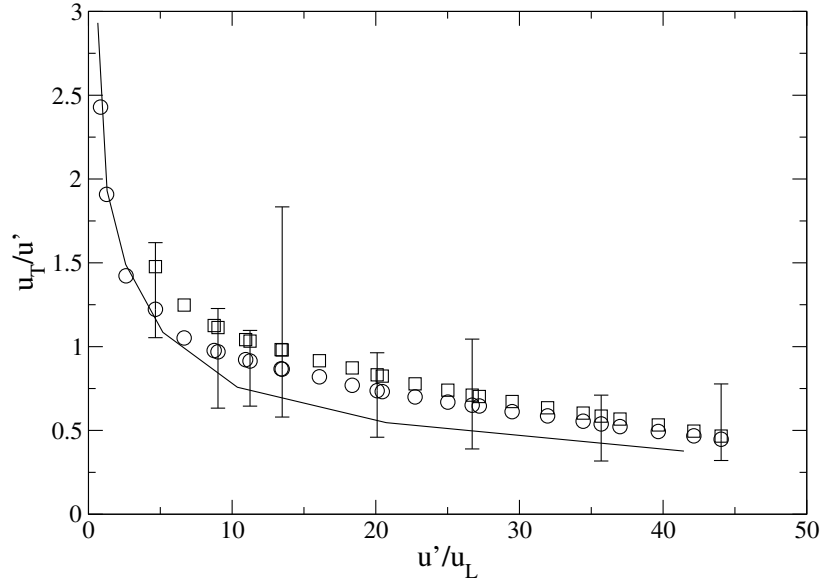


Figure 5.24: Predicted turbulent burning velocities for the slightly lean ($\phi = 0.88$) methane flames ($l_T = 40$ mm) using 200 ppc. Experimental data, measured ($\circ$), corrected for fully developed flames ($\square$) and error bars by Abdel-Gayed *et al.* [1]. Reaction rate expression given by Eq. (5.36) with $A = 12$ $A_\mu = 1.0$ and $\delta_L = 1$ mm. τ_ϕ^{-1} given by Eq. (5.15) with $C_\phi = 0.0$ and $C_\phi^* = 2.4$ (—).

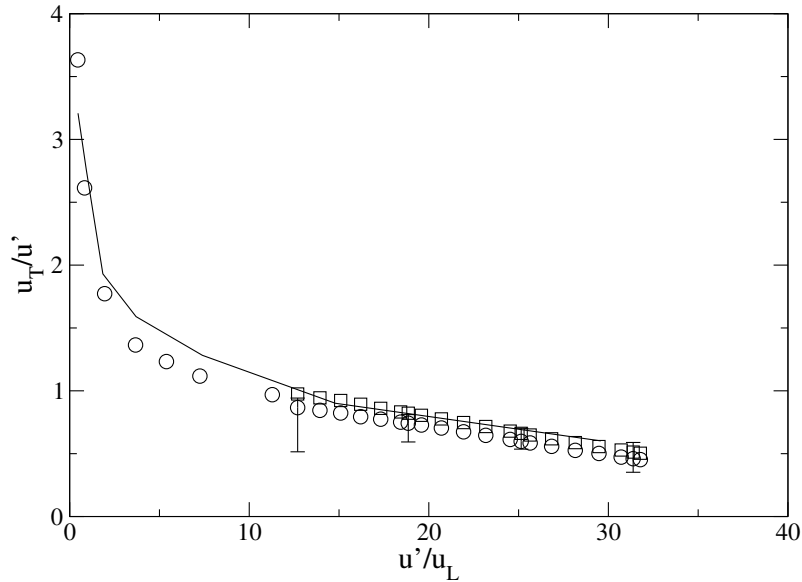


Figure 5.25: Predicted turbulent burning velocities for stoichiometric ethane flames ($l_T = 40$ mm) using 200 ppc. Symbols as in Fig. 5.24 except $\delta_L = 0.7$ mm.

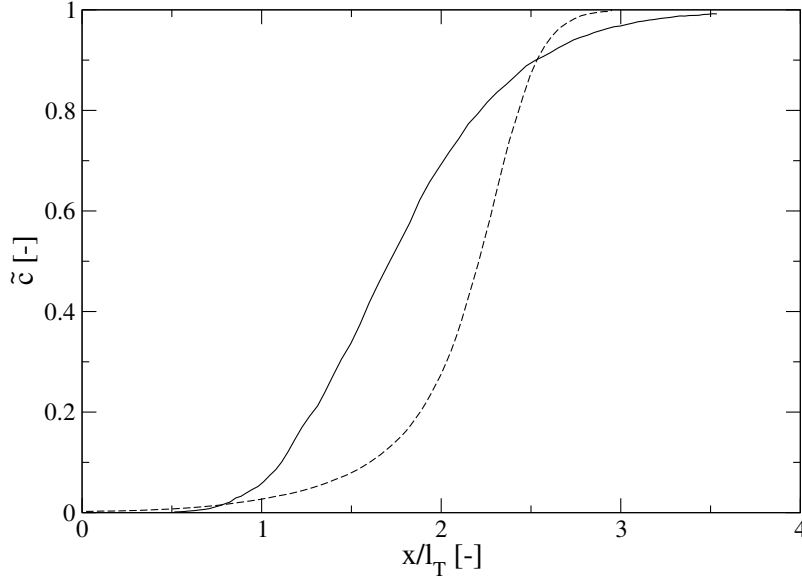


Figure 5.26: Computed reaction progress variable profiles, $u' = 1$ m/s and $l_T = 40$ mm. Predicted profile with diffusion term correction of Eq. (5.36) with $A_c = 12$, $A_\mu = 1.0$, $\delta_L = 1$ mm and 200 ppc, τ_ϕ^{-1} given by Eq. (5.15) with $C_\phi = 0.0$ and $C_\phi^* = 2.4$ (—) and without diffusion term correction using 1600 ppc, τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (- -).

explored by computing stoichiometric CH_4 flames using 200 ppc. The computed results using the mixing time scale expression given by Eq. (5.14) with $C_\phi = 2.0$, $C_\phi^* = 2.4$ and $A_\mu = 1.0$ are shown in Fig. 5.23. Consistent with the extracted diffusion terms, a slight over-prediction can be observed. However, the improved agreement compared with results obtained without laminar diffusion correction are encouraging. The sensitivity to the A_μ parameter was also investigated and a value of $A_\mu = 0.5$ improved predictions. The best overall agreement is obtained without the standard mixing time scale expression ($C_\phi = 0.0$) and the exponential Le number scaling given by Eq. (5.15). The latter is encouraging since it is consistent with the earlier findings obtained for the hydrogen flames. The same closure was also applied to compute the slightly lean ($\phi = 0.88$) methane flames. The predicted turbulent burning velocities are slightly low compared to the measurements for high Re numbers as shown in Fig. 5.24. In the high Da number limit, on the other hand, the predictions are in excellent agreement with experimental data. Overall

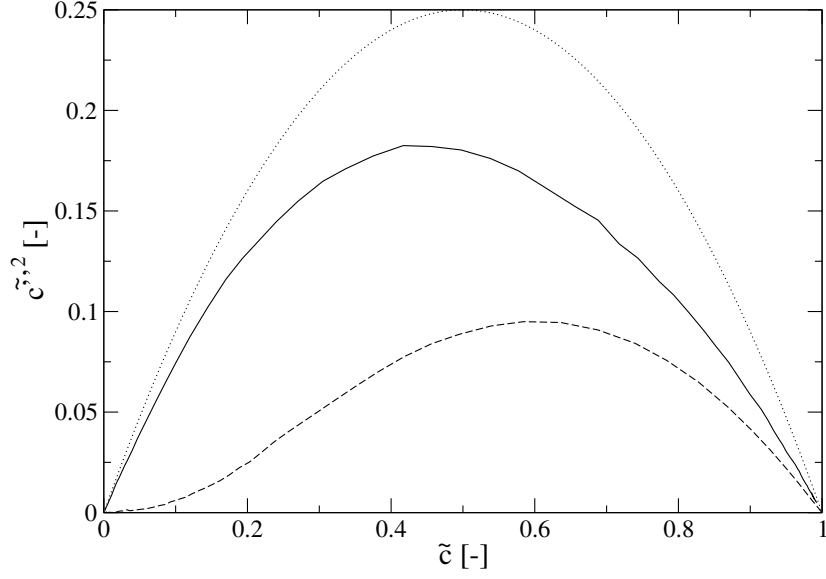


Figure 5.27: Computed reaction progress variable variance profiles, $u' = 1$ m/s and $l_T = 40$ mm. Predicted variance with diffusion term correction of Eq. (5.36) with $A_c = 12$, $A_\mu = 1.0$, $\delta_L = 1$ mm and 200 ppc, τ_ϕ^{-1} given by Eq. (5.15) with $C_\phi = 0.0$ and $C_\phi^* = 2.4$ (—) and without diffusion term correction using 1600 ppc, τ_ϕ^{-1} given by Eq. (5.14) with $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (- - -) and theoretical maximum variance $\tilde{c}''^2 = \tilde{c}(1 - \tilde{c})$ (····).

the computed results are well within experimental uncertainties.

The computed stoichiometric ethane flames shown in Fig. 5.25 agree reasonably well with experimental data, especially at high Da numbers. As expected, the impact of the laminar diffusion correction term is significantly smaller compared to the methane flames. Overall, it appears that the standard closure for the scalar flux term in Eq. (5.18) is sufficient when combined with the extended closure for the mixing frequency shown in Eq. (5.15), apart from at high Zeldovich numbers when a comparatively simple analytical correction for the contribution of molecular diffusion towards the leading edge can be applied. In Figs. 5.26 and 5.27, the predicted profiles of the reaction progress variable and the reaction progress variable variance are compared with the computed profiles without the modelled diffusion correction term for one selected flame in the flamelet regime of combustion. The turbulence, for the selected flame, is characterised by a turbulence intensity of $u' = 1$ m/s and a turbulent integral length scale of $l_T = 40$ mm. The predicted reaction progress

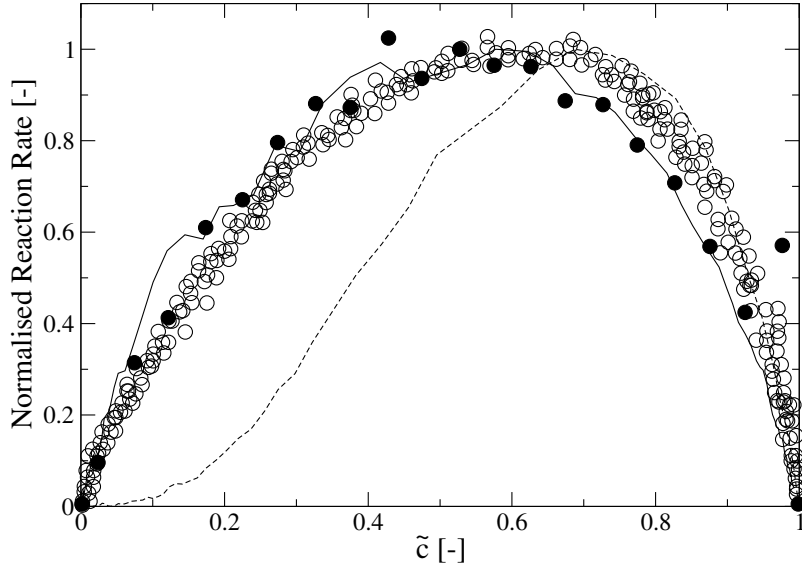


Figure 5.28: Predicted normalised turbulent reaction rates for stoichiometric CH_4 flames, $u' = 1$ m/s and $l_T = 40$ mm. No diffusion model, 1600 ppc, τ_ϕ^{-1} via Eq. (5.14), $C_\phi = 2.0$ and $C_\phi^* = 2.4$ (- -). Diffusion model of Eq. (5.36), 200 ppc, τ_ϕ^{-1} via Eq. (5.15), $C_\phi = 0.0$, $C_\phi^* = 2.4$, $A_c = 12$, $A_\mu = 1.0$ and $\delta_L = 1$ mm (—). Experimental data: Cheng & Shepherd [29] (o) and Lawn & Schefer [101] (●).

profile for the case with laminar diffusion correction is close to the shape of an error function, a function commonly used to represent turbulent $\tilde{c}$ -profiles [20, 119], while the predictions without the correction term has an extended leading edge of the flame due to the low reaction rate in this region. The predicted peak value of the variance is significantly lower than the theoretical $\widetilde{c'^2} = \tilde{c}(1 - \tilde{c})$ for the case without laminar diffusion correction while a significant improvement can be seen both in terms of the shape and the peak value for the case with the correction term. A slight shift towards fresh gases can also be observed. Similar to the work of Lindstedt & Város [115], the mean reaction rate predictions are shown in Fig. 5.28. In the latter figure, the normalised turbulent reaction rates are shown for the cases with and without diffusion correction together with the experimental data of Cheng & Shepherd [29] and Lawn & Schefer [101]. The measured reaction rates of Cheng & Shepherd are obtained for a range of burner geometries including rod-stabilised v-flames, tube stabilised conical flames and flames stabilised in stagnation point flow. The measured turbulent rates are consistent and independent of burner geometry

or flame type. All flames are in the wrinkled laminar flamelet regime of combustion. Lawn & Schefer determined the position of the flame front through planar laser-induced fluorescence. The ensemble average of a collection of 200 images allowed the statistics for the 2-D flamelet surface density to be measured. The fuel was a mixture of 75% CH_4 and 25% H_2 at equivalence ratio 0.9. The prediction using the diffusion correction term with $C_\phi = 0.0$ and $C_\phi^* = 2.4$ agrees comparatively well with experimental data while significant deviations can be seen for the predictions without the correction term.

5.7 Summary

The ability of a transported PDF method closed at the joint scalar level to predict the turbulent burning velocity data of Abdel-Gayed et al. [1] has been evaluated. It is shown that the standard closure for the scalar dissipation rate results in a qualitatively incorrect behaviour in terms of the turbulent burning velocity scaling with respect to turbulence intensity variations. An extended scalar dissipation rate closure, featuring a scaling on the Kolmogorov velocity, provides a qualitatively correct behaviour at all Damköhler numbers for all tested fuels. Reasonable quantitative agreement was also obtained for the C_2H_6 and H_2 flames. In the case of fuel-air mixtures with Lewis numbers departing from unity, the introduction of a Lewis number scaling in the model for the mixing frequency is found to be beneficial. The results suggest that fuels with Zeldovich numbers not greater than ethane can be computed directly with the current methodology and that a derived additional analytic term that explicitly takes into account the impact of molecular transport at the leading edge of the flame can alleviate difficulties encountered for less reactive fuels. The approach can readily be extended to incorporate differential transport of energy. It may be noted that the current results were obtained with a comparatively simple mixing model and that further improvements can be expected by the application of models that enforce locality in composition space.

Chapter 6

Simulation of a partially premixed flame in an industrial burner

6.1 Introduction

The introduction and development of lean (partially) premixed prevaporised (LPP) combustion systems in industrial gas turbines has led to a significant reduction of nitric oxides (NO_x) compared to conventional non-premixed diffusion-type flame techniques. On the other hand, lean mixtures make the system very sensitive to shear layer instabilities and equivalence ratio fluctuations producing vortex shedding, steep velocity gradients, non-uniform heat release and local extinction/re-ignition phenomena. The occurrence of combustion instabilities and the coupling to acoustic waves might cause severe damage to the combustion chamber [42], even though the amplitudes of the pressure fluctuations are of the order of a few percent [175] of the operating pressure. Other key aspects of a practical combustion system are suppressed part load emissions and stable operation over a wide range of load conditions, fuels and equivalence ratios. These features might be possible to achieve to some extent by considering Rich-Quench-Lean (RQL) pilot [60] stabilisation of the swirling main flame or the flameless oxidation principle [114] or a combination of both. The RQL piloting system features a small pre-combustion chamber generating a pool of radicals fed to the forward stagnation point of the

swirling main flame. The flameless oxidation principle consists of mixing between a jet of fuel and preheated air and dilution by products of combustion. The dilution process generates lower overall temperatures and less air is needed for cooling of the combustion chamber. A practical combustion system features complex aerodynamics interacting with chemical reaction at a range of time scales. Numerical tools that can deal with the relatively fast heat release and the slow pollutant formation in the post flame region and at the same time predict global extinction/re-ignition is a prerequisite.

In the review paper of Brewster et al. [23], it was concluded that transported PDF methods are the most suitable approach for land-based gas turbines. The approach is general and applicable in non-premixed, partially premixed and premixed modes and allow arbitrarily complex chemistry to be incorporated. Furthermore, it is argued that joint velocity-scalar PDF are preferred over joint scalar approaches in order to include a higher order closure for transport in physical space. Anand et al. [5, 6] computed two axi-symmetric laboratory non-premixed swirl combustor configurations using the joint velocity-scalar-frequency transported PDF approach. The thermochemistry for the swirling hydrogen diffusion flame was represented by a single scalar, the mixture fraction, while a two-step chemical mechanism was applied for the methane step-swirl combustor. Cannon et al. [24] simulated lean premixed combustion in a axi-symmetric can combustor with a bluff body stabilised flame using a reduced 5-step mechanism combined with the ISAT methodology. James et al. [74] solved a piloted jet diffusion flame and a low-emissions premixed gas turbine combustor using the joint scalar PDF method with in situ adaptive tabulation of the chemistry and the $k - \epsilon$ turbulence model. A 16-species 41-step C_1 and a reduced 16-species 12-step C_2 mechanism were applied and it was concluded that a C_2 mechanism is a minimum requirement for accurate CO predictions. Furthermore, it was also shown that the $k - \epsilon$ model fails to predict the tangential (swirl) component of velocity while the axial component were in reasonable agreement with experimental data. The physical domains were represented by two-dimensional axi-symmetric geometries. James et al. [75, 76] applied the Eulerian and the Lagrangian joint scalar

transported PDF method to three three-dimensional geometries and concluded that both approaches can be used in practical combustor design. It was also shown that it was possible to obtain reasonable results with as little as 10 ppc [76] in the case of a Lagrangian approach. The $k - \epsilon$ model was applied in both cases. More examples can be found in the recent review paper by Haworth [68].

6.1.1 The present contribution

In the current Chapter simulations of a small gas turbine burner is performed at realistic gas turbine operating conditions. The partially premixed flame is swirl stabilised through the formation of a central recirculation zone. Adopted closures range from Reynolds stress/gradient diffusion/presumed PDF (PPDF) to Reynolds stress/transported PDF (TPDF) approaches. The purpose of the current work is to (i) apply transported PDF methods in a fully unstructured three-dimensional geometry, to further investigate (ii) the potentially low turbulent burning velocity predictions in a practical flow situation due to the uncertainties of experimentally derived values and modelling approaches (planar and spherical flames). No experimental data are available at this time, instead two sets of simulations are performed and compared. The PPDF simulation has dual purposes, to initialise the flow field for the PDF solver and to get a reference solution. The reference solution represent a “standard” solution in industry while the TPDF solution represents a more advanced modelling technique which has the potential to accurately model extinction/re-light and emissions — phenomena relevant to industry. In the present work, the node-based Eulerian joint scalar transported PDF is applied and the chemistry is represented by the global mechanism of Jones & Lindstedt [81] featuring four reactions and seven solved species (CH_4 , O_2 , H_2O , CO_2 , H_2 , CO and N_2).

6.2 Flow configuration

The current industrial gas turbine burner geometry represents a small pre-combustion chamber, the RPL (Rich-Pilot-Lean) burner, that is operated predominantly in the

fuel rich regime at a flame temperature higher than the main flame. This small device has two major purposes: (i) it acts as an ignition burner, a small torch, that ignites the pilot and the main burners. (ii) to support the main flame and to widen the operating window of the main burner. The RPL burner constantly feeds, over the entire load range, the forward stagnation point of the main burner with energy. The energy transfer materialise in two ways, first through heat, since the RPL burner is operated at a higher flame temperature as compared to the main flame. Secondly, through radicals from the products of combustion of the fuel rich flame.

The fuel and the oxidiser are introduced separately, but mixed before the entrance of the small combustion chamber. The air is introduced at the back end of the plenum and is swirled as it enters the mixing channel where the fuel is introduced. The fuel/air mixture enters the combustion chamber and forms the central recirculation zone and thereby creating the shear layer that is used to stabilise the (partially) premixed flame. The central recirculation zone recirculates the hot products of combustion to ensure a continuous combustion process.

6.3 Closure considerations

The node-based Eulerian joint scalar transported PDF approach described in Section 4.3.2 is here applied to an industrial gas turbine burner geometry at realistic conditions. The chemistry is represented by the global reaction scheme of Jones & Lindstedt [81, 82], described in detail in Section 4.3.2.3.

In Chapter 4 it was indicated that the turbulent burning velocity is under-predicted using the transported PDF approach and in Chapter 5 it was shown that extended mixing frequency expressions and additional laminar diffusion terms are needed in combination with Modified Curl's model for flows approaching the high Da number limit. The current flow is expected to approach the distributed reaction zones or the well stirred reactor regime where the impact of the extended mixing frequency and the laminar diffusion terms will weaken. Furthermore, sim-

plicity and computational cost are increasingly important in three-dimensional cases featuring unstructured grids. Therefore, the molecular mixing term in the transport equation of the joint scalar PDF is closed by Modified Curl's model described in Section 3.3.3.1. During a small time increment Δt , N_{pq} pairs of particles out of N are selected without replacement and N_{pq} is given by Eq. (3.37) where $\beta_\phi = 3.0$ to ensure the correct decay rate of the scalar variance. The scalar dissipation rate (τ_ϕ^{-1}) is given by Eq. (3.41) and the standard value of 2.0 is maintained for C_ϕ .

6.4 Numerical procedure

The physical domain is represented by a 45° sector of the burner geometry. The physical domain is discretised in control volumes by means of an unstructured mesh featuring 5.0×10^4 tetrahedral and hexahedral cells with a maximum cell skewness of 0.85 and local refinement around the position of the flame front. The grid was prepared using ANSYS Gambit and may be viewed in Fig. 6.1. The presence of

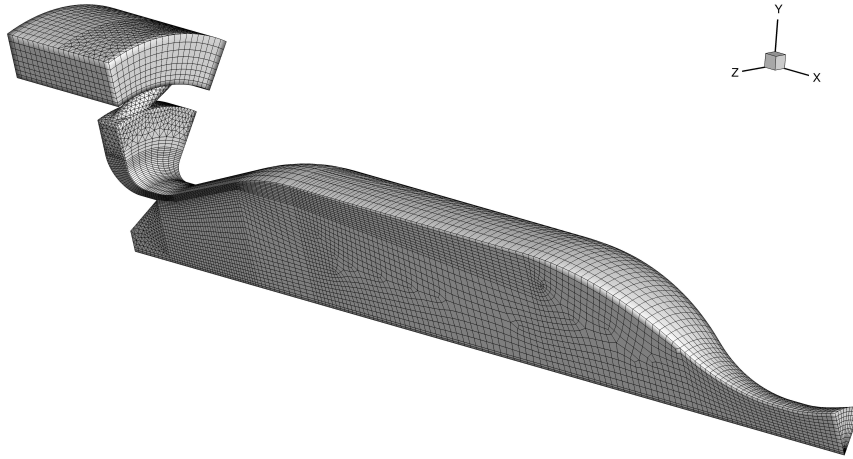


Figure 6.1: The unstructured grid featuring 5.0×10^4 tetrahedral and hexahedral cells.

swirl does not allow the use of symmetry boundary conditions as mass is transferred through these boundaries. Instead cyclic/periodic boundary conditions are applied where appropriate and standard wall functions are applied on all walls. The air is introduced at the back end of the plenum and is swirled as it enters the mixing

channel where the fuel is introduced. The outlet boundary condition is located downstream of the contraction. The velocity-pressure coupling is handled via a PISO [73] algorithm allowing a free number of correctors.

6.4.1 Initialisation

Before the PDF solver is introduced, the flow field is initialised using the two-scalar approach described in Section 4.3 — the joint β -bimodal presumed PDF approach. Similar to the work in Chapter 4, propagating laminar premixed flames ranging roughly from the lean to the rich limit ($0.30 \leq \phi \leq 4.00$), are computed to obtain primarily the laminar burning velocity (u_L), the temperature (T_b) and the viscosity (μ_b) of the burnt gases as a function of the mixture fraction. For these calculations the $C_1 - C_3$ mechanism of Leung & Lindstedt [102] was applied. In this case, however, the temperatures of the two streams are different which means that the reactant temperature (T_u) is also a function of equivalence ratio as shown in Fig. 6.2. This effect is taken into account in the laminar flame calculations and the result is shown in Figs 6.3-6.4.

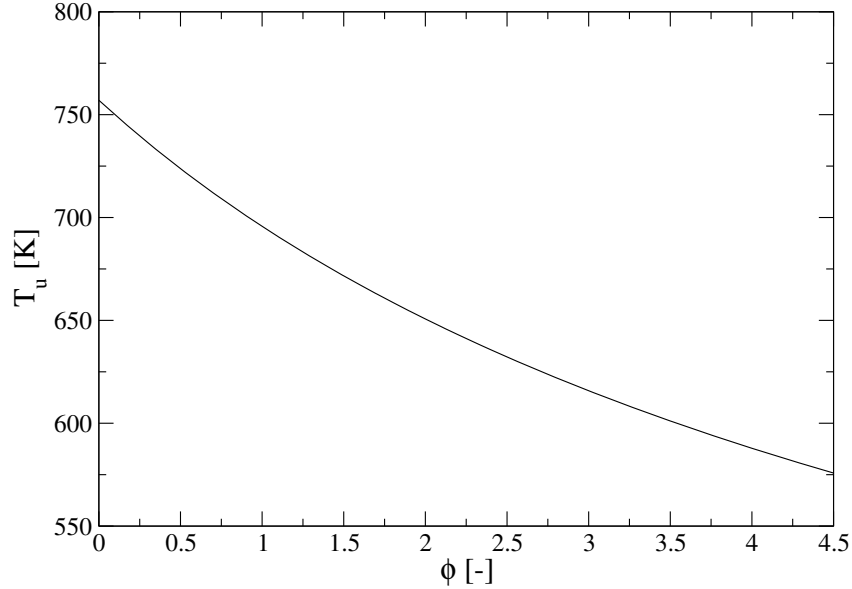


Figure 6.2: Fuel/air mixture temperature as a function of equivalence ratio at 23.8 bar, $T_O = 757$ K and $T_F = 300$ K (—).

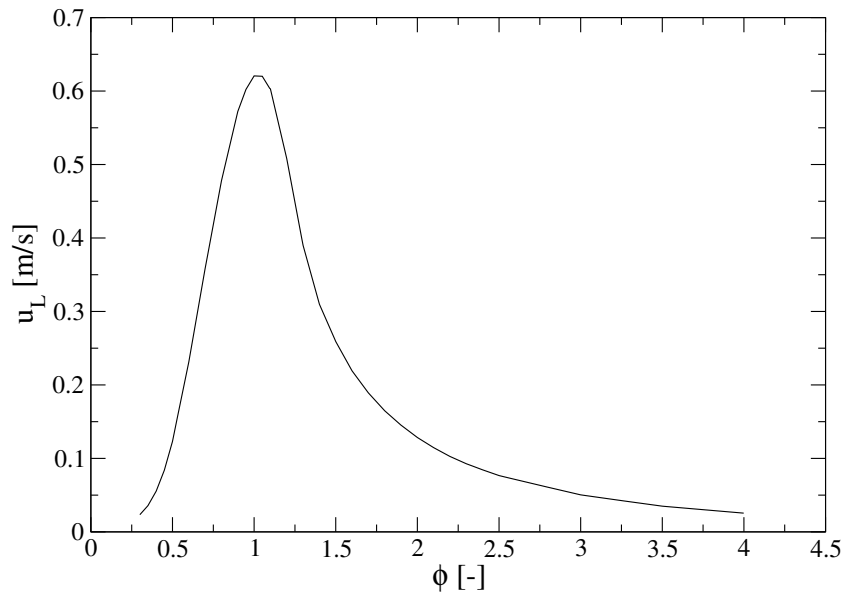


Figure 6.3: Laminar burning velocity as a function of equivalence ratio for CH_4 at 23.8 bar and temperatures according to Fig. 6.2 (—) [102].

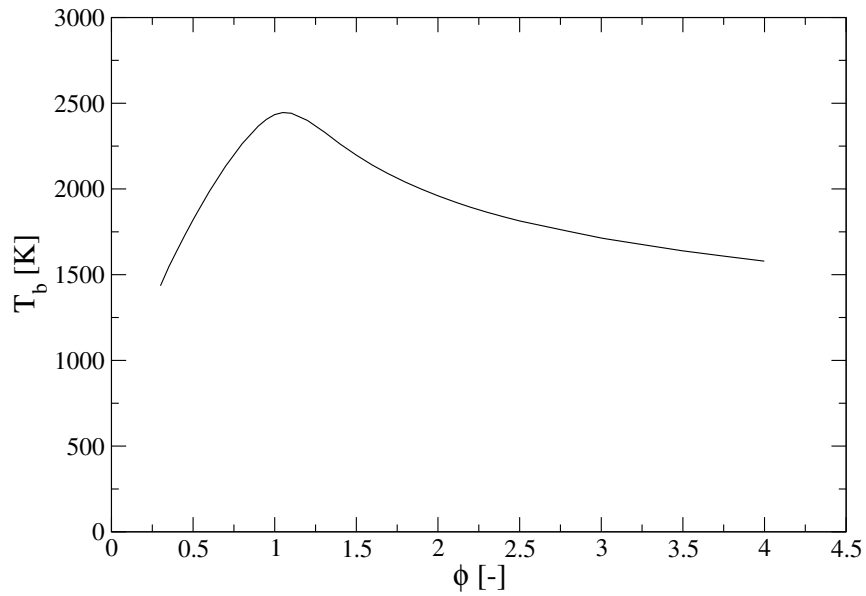


Figure 6.4: Adiabatic flame temperature as a function of equivalence ratio for CH_4 at 23.8 bar and temperatures according to Fig. 6.2 (—) [102].

For initialisation purposes, the governing equations are closed at the second moment level for the velocity field while a gradient diffusion closure is used for the scalar equations. The latter was considered appropriate as this closure level is consistent with the level of closure of the PDF solver. The Reynolds stress model of Jones & Musonge [83] was selected for this particular case as it has been validated for swirling flows [84]. The mean reaction rate is closed by the fractal model given by Eq. (1.57). A reaction rate constant of 4.0 was used to compensate for errors introduced by the gradient diffusion assumption [108] for scalar transport.

Spatial numerical diffusion is minimised through a blending scheme with the blending factor set to 0.5 for momentum and scalars and 0.0 for the turbulence equations. Temporal discretisation is approximated by implicit Euler expressions and the time step is limited to a local Courant number of 10 as a steady-state solution is expected. The rather large time step require the use of under-relaxation factors that limits the change of the variables during each time step. The under-relaxation factors were set to 0.50 for mixture fraction, reaction progress variable and turbulent kinetic energy dissipation, 0.25 for the remaining turbulence equations, 0.70 for momentum and 0.99 for pressure. The solution procedure is block structured featuring a momentum/scalar block and a turbulence block and the solver was forced to do a minimum of three iterations within each equation block. Furthermore, the numerical procedure features convergence adaptive time step control including step splitting on error. Convergence check is handled through four monitors, one for pressure, one for each block and one overall. The block convergence monitors allowed an error of 10^{-2} , the overall 10^{-3} and the pressure 10^{-6} .

6.4.2 The PDF solver

The steady state solution obtained with the PPDF closure is used as an initial field for the PDF solver. Each computational cell is allocated with 100 particles and particle values are initialised assuming a bimodal distribution followed by ten virtual PDF solver steps to smooth the first initial guess. After the ten virtual PDF solver steps, the PDF solver stops, and the field is initialised. The solution

procedure is structured so that the FV and the PDF solvers are completely decoupled but synchronised in time and the equations are solved in a fully transient manner. After particle initialisation, the density and viscosity fields are fed back to the block structured FV solver to update the velocity field during two FV steps. Within each FV step the momentum and turbulence blocks are forced to do a minimum of three iterations. The FV solver stops as the velocity field converges and particle values are updated during a free number of steps to ensure synchronisation in time.

The settings for the FV solver are maintained from the presumed PDF approach while the time step for the PDF solver is limited by requiring a turbulent time scale resolution of 0.03. A larger value resulted in an upstream propagation of the flame (i.e. an increase of the turbulent burning velocity). At time steps larger than a critical value the turbulent burning velocities increase exponentially as shown by Lindstedt & Város [115]. The particle values are ensemble averaged during eight PDF solver time steps and the moments are under-relaxed to ensure numerical stability. The under-relaxation factor was set to 0.3.

6.4.3 Boundary conditions

Prescribed values of mass flow of air and fuel are specified at separate inlet boundaries. The amount of fuel and air into the system corresponds to a global equivalence ratio of 1.4. The air and fuel temperatures are at 757 K and 300 K, respectively, and the operating pressure is set to 23.8 bar. Cyclic boundary conditions and standard wall functions are applied where appropriate. A small pressure drop is assumed over the domain and the pressure at the outlet is specified to 23.5 bar.

6.5 Results

In the current Section results of the PPDF and TPDF simulations are presented and compared. The same closure level applies for the velocity field while the representation of the scalar fields are different. In the presumed PDF approach only two scalars are solved, the mixture fraction and the reaction progress variable. The temperature is obtained from the look-up table. In the transported PDF approach, on the other hand, the mass fractions of species CH_4 , O_2 , H_2O , CO_2 , H_2 , CO , N_2 and temperature are solved scalars. In order to compare the scalar fields, temperature and mixture fraction are selected as representative scalars. The mixture fraction is not known directly from the transported PDF solution. From the species mass fractions it is, however, possible to compute the mixture fraction via Eq. (4.7). All results are time averaged.

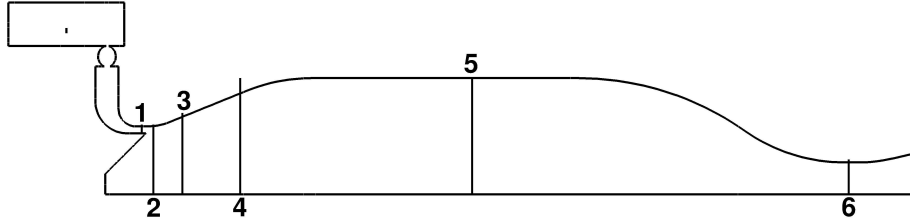


Figure 6.5: Locations of the various cross sections

Results are presented at six different axial locations as shown in Fig. 6.5. The first represents inlet conditions for the small combustor, while the following three cross-sections are representative for the location of the flame. The last two axial locations are representative for the combustion chamber where the first is roughly at the backward stagnation point and the last position is at the throat. The radial profiles are normalised by a characteristic radius (R_0). Contour plots of the TPDF simulation of the near field aerodynamics are shown in Figs. 6.6-6.9 and of the predicted species mass fractions in Figs. 6.10-6.15.

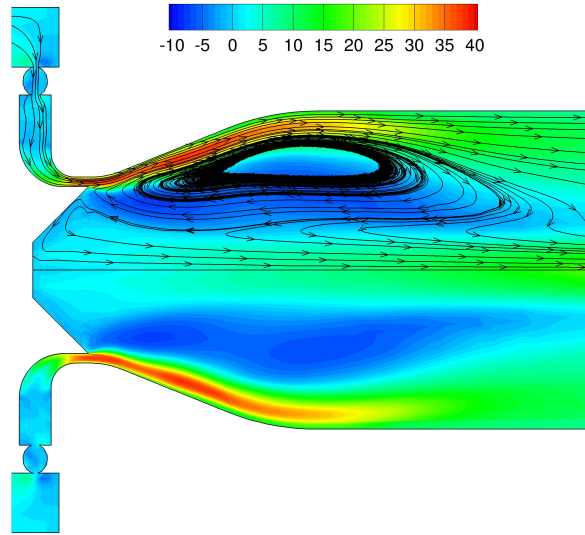


Figure 6.6: Computed axial velocity using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.

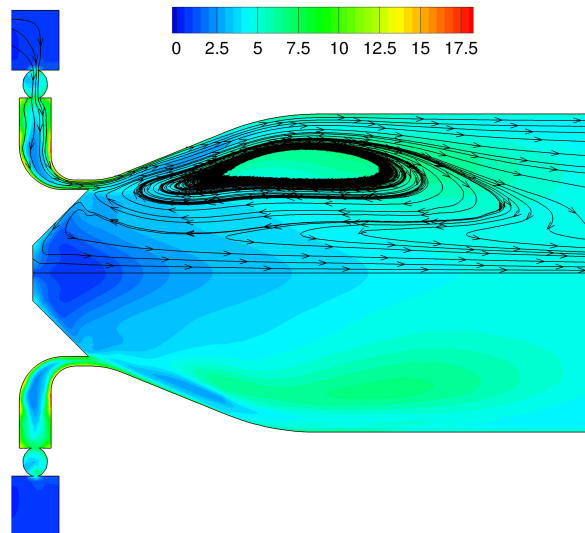


Figure 6.7: Computed turbulence intensity using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.

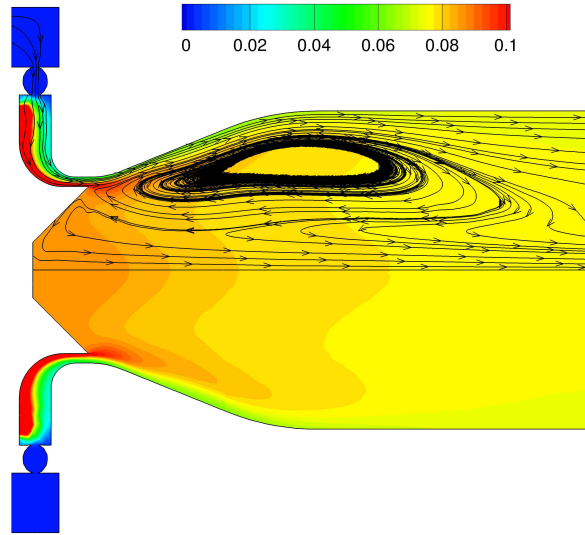


Figure 6.8: Computed mixture fraction using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.

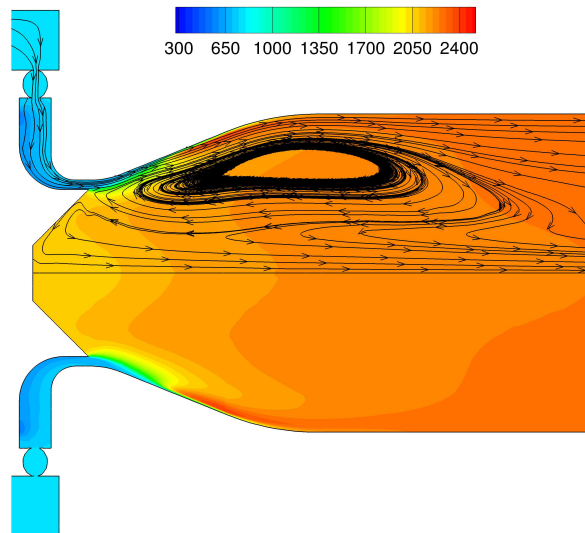


Figure 6.9: Computed temperature using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.

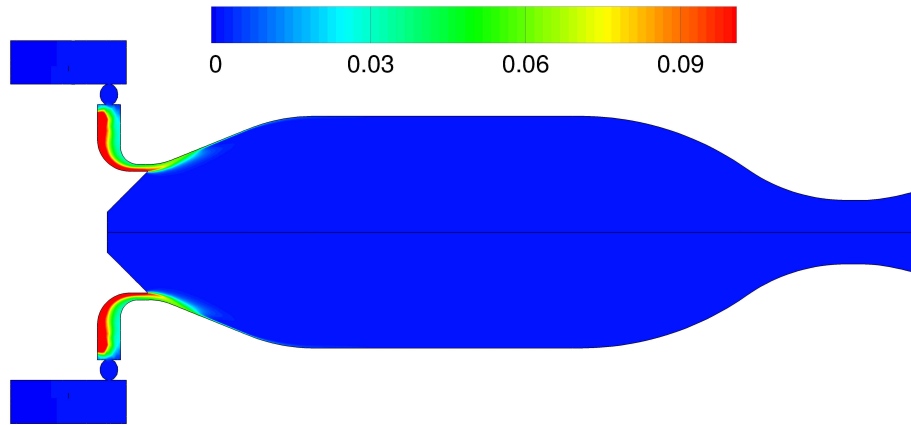


Figure 6.10: Computed mass fractions of CH_4 using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.

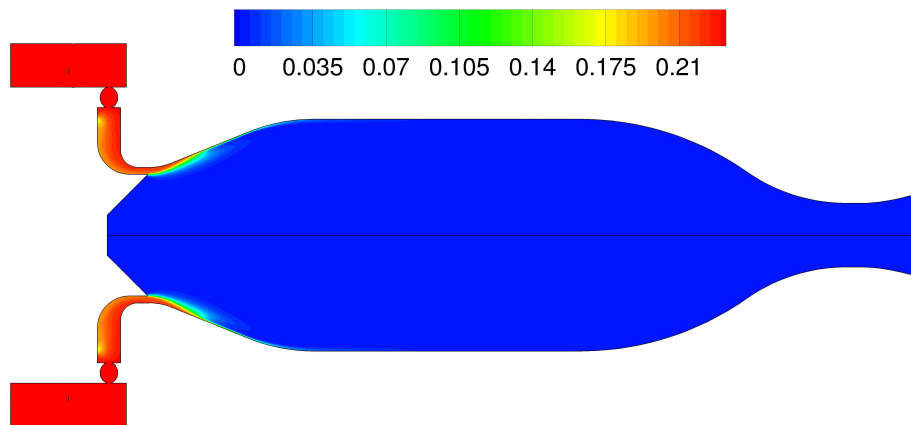


Figure 6.11: Computed mass fractions of O_2 using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.

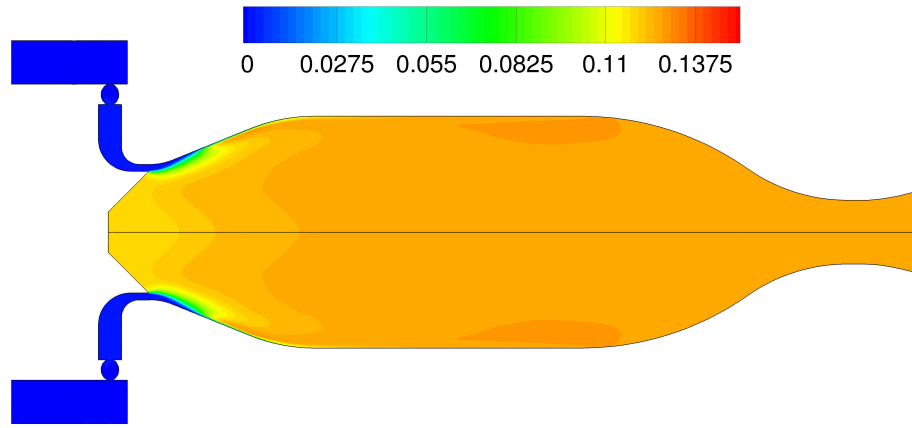


Figure 6.12: Computed mass fractions of H_2O using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.

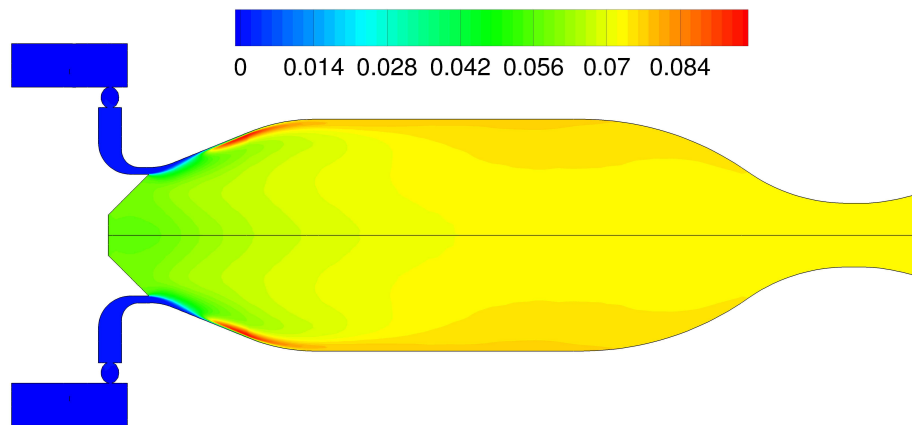


Figure 6.13: Computed mass fractions of CO_2 using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.

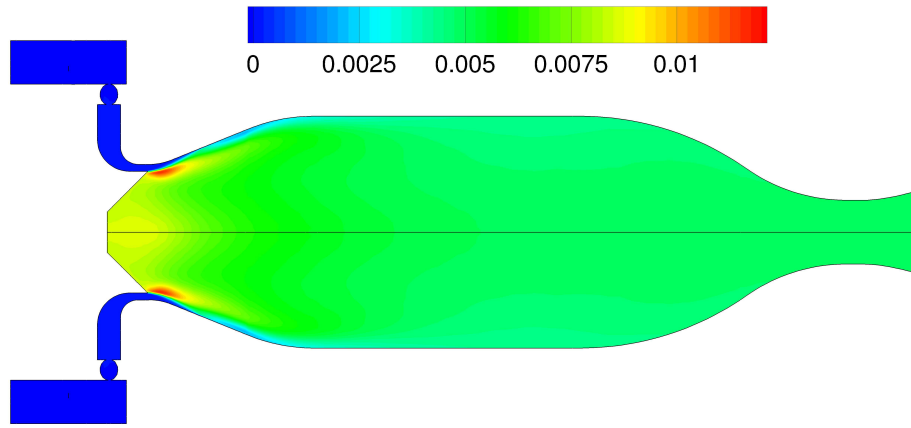


Figure 6.14: Computed mass fractions of H_2 using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.

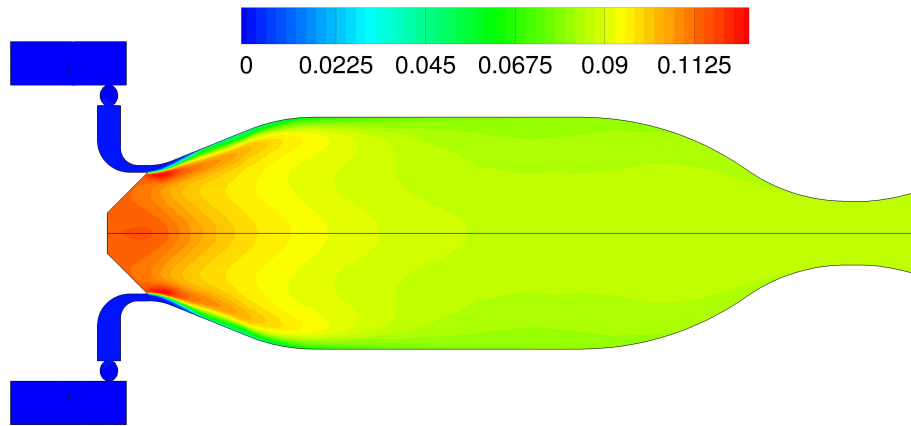


Figure 6.15: Computed mass fractions of CO using the TPDF approach, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K.

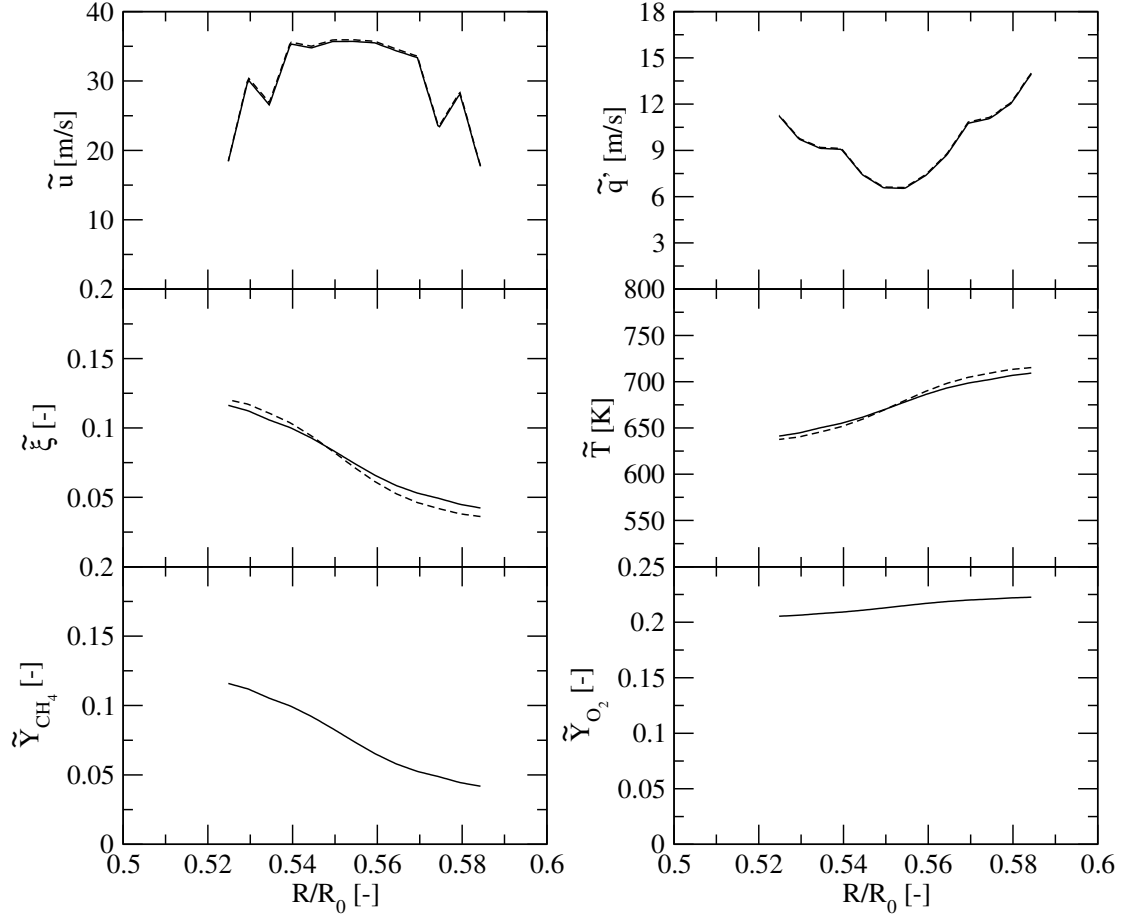


Figure 6.16: Predictions at the first cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. Top left (TL): Mean axial velocity, top right (TR): Turbulence intensity, middle left (ML): Mixture fraction, middle right (MR): Temperature, bottom left (BL): Mass fraction of CH_4 , bottom right (BR): Mass fraction of O_2 . Presumed (---) and transported (—) PDF.

In Fig. 6.16, profiles of mean velocity, turbulence intensity, mixture fraction, temperature and mass fractions of CH_4 and O_2 entering the small combustion chamber are shown. The mean velocity and turbulence intensity profiles indicate a rather poor grid resolution in this region. All scalar profiles, on the other hand, are smooth. Small differences in the mixing patterns are noticeable between the PPDF and TPDF closures. The mixture fraction profile of the PPDF closure has sharper gradients than the TPDF profile. This finding is not surprising as the current TPDF approach is first order accurate only. Figs. 6.17 and 6.18 show predictions at the second cross-section that represents the first location across the flame front. Small

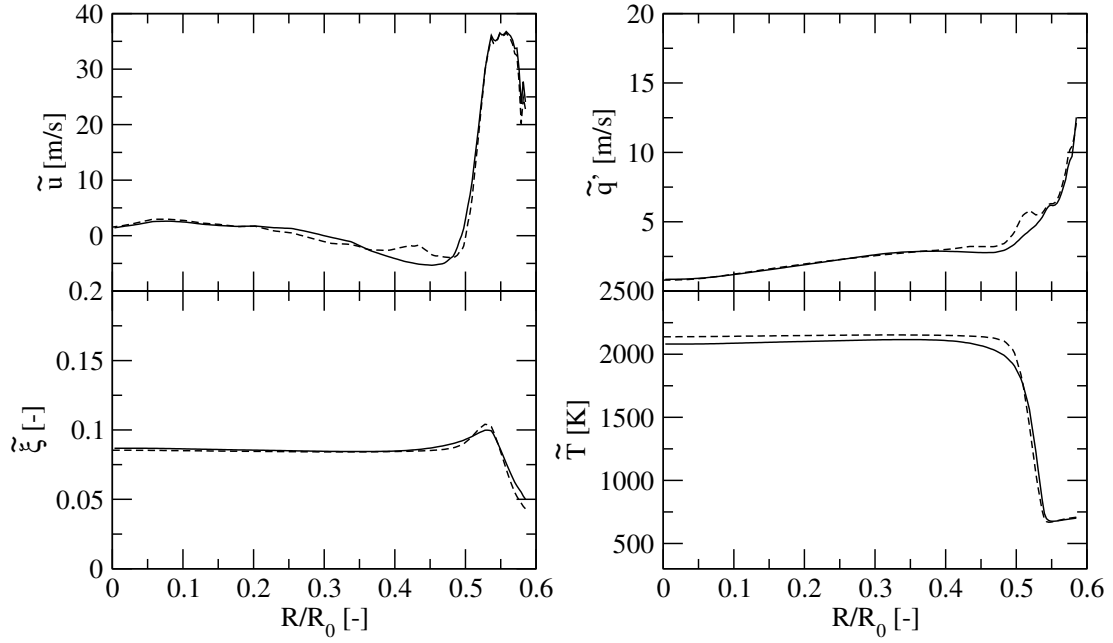


Figure 6.17: Predictions at the second cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. TL: Mean axial velocity, TR: Turbulence intensity, BL: Mixture fraction, BR: Temperature. Presumed (---) and transported (—) PDF.

differences may be noticed in the velocity fields at R/R_0 larger than 0.35. At this location the axial velocity becomes negative due to the central recirculation zone formed by the swirling flow and the TPDF solution indicates a slightly stronger recirculation zone. The mixture fraction profiles are almost identical with slightly sharper gradients close to the location of the flame front for the PPDF solution while the temperature rise occurs at the same position in both cases. At the back end of the flame, the maximum temperature is reached immediately for the PPDF solution while the kinetically controlled TPDF solution has a longer tail. From the predicted species mass fraction profiles in Fig. 6.18 it is clear that reaction (i) dominates over the competing fuel breakdown reaction (ii). Both reactions (i) and (ii) produces CO and H_2 which peaks at around $R/R_0 = 0.5$ where the majority of the fuel is consumed. A small increase can be seen in CO and H_2 towards the centreline while CO_2 and H_2O decreases. This is an indication that reactions (iii) and (iv) are reversed in this region. The velocity and scalar fields shown in Fig. 6.19 have the same tendency as the previous cross-section. There are, however, differences in the flame

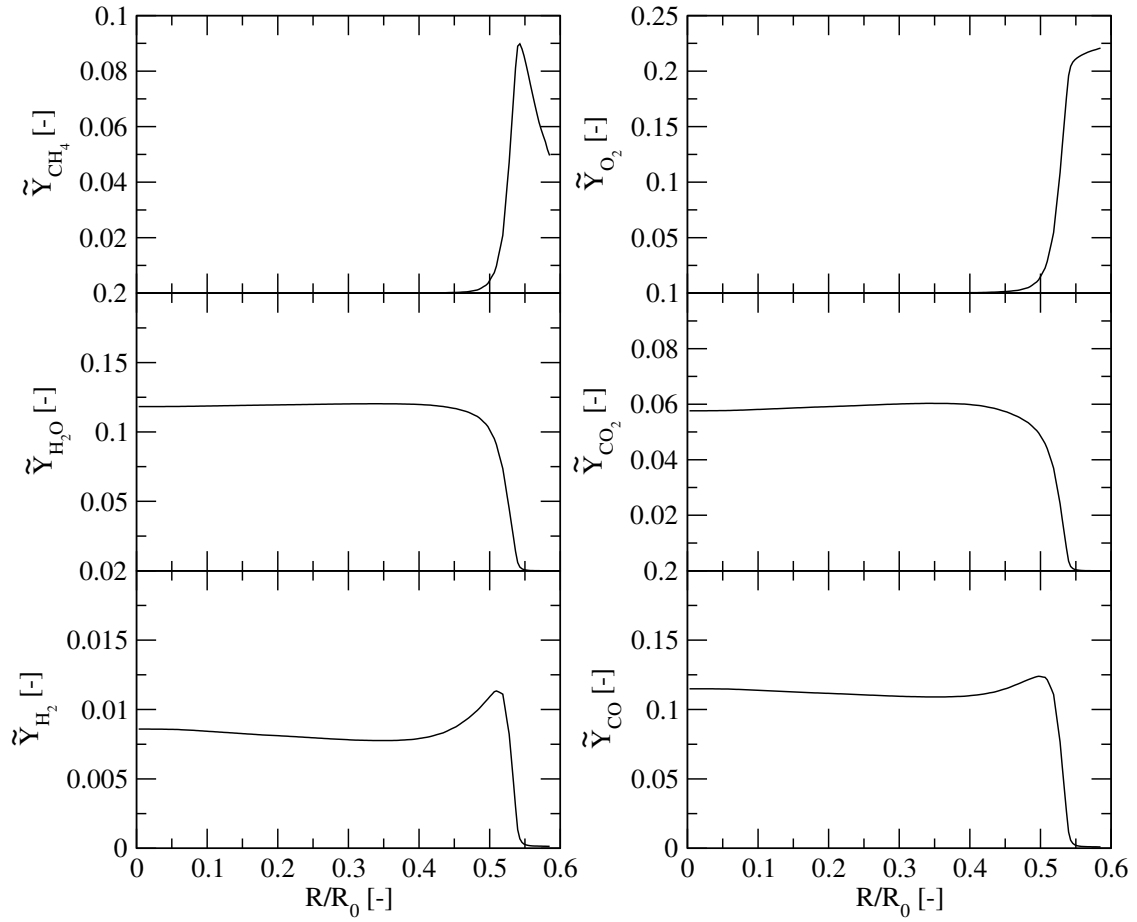


Figure 6.18: Predictions at the second cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. Mass fractions of TL: CH_4 , TR: O_2 , ML: H_2O , MR: CO_2 , BL: H_2 , BR: CO . Transported PDF (—).

structure towards the wall between the PPDF and TPDF solutions. The former has a local temperature peak close to the wall while the reaction rates goes smoothly to zero for the latter. The radial profiles of species mass fractions in Fig. 6.20 show an identical behaviour compared to the ones shown in Fig 6.18 but the CO and H_2 profiles are a bit smoother. At the fourth cross-section, at $R/R_0 > 0.6$, differences in the predicted mixture fraction profiles can be noticed as shown in Fig. 6.21. This difference affects the computed temperature and shifts the peak of the expansion to a larger radius for the PPDF as shown in the predictions of the velocity field. The species predictions, shown in Fig. 6.22, indicates that the back end of the flame (in axial direction) is approached as the majority of the reactants are consumed.

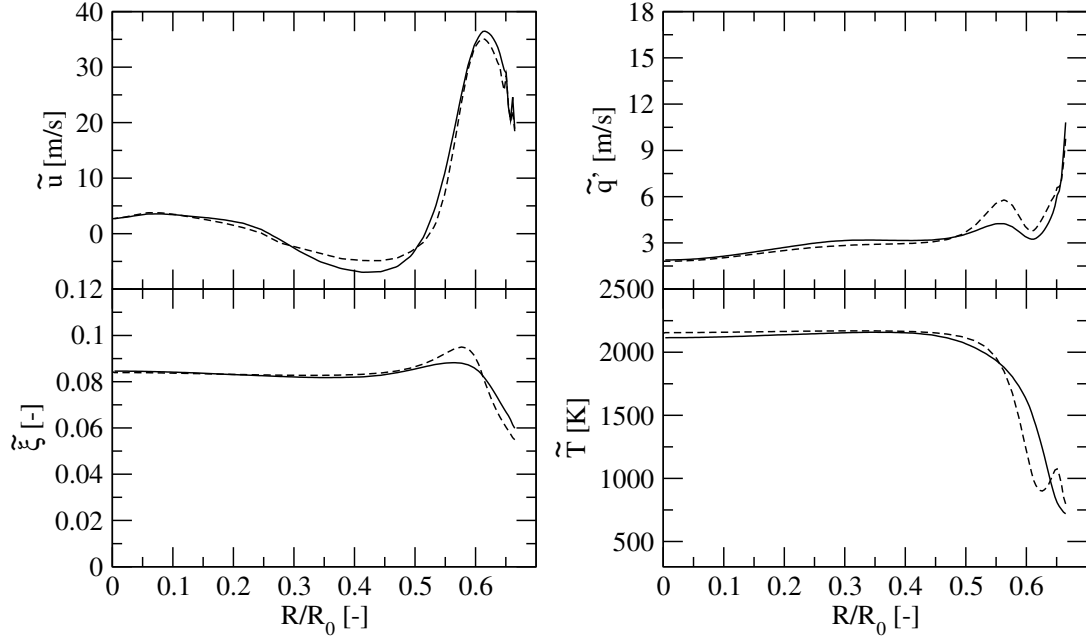


Figure 6.19: Predictions at the third cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. TL: Mean axial velocity, TR: Turbulence intensity, BL: Mixture fraction, BR: Temperature. Presumed (---) and transported (—) PDF.

At $R/R_0 > 0.8$, a distinct CO_2 peak appears due to the high temperature in this region.

None of the cross-sections across the flame gives a clear indication of a significant difference in the turbulent burning velocities from the PPDF and TPDF solutions. The fractal based mean reaction rate closure given by Eq. (1.57) has been applied successfully in previous studies [129] at comparable conditions. In Chapter 5 it was shown that the turbulent burning velocity is under-predicted for fuels with high Zeldovich numbers, such as methane. The methane flames presented in Chapter 5 range from the flamelet regime to the distributed reaction zones regime as shown in the Borghi diagram in Fig. 1.1. From the computational results in the current study it is possible to estimate the Da and the Ka numbers and thereby the combustion regime. From Fig. 6.3 the unstrained laminar burning velocity is known. The current burner is operated at equivalence ratio of 1.4 and at the present conditions, $u_L^0 = 0.31$ m/s and $\delta_L = 0.1$ mm. From the TPDF solution, the turbulence intensity and the turbulent integral length scale may be obtained. At $\tilde{c} = 0.5$, $l_T = 0.45$ mm

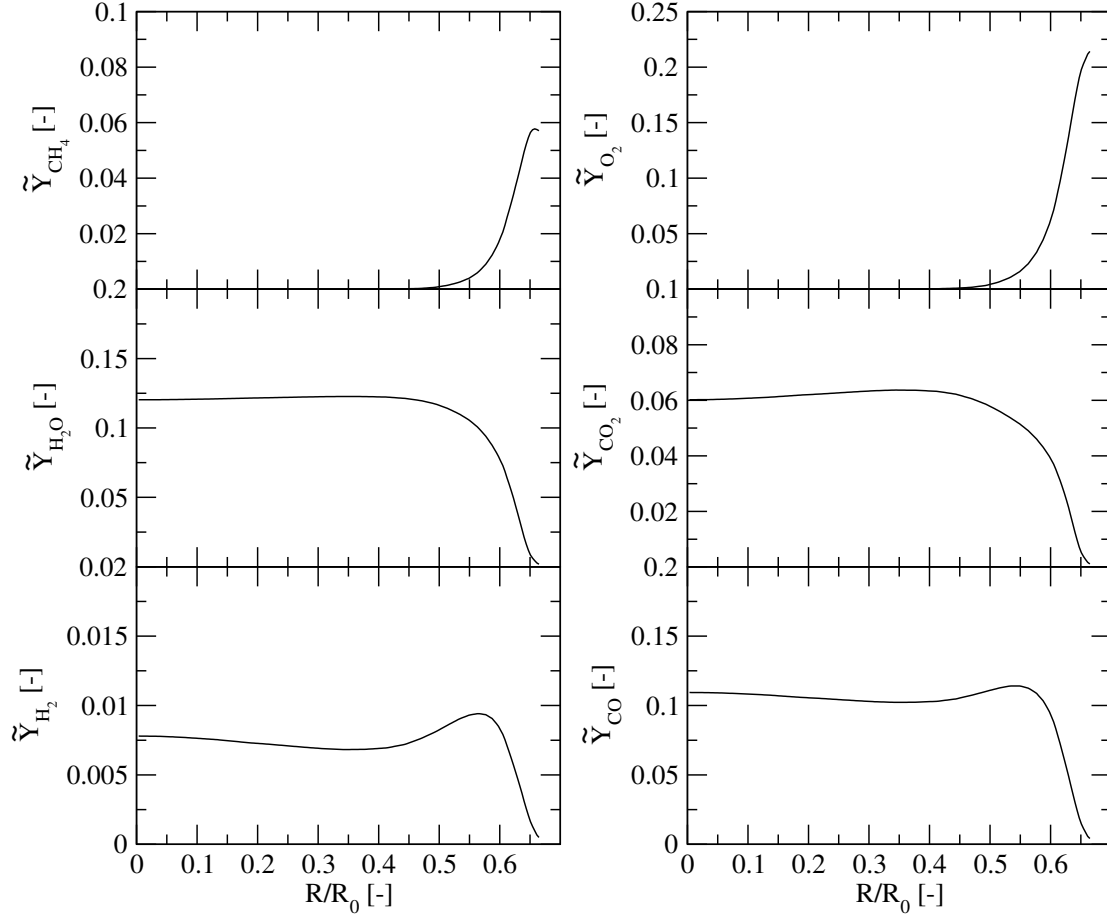


Figure 6.20: Predictions at the third cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. Mass fractions of TL: CH_4 , TR: O_2 , ML: H_2O , MR: CO_2 , BL: H_2 , BR: CO . Transported PDF (—).

and $q' = 3.4$ m/s giving $Da = 0.41$ and $Ka = 17.1$ from Eqs. (1.6)-(1.7). The current Da and Ka numbers indicates that at the present conditions the combustion regime is the well stirred reactor regime and the reaction rate is solely controlled by chemical kinetics. It is thus likely that the impact of molecular transport terms are small in this regime.

The predicted axial velocity at cross-section five, roughly indicates the position of the backward stagnation point, as shown in Fig. 6.23. The predicted mixture fraction and temperature profiles, as well as species mass fractions shown in Fig. 6.24, are almost flat at this cross-section indicating that combustion is completed. The mean velocity profiles shown in Fig. 6.25 require further comments, the profiles

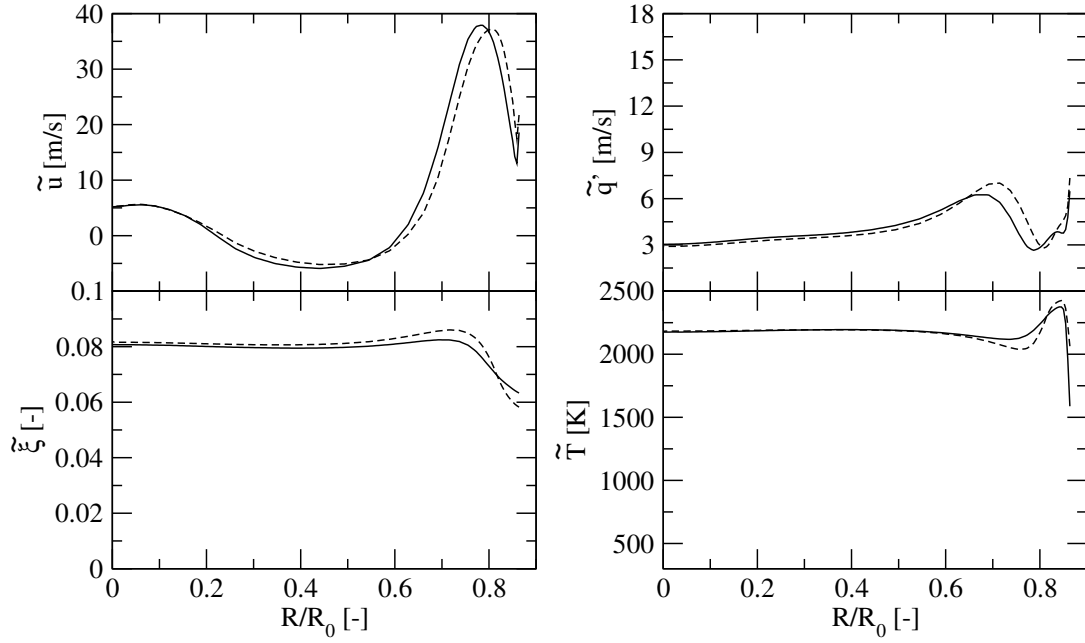


Figure 6.21: Predictions at the fourth cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. TL: Mean axial velocity, TR: Turbulence intensity, BL: Mixture fraction, BR: Temperature. Presumed (---) and transported (—) PDF.

are almost identical except the actual level which differs by the order of 7%. In order for continuity to be satisfied the density fields between the presumed and the transported PDF solutions must be different. The predicted density fields reveals a difference of the same order as the velocity fields. The temperature predictions does not explain the differences in the density fields as temperatures are within 10 K. In the presumed PDF approach only two scalars are solved and the thermochemistry is in principle represented by a global reaction step given by Eq. (1.1). In both cases, the density is obtained from Eq. (1.28) which is a function of the molecular weight (M). In the presumed PDF approach the molecular weight is obtained using five species whereas in the transported PDF approach seven species are taken into account and as a consequence, small differences in the density fields are inevitable. All computed scalar profiles are flat at this location.

In Fig. 6.27 traces of the axial velocity close to the flame front at one location along the first cross section are shown for the presumed and the transported PDF approach. The presumed PDF approach has clearly converged to steady state while

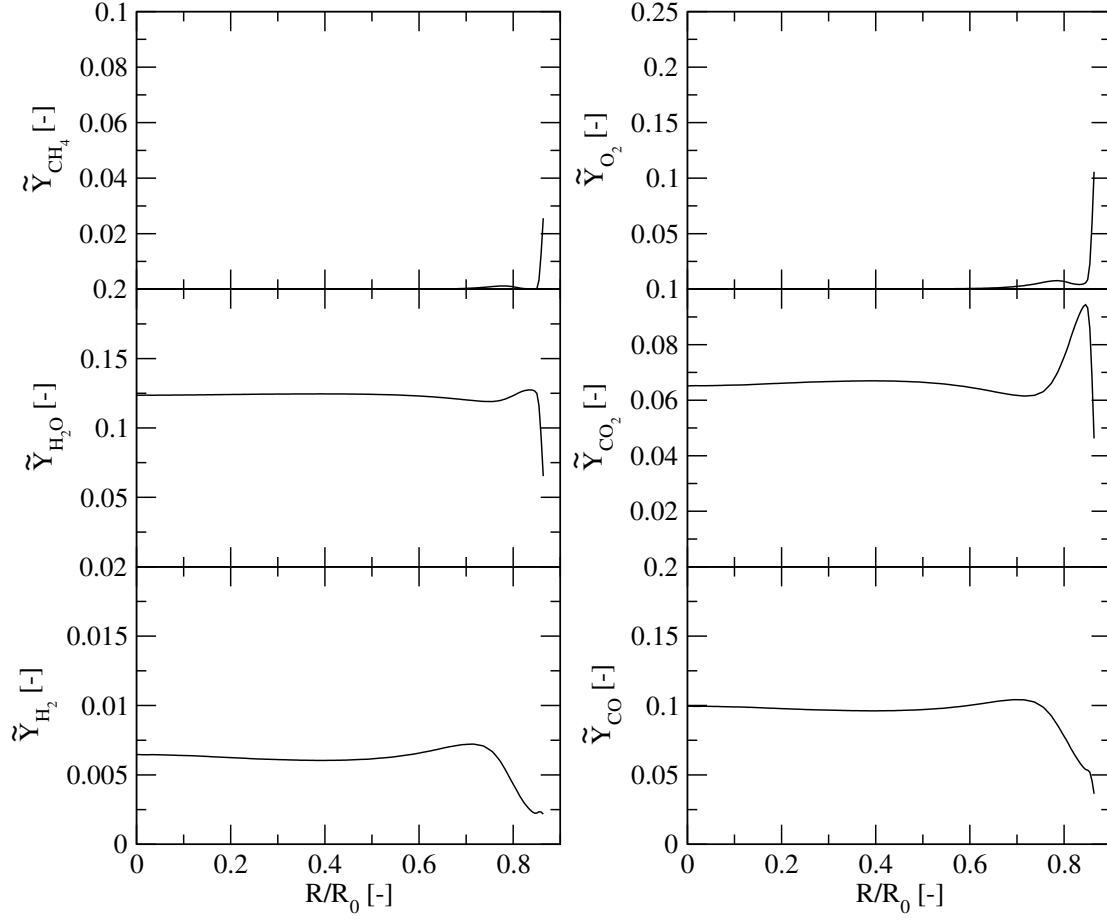


Figure 6.22: Predictions at the fourth cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. Mass fractions of TL: CH_4 , TR: O_2 , ML: H_2O , MR: CO_2 , BL: H_2 , BR: CO . Transported PDF (—).

the transported PDF solution indicates a potential transient nature of this flow. The time has been normalised by the residence time (t_{res}) of the device. The total simulation time for the presumed PDF approach is of the order of four residence times while the transported PDF approach is limited to close to two residence times. A fast fourier transform (fft) is performed to find the dominant frequencies from the trace of the axial velocity in the transported PDF solution. A number of frequencies are obtained ranging roughly from 800 - 1100 Hz. An extended simulation time is required to capture lower frequencies. A dominant peak at around 70 kHz can also be seen in the figure. The latter frequency is not physical, rather a consequence of the switch (numerically induced) between the FV and PDF solvers, and is well

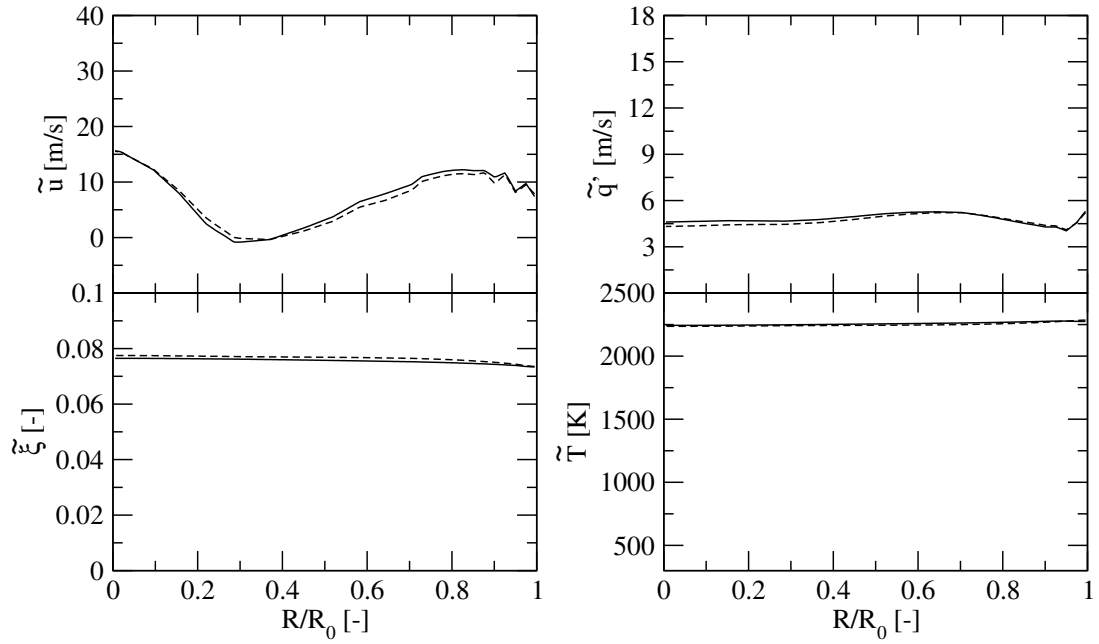


Figure 6.23: Predictions at the fifth cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. TL: Mean axial velocity, TR: Turbulence intensity, BL: Mixture fraction, BR: Temperature. Presumed (---) and transported (—) PDF.

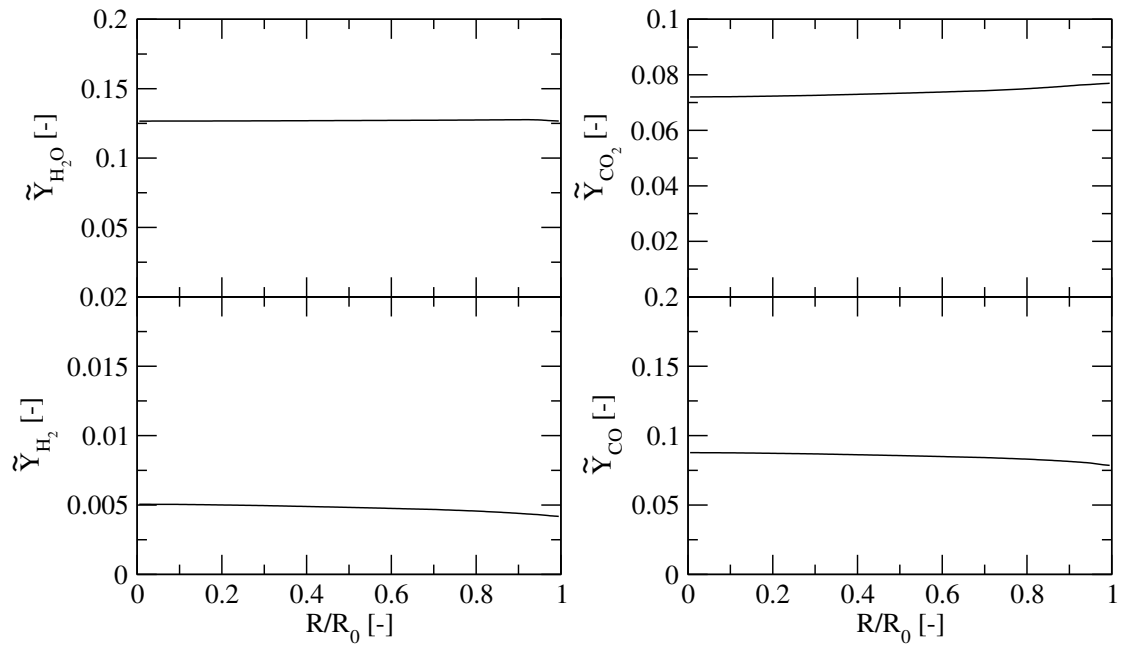


Figure 6.24: Predictions at the fifth cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. Mass fractions of TL: H_2O , TR: CO_2 , BL: H_2 , BR: CO . Transported PDF (—).

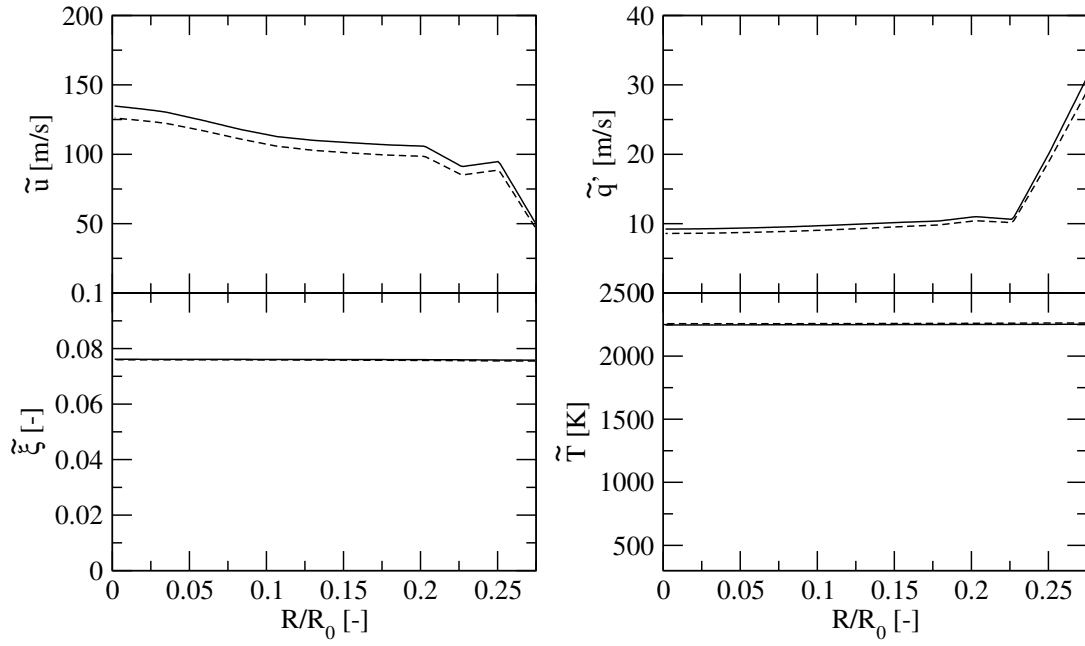


Figure 6.25: Predictions at the sixth cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. TL: Mean axial velocity, TR: Turbulence intensity, BL: Mixture fraction, BR: Temperature. Presumed (- -) and transported (—) PDF.

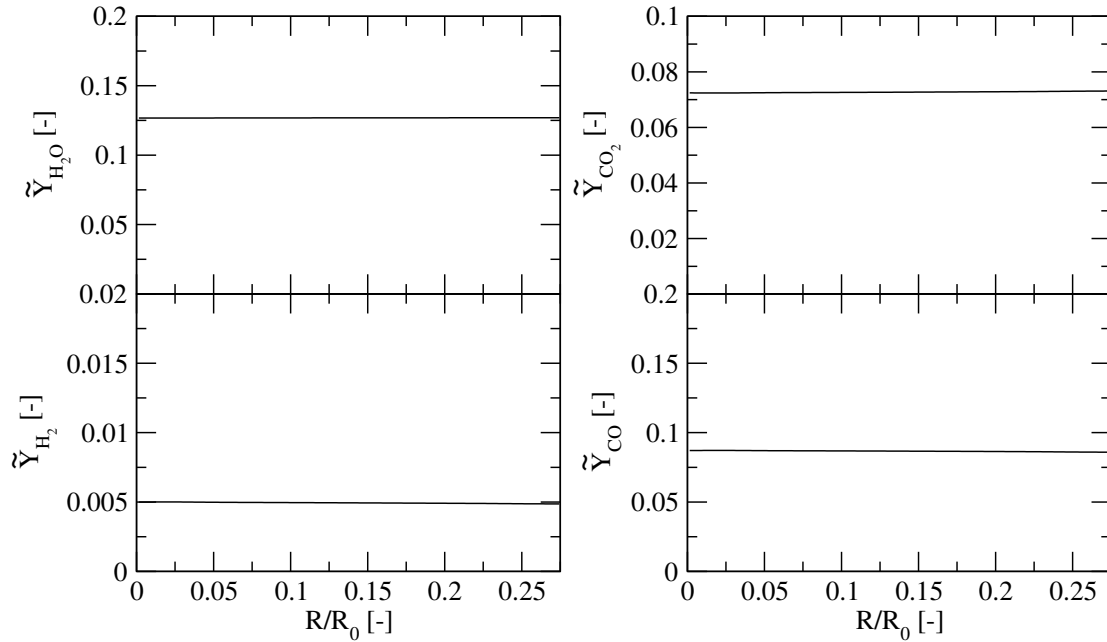


Figure 6.26: Predictions at the sixth cross-section, 23.8 bar, $T_O = 757$ K and $T_F = 300$ K. Mass fractions of TL: H_2O , TR: CO_2 , BL: H_2 , BR: CO . Transported PDF (—).

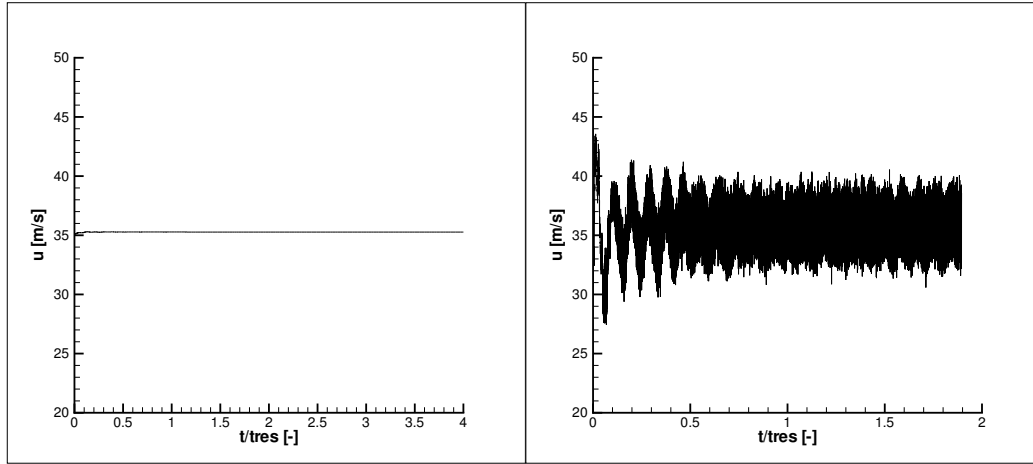


Figure 6.27: Time trace of the axial velocity at the swirler channel exit, left: PPDF, right: TPDF.

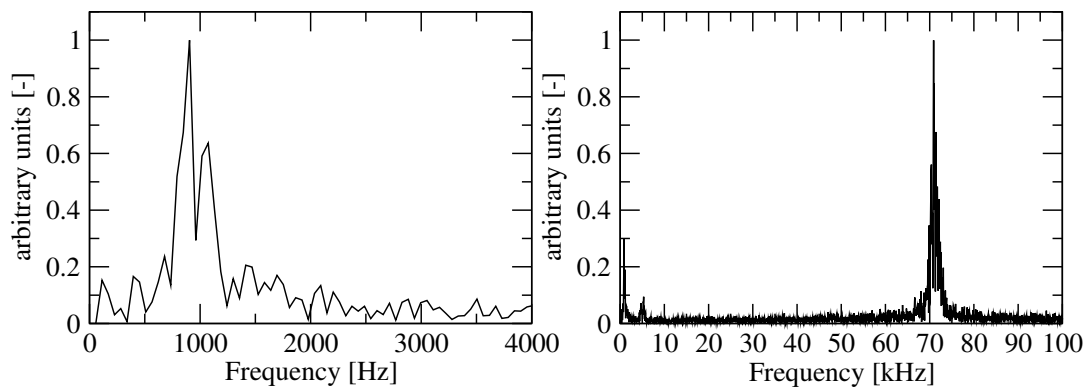


Figure 6.28: Dominant frequencies using the TPDF approach based on the axial velocity trace at the swirler channel exit. Left: Frequency peaks ranging roughly from 800 - 1100 Hz. Right: Unphysical frequency at around 70 kHz obtained as a result of the solution strategy.

separated from any physical scales.

6.6 Summary

A small industrial gas turbine burner was computed at realistic conditions using the joint β -bimodal presumed PDF approach and the node-based joint scalar transported PDF approach described in previous chapters. In both cases, the JM second moment closure is applied for the velocity field. The computational domain is represented by a 45° sector and the geometry is discretised using an unstructured mesh featuring 5.0×10^4 computational cells. The flame in this case is swirl-stabilised and may be characterised as partially premixed. In the case of a presumed PDF approach, a gradient diffusion type model, consistent with the level of closure for the transported PDF approach, is applied to obtain closure for the unknown turbulent scalar flux term. Again, the algebraic fractal-based flame surface density model is used to close the mean reaction rate. In the case of a transported PDF approach, closure for the molecular mixing term is obtained using Modified Curl's model and the chemistry is represented by a four-step global reaction scheme featuring seven solved species. The presumed PDF solution has dual purposes, to initialise the flow field for the PDF solver and to serve as a reference solution to compare the transported PDF predictions with due to lack of experimental data at these conditions. Overall, the predictions are very similar using both methodologies. Of special interest is the point of flame stabilisation in the two cases as the calculations in previous chapters indicate that the computed turbulent burning velocity is rather low when the transported PDF approach is applied, especially for cases approaching the high Da number limit. In this particular case there are, however, no such indications as the computed point of stabilisation are very similar in the two cases. A possible explanation is that the current case is in the well stirred reactor regime in the Borghi diagram — a regime that is well separated from high Da numbers. The presumed PDF approach converges to steady state while the transported PDF approach indicates a potential transient nature of this flow as a range of frequencies are obtained.

The simulation time is, however, limited and comparison with experimental data is required to confirm such findings.

Chapter 7

Summary and concluding remarks

The present thesis constitutes a modelling study of turbulent premixed or partially premixed flames over a wide range of conditions using state of the art combustion and turbulence closures. The cases studied are ranging from simple one-dimensional propagating premixed flames to three-dimensional flames stabilised by swirl or stagnating turbulence. Each case is characterised in terms of the Borghi diagram and the flames are ranging from the flamelet to the well stirred reactor regime. Some important conclusions are drawn regarding the applicability of closures in different combustion regimes. The models applied range from eddy viscosity based closures to full second moment closures coupled with a presumed PDF approach for scalar statistics to the joint scalar transported PDF approach coupled with a second moment closure for the velocity field.

7.1 The present contributions and conclusions

The isothermal and reacting opposed flows featuring fractal-generated turbulence of Geipel [52] and Geipel et al. [53] have been studied numerically using different classes of models. The case is characterised by a nozzle separation of one nozzle diameter and in the reacting case, a methane-air mixture of equivalence ratio 0.9. The computational domain is represented by a 90° sector of one of the nozzles and the geometry is discretised using an unstructured hexahedral mesh featuring 3.5×10^5

computational cells. In the isothermal case, the standard $k - \epsilon$ model along with the transport equation based Reynolds stress models of Haworth & Pope [66, 67] (HP) and Jones & Musonge [83] (JM) are applied and compared. In contrast to previous studies (cf. [112, 121]), where the turbulence peak at the stagnation point were significantly over-predicted, the standard $k - \epsilon$ model performs comparatively well in this case. Possible explanations are the significant increase in turbulent Reynolds number as a result of the fractal-generated turbulence and the reduction in strain along the centreline due to the largest fractal cross in the fractal plates. Predictions along the stagnation plane and at the nozzle exit are also in a close agreement with the experimental data. Both Reynolds stress models have a slight tendency to over-predict the axial velocity fluctuation at the stagnation point. All turbulence models tested are predicting a more narrow turbulence peak along the burner centreline compared to the experimental data. The width in the experiments is a result of stagnation point movement [53] which is not captured in the numerical approach due to the use of symmetry boundary conditions. The predictions at the nozzle exit are similar for all models tested. Overall the predictions are in a reasonable agreement with the experimental data for both the HP and the JM models but the HP model is in general closer to the experimentally derived values. The HP model is therefore the only Reynolds stress model considered for the reacting opposed case.

In the reacting opposed case, the standard $k - \epsilon$ and the HP models are applied to close the unknown Reynolds stresses. Both models are applied together with a gradient diffusion model for the unknown turbulent scalar flux term coupled with a joint β -bimodal presumed PDF approach. The HP model is also combined with a consistent [142] transport equation based closure for the turbulent scalar flux term, with or without additional acceleration redistribution/scrambling models [108]. In all these cases, the mean reaction rate is closed by the algebraic fractal-based flame surface density model of Lindstedt & Város [108]. Furthermore, the HP model is combined with the node-based Eulerian joint scalar transported PDF approach. In this case, the molecular mixing term is closed by Modified Curl's Model [41, 77] and the chemistry is represented by the global reaction scheme for hydrocarbon

combustion of Jones & Lindstedt [81, 82] featuring four reactions and seven solved species. The experimental data in the reacting case is arguably conventionally averaged while the solved quantities are represented by Favre averages. The latter are therefore transformed into conventional averages using relations from the BML theory. Both the standard $k - \epsilon$ model and the HP model fails to predict the reacting opposed case when combined with a gradient diffusion model. In essence, the predicted turbulent flame is too thin resulting in deviations in the mean axial velocity profile along the burner centreline and, as a consequence, deviations are observed in the turbulence profiles. The predictions along the stagnation plane are in a reasonable agreement for both models. A significant improvement is achieved using the full second moment closure without additional acceleration redistribution/scrambling models. The computed flame thickness and the reaction progress variable variance are in a very close agreement with the experimental data. As a result, the computed mean axial velocity profile and the axial velocity fluctuation along the burner centreline are reasonably well predicted with properties along the stagnation plane. The addition of acceleration redistribution/scrambling models results in a slight over-prediction of the turbulent flame thickness. The axial velocity fluctuation at the stagnation point is also over-predicted while the predicted turbulent kinetic energy is approaching the measured value in contrast to the other models. None of the models are able to predict the radial velocity fluctuation along the burner centreline. Surprisingly, the experimental data suggests a higher radial than axial velocity fluctuation at the stagnation point. In general, along the burner centreline, the flow leaving the nozzle is purely axial and turbulence is produced in the axial direction due to strain. The turbulent kinetic energy is unaltered but part of the energy is redistributed to the radial component. One possible explanation is stagnation point movement [53] in the radial direction in the experiments and this movement is not captured in the simulations as the position of the stagnation point is dictated by the symmetry boundary conditions. The application of the node-based Eulerian joint scalar transported PDF approach combined with the HP model indicates an under-prediction of the turbulent burning velocity as the peak value of

the reaction progress variable is lower than the experimentally derived values and values obtained with the algebraic fractal-based flame surface density model.

The ability of the transported PDF approach to predict turbulent burning velocities is explored in detail for a wide range of conditions and fuel/air mixtures as this matter is of great importance in the development of practical devices as the propagation speed will dictate the flame stabilisation point. The computed values are compared against the experimental data of Abdel-Gayed et al. [1] for lean ($\phi = 0.88$) and stoichiometric CH_4 , stoichiometric C_2H_6 as well as the fuel rich ($\phi = 1.6$) H_2 flames. Turbulent burning velocities are computed for a wide range of Damköhler numbers using detailed or systematically reduced chemistry. It is shown that the standard expression for the scalar dissipation rate results in a qualitatively incorrect behaviour in terms of the turbulent burning velocity scaling with respect to turbulence intensity variations. The turbulent burning velocity scales linearly with turbulence intensities in contrast to the experimental data. The solution at high Re numbers approaches the correct value for the hydrogen flames. The multi-scale scalar dissipation rate closure proposed by Lindstedt & Város [115] that accounts for the influence of the Da number is extended in a simple manner to include Le number effects in order to explore the sensitivity of predictions. The extended closure results in a significant improvement in terms of the scaling of turbulent burning velocities while the computed value is lower than the experimentally derived value for the hydrocarbon fuels, especially for methane. Extracted turbulent reaction rates indicates a rather low flame front activity compared to the reaction progress variable variance expression from the BML theory. The low flame front activity is traced to the mixing model and the impact of molecular transport on the turbulent burning velocity is explored and analysed in terms of the Zeldovich (β) number through the inclusion of an explicit analytical formulation. The results suggest that fuels with Zeldovich numbers not greater than ethane can be computed directly with the current methodology and that a derived additional analytic term that explicitly takes into account the impact of molecular transport at the leading edge of the flame can alleviate difficulties encountered for less reactive fuels. Also, computed turbulent

reaction rates of methane are compared with the experimental data of Cheng & Shepherd [29] and Lawn & Schefer [101] and a significant improvement is achieved with the explicit correction term.

The node-based Eulerian joint scalar transported PDF approach is applied to model a swirl-stabilised fuel-rich partially premixed methane flame in an industrial gas turbine burner at realistic operating conditions. The chemistry is represented by the global reaction scheme for hydrocarbon combustion of Jones & Lindstedt [81, 82] featuring four reactions and seven solved species and the unknown molecular mixing term is closed by Modified Curl's Model in its standard form. The JM [83] model is used to obtain closure for the unknown Reynolds stresses as this model have been applied to swirling flows in previous studies [84]. The computational domain is represented by a 45° sector with cyclic boundary conditions and the geometry is discretised using an unstructured mesh featuring 5.0×10^4 computational cells. The current case is expected to be in the distributed reaction zones or the well stirred reactor regime. In the latter regime, all scales of turbulence can enter the inner structure of the flame and all chemical time scales are longer than the relevant turbulent time scale and the overall reaction rate is solely controlled by the chemical kinetics. It is thus expected that the influence of additional explicit correction term is small in this regime. To initialise the flow field, the JM model is combined with a gradient diffusion model coupled with the joint β -bimodal presumed PDF approach for scalar statistics. The initial solution also serves as a reference to compare the transported PDF predictions with, due to the lack of experimental data at these conditions. In this case, no major differences in the point of flame stabilisation can be observed and it is shown that the case is in the well stirred reactor regime. Furthermore, the solutions obtained with the two approaches are very similar in general but the presumed PDF approach converges to steady state while the transported PDF approach indicates a potential transient nature of this flow as a range of frequencies are obtained.

7.2 Suggestions for future work

- The experimental data for the isothermal and reacting opposed flows used in the current study indicate a potential stagnation point movement. The stagnation point movement is a possible explanation for the high radial turbulence intensity peak which is not captured with the use of symmetry boundary conditions. It would therefore be useful to do a full three-dimensional transient simulation as the next step.
- In the present work, the modified Curl's model is used to close the molecular mixing term in the evolution equation for the scalar PDF. For freely propagating turbulent premixed flames it appears that the use of the current mixing model results in a low flame front activity for fuel-air mixtures with a relatively high Zeldovich number. One possible way forward is to explore the predictive capabilities of more recent mixing models such as the EMST model of Subramaniam & Pope [166] applied to similar flames. A key feature of the model is that it ensures localness in composition space.
- The strong impact of the mixing time scale expression prevails with multiple scalars. It would be beneficial to formulate a more general expression that is valid in both combustion mode extremes — for both diffusion and premixed flames. Also, to alleviate the need to pre-compute input parameters. This is, however, not a major concern for practical purposes since it is advantageous to initialise the field using a simpler (flamelet) combustion closure.
- In the work of Lindstedt & Város [110] it is shown that more sophisticated closures for transport in physical space increases the predicted turbulent burning velocity. A closure at the second moment level can be achieved on the basis of the joint velocity-scalar transported PDF approach. On the other hand, a closure at this level significantly increases the complexity and the computational burden. Instead, explore a possible intermediate step — to formulate algebraic turbulence scalar flux models to increase the closure level of the transport in

physical space term in the joint scalar PDF equation.

- Investigate the possibility of formulating a particle reactivity biased particle interaction model to overcome the low flame front activity issue. In this case the particles are not selected at random but selected based on their value of, for example, the Jacobian. The idea is to mix a high reactivity particle with a low reactivity particle. One issue is of course the violation of the locality criterion. On the other hand, the modified Curl's model does not satisfy this criterion either.
- Investigate the potential of LES in combination with filtered density functions. McDermott & Pope [126] have formulated models that converge to a DNS at zero filter width and allow the inclusion of differential diffusion effects. The major disadvantage is of course the extremely high computational burden. Nevertheless, it appears to be a very promising approach that resolves many of the known issues of RANS/PDF and traditional combustion modelling in LES.

Appendices

Appendix A

Reduced and detailed mechanisms

Table A.1: Reduced hydrocarbon mechanism

No	Reaction			A $m^3 kmol^{-1} s^{-1}$	n	E $Jmol^{-1}$
1	$H + O_2$	$\rightleftharpoons$	$OH + O$	0.2000E+12	0.00	0.7030E+05
2	$O + H_2$	$\rightleftharpoons$	$OH + H$	0.5120E+02	2.67	0.2630E+05
3	$OH + H_2$	$\rightleftharpoons$	$H_2O + H$	0.1000E+06	1.60	0.1380E+05
4	$OH + OH$	$\rightleftharpoons$	$H_2O + O$	0.3570E+02	2.40	-0.8840E+04
5	$O_2 + H + M$	$\rightleftharpoons$	$HO_2 + M^a$	0.2300E+13	-0.80	0.0000E+00
6	$HO_2 + H$	$\rightleftharpoons$	$OH + OH$	0.1680E+12	0.00	0.3660E+04
7	$HO_2 + H$	$\rightleftharpoons$	$H_2 + O_2$	0.4270E+11	0.00	0.5900E+04
8	$HO_2 + OH$	$\rightleftharpoons$	$H_2O + O_2$	0.2890E+11	0.00	-0.2080E+04
9	$HO_2 + H$	$\rightleftharpoons$	$H_2O + O$	0.3000E+11	0.00	0.7200E+04
10	$HO_2 + O$	$\rightleftharpoons$	$OH + O_2$	0.3190E+11	0.00	0.0000E+00
11	$H + H + M$	$\rightleftharpoons$	$H_2 + M^b$	0.6530E+12	-1.00	0.0000E+00
12	$H + H + M$	$\rightleftharpoons$	$H_2 + M^c$	0.9200E+11	-0.60	0.0000E+00
13	$H + H + M$	$\rightleftharpoons$	$H_2 + M^d$	0.6000E+14	-1.25	0.0000E+00
14	$H + H + M$	$\rightleftharpoons$	$H_2 + M^e$	0.5490E+15	-2.00	0.0000E+00
15	$H + OH + M$	$\rightleftharpoons$	$H_2O + M^f$	0.2200E+17	-2.00	0.0000E+00
16	$O + O + M$	$\rightleftharpoons$	$O_2 + M^f$	0.1000E+12	-1.00	0.0000E+00
17	$CO + OH$	$\rightleftharpoons$	$CO_2 + H$	0.4400E+04	1.50	-0.3100E+04
18	$CO + HO_2$	$\rightleftharpoons$	$CO_2 + OH$	0.1500E+12	1.50	0.9893E+05
19	$CO + O + M$	$\rightleftharpoons$	$CO_2 + M^f$	0.5300E+08	1.50	-0.1900E+05

Table A.1: continued

No	Reaction			A $m^3 kmol^{-1} s^{-1}$	n	E $Jmol^{-1}$
20	$CO + O_2$	$\rightleftharpoons$	$CO_2 + O$	0.2500E+10	1.50	0.2000E+06
21	$CH + O_2$	$\rightleftharpoons$	$CHO + O$	0.7500E+11	0.00	0.0000E+00
22	$CH + CO_2$	$\rightleftharpoons$	$CHO + CO$	0.3400E+10	0.00	0.2900E+04
23	$CH + O$	$\rightleftharpoons$	$CO + H$	0.4000E+11	0.00	0.0000E+00
24	$CH + OH$	$\rightleftharpoons$	$CHO + H$	0.3000E+11	0.00	0.0000E+00
25	$CH + H_2O$	$\rightleftharpoons$	CH_2OH	0.5730E+10	0.00	-0.3150E+04
26	$CH + CH_2O$	$\rightleftharpoons$	$C_2H_2O + H$	0.9460E+11	0.00	-0.2160E+04
27	$CH + CH_2$	$\rightleftharpoons$	$C_2H_2 + H$	0.4000E+11	0.00	0.0000E+00
28	$CH + CH_3$	$\rightleftharpoons$	$C_2H_3 + H$	0.3000E+11	0.00	0.0000E+00
29	$CH + CH_4$	$\rightleftharpoons$	$C_2H_4 + H$	0.6000E+11	0.00	0.0000E+00
30	$CHO + H$	$\rightleftharpoons$	$CO + H_2$	0.9000E+11	0.00	0.0000E+00
31	$CHO + O$	$\rightleftharpoons$	$CO + OH$	0.3000E+11	0.00	0.0000E+00
32	$CHO + O$	$\rightleftharpoons$	$CO_2 + H$	0.3000E+11	0.00	0.0000E+00
33	$CHO + OH$	$\rightleftharpoons$	$CO + H_2O$	0.1000E+12	0.00	0.0000E+00
34	$CHO + O_2$	$\rightleftharpoons$	$CO + HO_2$	0.4520E+15	-1.85	0.1468E+04
35	$CHO + M$	$\rightleftharpoons$	$CO + H + M^g$	0.1860E+15	-1.00	0.7110E+05
36	$^1CH_2 + H_2$	$\rightleftharpoons$	$CH_3 + H$	0.7230E+11	0.00	0.0000E+00
37	$^1CH_2 + H$	$\rightleftharpoons$	$CH + H_2$	0.7000E+11	0.00	0.0000E+00
38	$^1CH_2 + O$	$\rightleftharpoons$	$CO + H + H$	0.1500E+11	0.00	0.0000E+00
39	$^1CH_2 + O$	$\rightleftharpoons$	$CO + H_2$	0.1500E+11	0.00	0.0000E+00
40	$^1CH_2 + OH$	$\rightleftharpoons$	$CH_2O + H$	0.3000E+11	0.00	0.0000E+00
41	$^1CH_2 + O_2$	$\rightleftharpoons$	$CO + OH + H$	0.3000E+11	0.00	0.0000E+00
42	$^1CH_2 + CO_2$	$\rightleftharpoons$	$CH_2O + CO$	0.3000E+10	0.00	0.0000E+00
43	$^1CH_2 + CH_3$	$\rightleftharpoons$	$C_2H_4 + C$	0.1800E+11	0.00	0.0000E+00
44	$^1CH_2 + CH_4$	$\rightleftharpoons$	$CH_3 + CH_3$	0.4270E+11	0.00	0.0000E+00
45	$^1CH_2 + M$	$\rightleftharpoons$	$CH_2 + M^h$	0.1000E+11	0.00	0.0000E+00
46	$CH_2 + H_2$	$\rightleftharpoons$	$CH_3 + H$	0.3000E+07	0.00	0.0000E+00
47	$CH_2 + H$	$\rightleftharpoons$	$CH + H_2$	0.1100E+12	0.00	0.0000E+00
48	$CH_2 + O$	$\rightleftharpoons$	$CO + H + H$	0.4880E+11	0.00	0.0000E+00
49	$CH_2 + O$	$\rightleftharpoons$	$CO + H_2$	0.3250E+11	0.00	0.0000E+00
50	$CH_2 + OH$	$\rightleftharpoons$	$CH + H_2O$	0.1130E+05	2.00	0.1256E+05

Table A.1: continued

No	Reaction	A $m^3 kmol^{-1} s^{-1}$	n	E $Jmol^{-1}$
51	$CH_2 + OH \rightleftharpoons CH_2O + H$	0.2500E+11	0.00	0.0000E+00
52	$CH_2 + O_2 \rightleftharpoons CO + H + OH$	0.1642E+19	-3.30	0.1200E+05
53	$CH_2 + O_2 \rightleftharpoons CO_2 + H + H$	0.3285E+19	-3.30	0.1200E+05
54	$CH_2 + O_2 \rightleftharpoons CH_2O + O$	0.3285E+19	-3.30	0.1200E+05
55	$CH_2 + O_2 \rightleftharpoons CO_2 + H_2$	0.2630E+19	-3.30	0.1200E+05
56	$CH_2 + O_2 \rightleftharpoons CO + H_2O$	0.2240E+20	-3.30	0.1200E+05
57	$CH_2 + CO_2 \rightleftharpoons CH_2O + CO$	0.1100E+09	0.00	0.4187E+04
58	$CH_2 + CH_2 \rightleftharpoons C_2H_2 + H + H$	0.1200E+12	0.00	0.3320E+04
59	$CH_2 + CH_3 \rightleftharpoons C_2H_4 + H$	0.4000E+11	0.00	0.0000E+00
60	$CH_2O + H \rightleftharpoons CHO + H_2$	0.2180E+06	1.77	0.1255E+05
61	$CH_2O + O \rightleftharpoons CHO + OH$	0.4150E+09	0.57	0.1156E+05
62	$CH_2O + OH \rightleftharpoons CHO + H_2O$	0.1130E+07	1.18	-0.1870E+04
63	$CH_2O + O_2 \rightleftharpoons CHO + HO_2$	0.6000E+11	0.00	0.1700E+06
64	$CH_2O + CH_3 \rightleftharpoons CHO + CH_4$	0.4090E+10	0.00	0.3700E+05
65	$CH_3 + CH_3 \rightleftharpoons C_2H_5 + H$	0.5000E+10	0.10	0.4436E+05
66	$CH_3 + CH_3 \rightleftharpoons C_2H_6^{i,1}$	0.3600E+11	0.00	0.0000E+00
		0.1270E+36	-7.00	0.1155E+05
67	$CH_3 + O \rightleftharpoons CH_2O + H$	0.8430E+11	0.00	0.0000E+00
68	$CH_3 + OH \rightleftharpoons CH_2OH + H$	0.1500E+12	0.00	0.3446E+05
69	$CH_3 + OH \rightleftharpoons {}^1CH_2 + H_2O$	0.4000E+11	0.00	0.1047E+05
70	$CH_3 + OH \rightleftharpoons CH_2O + H_2$	0.1024E+10	0.00	0.0000E+00
71	$CH_3 + OH \rightleftharpoons CH_3O + H$	0.5740E+10	-0.23	0.5828E+05
72	$CH_3 + O_2 \rightleftharpoons CH_3O + O$	0.1320E+12	-0.23	0.1314E+06
73	$CH_3 + O_2 \rightleftharpoons CH_2O + OH$	0.3300E+09	0.00	0.3740E+05
74	$CH_3 + HO_2 \rightleftharpoons CH_3O + OH$	0.1800E+11	0.00	0.0000E+00
75	$CH_3 + CHO \rightleftharpoons CH_4 + CO$	0.1200E+12	0.00	0.0000E+00
76	$CH_3O + M \rightleftharpoons CH_2OH + M$	0.3010E+09	0.00	0.1704E+05
77	$CH_3O + H \rightleftharpoons CH_2O + H_2$	0.2000E+11	0.00	0.0000E+00
78	$CH_3O + O \rightleftharpoons CH_2O + OH$	0.6000E+10	0.00	0.0000E+00
79	$CH_3O + OH \rightleftharpoons CH_2O + H_2O$	0.1800E+11	0.00	0.0000E+00
80	$CH_3O + O_2 \rightleftharpoons CH_2O + HO_2$	0.6600E+08	0.00	0.1088E+05

Table A.1: continued

No	Reaction	A $m^3 kmol^{-1} s^{-1}$	n	E $Jmol^{-1}$
81	$CH_3O + M \rightleftharpoons CH_2O + H + M$	0.5450E+11	0.00	0.5650E+05
82	$CH_2OH + H \rightleftharpoons CH_2O + H_2$	0.3000E+11	0.00	0.0000E+00
83	$CH_2OH + O \rightleftharpoons CH_2O + OH$	0.4220E+11	0.00	0.0000E+00
84	$CH_2OH + OH \rightleftharpoons CH_2O + H_2O$	0.2400E+11	0.00	0.0000E+00
85	$CH_2OH + O_2 \rightleftharpoons CH_2O + HO_2$	0.6000E+10	0.00	0.0000E+00
86	$CH_2OH + M \rightleftharpoons CH_2O + H + M$	0.2300E+41	-8.00	0.1800E+06
87	$CH_3 + H \rightleftharpoons CH_4^{j,2}$	0.2100E+12	0.00	0.0000E+00
		0.6300E+18	-1.80	0.0000E+00
88	$CH_4 + H \rightleftharpoons CH_3 + H_2$	0.3860E+04	2.11	0.3242E+05
89	$CH_4 + O \rightleftharpoons CH_3 + OH$	0.9033E+06	1.56	0.3550E+05
90	$CH_4 + OH \rightleftharpoons CH_3 + H_2O$	0.1560E+05	1.83	0.1160E+05
91	$C_2H + H_2 \rightleftharpoons C_2H_2 + H$	0.5670E+08	0.90	0.8340E+04
92	$C_2H + O \rightleftharpoons CO + CH$	0.1000E+11	0.00	0.0000E+00
93	$C_2H + OH \rightleftharpoons C_2HO + H$	0.2000E+11	0.00	0.0000E+00
94	$C_2H + O_2 \rightleftharpoons CO + CO + H$	0.9040E+10	0.00	-0.1910E+04
95	$C_2H + H_2O \rightleftharpoons C_2H_2O + H$	0.1140E+11	0.00	0.1660E+04
96	$C_2HO + H \rightleftharpoons {}^1CH_2 + H$	0.1000E+12	0.00	0.0000E+00
97	$C_2HO + O \rightleftharpoons CO + CO + H$	0.9635E+11	0.00	0.0000E+00
98	$C_2HO + O_2 \rightleftharpoons CO + CO + OH$	0.1000E+11	0.00	0.0000E+00
99	$C_2HO + O_2 \rightleftharpoons CO_2 + CO + H$	0.1000E+11	0.00	0.0000E+00
100	$C_2H_2 + O \rightleftharpoons CH_2 + CO$	0.2893E+04	2.09	0.6535E+04
101	$C_2H_2 + O \rightleftharpoons C_2HO + H$	0.4340E+04	2.09	0.6535E+04
102	$C_2H_2 + OH \rightleftharpoons C_2H + H_2O$	0.3370E+05	2.00	0.5858E+05
103	$C_2H_2 + OH \rightleftharpoons C_2H_2O + H$	0.3750E+04	1.70	0.4184E+04
104	$C_2H_2 + O_2 \rightleftharpoons C_2HO + OH$	0.2000E+06	1.50	0.1260E+06
105	$CH_2 + CO \rightleftharpoons C_2H_2O$	0.6020E+06	0.00	0.0000E+00
106	$C_2H_2O + H \rightleftharpoons CH_3 + CO$	0.1110E+05	2.00	0.8368E+04
107	$C_2H_2O + H \rightleftharpoons C_2HO + H_2$	0.1800E+12	0.00	0.3598E+05
108	$C_2H_2O + O \rightleftharpoons CO_2 + CH_2$	0.2000E+11	0.00	0.9603E+04
109	$C_2H_2O + O \rightleftharpoons C_2HO + OH$	0.1000E+11	0.00	0.3350E+05
110	$C_2H_2O + OH \rightleftharpoons CH_2OH + CO$	0.1020E+11	0.00	0.0000E+00

Table A.1: continued

No	Reaction	A $m^3 kmol^{-1} s^{-1}$	n	E $Jmol^{-1}$
111	$C_2H_2O + OH \rightleftharpoons C_2HO + H_2O$	0.7500E+10	0.00	0.8370E+04
112	$C_2H_3 \rightleftharpoons C_2H_2 + H^{k,3}$	0.2000E+15	0.00	0.1663E+06
		0.4160E+39	-7.50	0.1904E+06
113	$C_2H_3 + H \rightleftharpoons C_2H_2 + H_2$	0.3000E+11	0.00	0.0000E+00
114	$C_2H_3 + O \rightleftharpoons C_2H_2O + H$	0.3000E+11	0.00	0.0000E+00
115	$C_2H_3 + OH \rightleftharpoons C_2H_2 + H_2O$	0.2000E+11	0.00	0.0000E+00
116	$C_2H_3 + O_2 \rightleftharpoons CHO + CH_2O$	0.3660E+10	0.00	-0.9900E+03
117	$C_2H_3 + O_2 \rightleftharpoons C_2H_2 + HO_2$	0.1500E+09	0.00	-0.9980E+03
118	$C_2H_4 + H \rightleftharpoons C_2H_3 + H_2$	0.1325E+04	2.53	0.5121E+05
119	$C_2H_4 + O \rightleftharpoons CH_3 + CHO$	0.1320E+06	1.55	0.1788E+04
120	$C_2H_4 + OH \rightleftharpoons C_2H_3 + H_2O$	0.1570E+02	2.75	0.1746E+05
121	$C_2H_5 + O_2 \rightleftharpoons C_2H_4 + HO_2$	0.1020E+09	0.00	-0.9140E+04
122	$C_2H_5 + O \rightleftharpoons CH_3 + CH_2O$	0.6600E+11	0.00	0.0000E+00
123	$C_2H_4 + H \rightleftharpoons C_2H_5^{j,4}$	0.3975E+07	1.28	0.5404E+04
		0.4714E+13	0.00	0.3159E+04
124	$C_2H_6 \rightleftharpoons C_2H_5 + H^{j,5}$	0.8850E+21	-1.23	0.4277E+06
		0.4900E+40	-6.43	0.4484E+06
125	$C_2H_6 + H \rightleftharpoons C_2H_5 + H_2$	0.1445E+07	1.50	0.3100E+05
126	$C_2H_6 + O \rightleftharpoons C_2H_5 + OH$	0.1000E+07	1.50	0.2430E+05
127	$C_2H_6 + OH \rightleftharpoons C_2H_5 + H_2O$	0.7226E+04	2.00	0.3616E+04
128	$CH_2 + M \rightleftharpoons C + H_2 + H + M$	0.1148E+12	0.00	0.2337E+06
129	$CH + M \rightleftharpoons C + H + M$	0.1000E+12	0.00	0.2680E+06
130	$CH + H \rightleftharpoons C + H_2$	0.3000E+11	0.00	0.0000E+00
131	$CH + OH \rightleftharpoons C + H_2O$	0.4000E+05	2.00	0.1250E+05
132	$C + OH \rightleftharpoons CO + H$	0.5000E+11	0.00	0.0000E+00
133	$C + O_2 \rightleftharpoons CO + O$	0.1200E+12	0.00	0.1671E+05
134	$C + CO_2 \rightleftharpoons CO + CO$	0.6000E+06	0.00	0.0000E+00
135	$C + CH_3 \rightleftharpoons C_2H_2 + H$	0.5000E+11	0.00	0.0000E+00
136	$C + CH_2 \rightleftharpoons C_2H + H$	0.5000E+11	0.00	0.0000E+00
137	$C_2H + C_2H \rightleftharpoons C_2H_2 + C_2$	0.1810E+10	0.00	0.0000E+00
138	$C_2H + H \rightleftharpoons C_2 + H_2$	0.3610E+11	0.00	0.1183E+06

Table A.1: continued

No	Reaction			A $m^3 kmol^{-1} s^{-1}$	n	E $Jmol^{-1}$
139	$C + C + M$	$\rightleftharpoons$	$C_2 + M$	0.1800E+16	-1.60	0.0000E+00
140	$C_2 + O$	$\rightleftharpoons$	$CO + C$	0.3610E+12	0.00	0.0000E+00
141	$C_2 + O_2$	$\rightleftharpoons$	$CO + CO$	0.8970E+10	0.00	0.4100E+04
142	$C_2H_2 + O_2$	$\rightleftharpoons$	$C_2H + HO_2$	0.1200E+11	0.00	0.3117E+06

Collision Efficiencies:

M^a : $N_2 = 0.4$, $O_2 = 0.35$, $CO = 0.7$, $CO_2 = 1.5$, $H_2O = 6.5$

M^b : $H_2 = 0.0$, $CO_2 = 0.0$, $H_2O = 0.0$

M^c : All species= 0.0 except $H_2 = 1.0$

M^d : All species= 0.0 except $H_2O = 1.0$

M^e : All species= 0.0 except $CO_2 = 1.0$

M^f : $H_2 = 2.5$, $CO = 1.9$, $CO_2 = 3.8$, $H_2O = 12.0$

M^g : $CH_4 = 7.5$, $H_2 = 2.5$, $CO = 1.9$, $CO_2 = 3.8$, $H_2O = 16.25$

M^h : $H = 20.0$, $H_2O = 3.0$, $C_2H_2 = 4.0$, $C_2H_4 = 1.4$, $C_2H_6 = 2.2$

M^i : $H_2 = 1.1$, $N_2 = 1.6$, $O_2 = 1.9$, $CO = 1.9$, $CO_2 = 3.3$, $H_2O = 5.7$

M^j : $H_2 = 2.0$, $O_2 = 1.5$, $CO = 1.5$, $CO_2 = 3.0$, $H_2O = 6.0$

M^k : $H_2 = 2.0$, $O_2 = 1.5$, $CO = 2.0$, $CO_2 = 3.0$, $H_2O = 5.0$

Fall-off parameters for pressure dependent reactions:

$$^1F_c = 0.38 \exp(-T/73.0) + 0.62 \exp(-T/1180.0) \text{ (Troe)}$$

$$^2F_c = 0.63 \exp(-T/3315.0) + 0.37 \exp(-T/61.0) \text{ (Troe)}$$

$$^3F_c = 0.35 \text{ (Linear)}$$

$$^4F_c = 0.24 \exp(-T/40.0) + 0.76 \exp(-T/1025.0) \text{ (Troe)}$$

$$^5F_c = \exp(-T/3371.0) + 47.6 \exp(-16182.0/T) \text{ (Troe)}$$

Table A.2: Detailed hydrogen mechanism

No	Reaction	A $m^3 kmol^{-1} s^{-1}$	n	E $Jmol^{-1}$
1	$H + O_2 \rightleftharpoons OH + O$	0.2000E+12	0.00	0.7030E+05
2	$O + H_2 \rightleftharpoons OH + H$	0.5120E+02	2.67	0.2630E+05
3	$OH + H_2 \rightleftharpoons H_2O + H$	0.1000E+06	1.60	0.1380E+05
4	$OH + OH \rightleftharpoons H_2O + O$	0.3570E+02	2.40	-0.8840E+04
5	$O_2 + H + M \rightleftharpoons HO_2 + M^a$	0.2300E+13	-0.80	0.0000E+00
6	$HO_2 + H \rightleftharpoons OH + OH$	0.1680E+12	0.00	0.3660E+04
7	$HO_2 + H \rightleftharpoons H_2 + O_2$	0.4270E+11	0.00	0.5900E+04
8	$HO_2 + OH \rightleftharpoons H_2O + O_2$	0.2890E+11	0.00	-0.2080E+04
9	$HO_2 + H \rightleftharpoons H_2O + O$	0.3000E+11	0.00	0.7200E+04
10	$HO_2 + O \rightleftharpoons OH + O_2$	0.3190E+11	0.00	0.0000E+00
11	$HO_2 + HO_2 \rightleftharpoons H_2O_2 + O_2$	0.1860E+10	0.00	0.6440E+04
12	$H_2O_2 + H \rightleftharpoons H_2O + OH$	0.1000E+11	0.00	0.1500E+05
13	$H_2O_2 + H \rightleftharpoons HO_2 + H_2$	0.1700E+10	0.00	0.1570E+05
14	$H_2O_2 + O \rightleftharpoons HO_2 + OH$	0.6600E+09	0.00	0.1660E+05
15	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$	0.7830E+10	0.00	0.5570E+04
16	$H_2O_2 + M \rightleftharpoons OH + OH + M^b$	0.1200E+15	0.00	0.1900E+06
17	$H + H + M \rightleftharpoons H_2 + M^c$	0.6530E+12	-1.00	0.0000E+00
18	$H + H + M \rightleftharpoons H_2 + M^d$	0.9200E+11	-0.60	0.0000E+00
19	$H + H + M \rightleftharpoons H_2 + M^e$	0.6000E+14	-1.25	0.0000E+00
20	$H + OH + M \rightleftharpoons H_2O + M^b$	0.2200E+17	-2.00	0.0000E+00
21	$O + O + M \rightleftharpoons O_2 + M^b$	0.1000E+12	-1.00	0.0000E+00

Collision Efficiencies:

M^a : $N_2 = 0.4$, $O_2 = 0.35$, $H_2O = 6.5$

M^b : $H_2 = 2.5$, $H_2O = 12.0$

M^c : $H_2 = 0.0$, $H_2O = 0.0$

M^d : All species= 0.0 except $H_2 = 1.0$

M^e : All species= 0.0 except $H_2O = 1.0$

Appendix B

Global activation energies

Table B.1: Computed global activation energies based on stoichiometric CH_4 mixtures with N_2 dilution.

X_{CH_4}	X_{O_2}	X_{N_2}	u_L^0 [m/s]	ρ_u [kg/m ³]	T_b [K]	E_a [kJ/mol]
0.08678	0.1736	0.73962	0.331	1.027	2082	
0.07985	0.1597	0.76045	0.251	1.028	1980	
0.07394	0.1479	0.77816	0.193	1.028	1891	
0.06885	0.1377	0.79345	0.146	1.029	1813	
0.06441	0.1288	0.80679	0.110	1.029	1743	
						196

Table B.2: Computed global activation energies based on slightly lean ($\phi = 0.88$) CH_4 mixtures with N_2 dilution.

X_{CH_4}	X_{O_2}	X_{N_2}	u_L^0 [m/s]	ρ_u [kg/m ³]	T_b [K]	E_a [kJ/mol]
0.07717	0.1754	0.74743	0.280	1.031	1978	
0.07095	0.1612	0.76785	0.210	1.032	1879	
0.06565	0.1492	0.78515	0.156	1.032	1791	
0.06110	0.1389	0.80000	0.116	1.032	1712	
0.05713	0.1298	0.81307	0.0856	1.033	1641	
0.05365	0.1219	0.82445	0.0627	1.033	1576	
0.05056	0.1149	0.83454	0.0455	1.033	1517	
						197

Table B.3: Computed global activation energies based on stoichiometric C_2H_6 mixtures with N_2 dilution.

$X_{C_2H_6}$	X_{O_2}	X_{N_2}	u_L^0 [m/s]	ρ_u [kg/m ³]	T_b [K]	E_a [kJ/mol]
0.05357	0.1875	0.75893	0.440	1.072	2191	
0.04839	0.1694	0.78221	0.337	1.068	2060	
0.04412	0.1544	0.80148	0.250	1.064	1937	
0.04054	0.1419	0.81756	0.189	1.059	1837	
0.03750	0.1313	0.83120	0.141	1.056	1753	
						168

Table B.4: Computed global activation energies based on fuel rich ($\phi = 1.6$) H_2 mixtures with N_2 dilution.

X_{H_2}	X_{O_2}	X_{N_2}	u_L^0 [m/s]	ρ_u [kg/m ³]	T_b [K]	E_a [kJ/mol]
0.3827	0.1196	0.4977	3.543	0.689	2053	
0.3652	0.1141	0.5207	3.224	0.705	1981	
0.3493	0.1091	0.5416	2.935	0.720	1915	
0.3347	0.1046	0.5607	2.671	0.733	1855	
0.3212	0.1004	0.5784	2.432	0.746	1798	
0.3088	0.0965	0.5947	2.218	0.757	1744	
0.2973	0.0929	0.6098	2.020	0.767	1695	
0.2867	0.0896	0.6237	1.842	0.777	1648	
0.2768	0.0865	0.6367	1.678	0.786	1604	
0.2675	0.0836	0.6489	1.528	0.795	1562	
0.2589	0.0809	0.6602	1.389	0.803	1522	
0.2507	0.0784	0.6709	1.263	0.810	1483	
0.2431	0.0760	0.6809	1.146	0.817	1446	
0.2360	0.0737	0.6903	1.040	0.824	1408	
0.2292	0.0716	0.6992	0.946	0.830	1370	
0.2228	0.0696	0.7076	0.868	0.836	1332	
						77

Appendix C

Transformation to the $t - \omega$ coordinate system

Parabolic flows are assumed to be steady, predominantly in one direction (the velocity vector in that direction is nowhere negative) and without recirculation and diffusion effects in that direction. Integration of the boundary layer type equations proceeds until a steady state is reached in flame space. The stationary, statistically two-dimensional boundary layer governing equations have the general form in cylindrical coordinates

$$\frac{\partial \langle \rho \rangle \tilde{u} \tilde{\phi}}{\partial x} + \frac{1}{r} \frac{\partial \langle \rho \rangle r \tilde{v} \tilde{\phi}}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left[r \Gamma_{\phi} \frac{\partial \tilde{\phi}}{\partial r} \right] + \langle \rho \rangle \tilde{S}_{\phi}. \quad (\text{C.1})$$

Now, since the x -direction is the only predominant direction of the flow, convection terms in any other direction are negligible, Eq. (C.1) reduces to

$$\frac{\partial \langle \rho \rangle \tilde{u} \tilde{\phi}}{\partial x} = \frac{1}{r} \frac{\partial}{\partial r} \left[r \Gamma_{\phi} \frac{\partial \tilde{\phi}}{\partial r} \right] + \langle \rho \rangle \tilde{S}_{\phi} \quad (\text{C.2})$$

where the term on the left hand side may be rewritten due to continuity

$$\langle \rho \rangle \tilde{u} \frac{\partial \tilde{\phi}}{\partial x} + \underbrace{\tilde{\phi} \frac{\partial \langle \rho \rangle \tilde{u}}{\partial x}}_0 = \frac{1}{r} \frac{\partial}{\partial r} \left[r \Gamma_{\phi} \frac{\partial \tilde{\phi}}{\partial r} \right] + \langle \rho \rangle \tilde{S}_{\phi}. \quad (\text{C.3})$$

Following Spalding [163], defining a stream function based cross-stream variable allows Eq. (C.3) to be written in a compact form. The stream function Ψ is constant along a streamline and is defined by (for fixed x)

$$\partial\Psi = r < \rho > \tilde{u} \partial r \quad \Leftrightarrow \quad \frac{1}{\partial r} = r < \rho > \tilde{u} \frac{1}{\partial\Psi}. \quad (\text{C.4})$$

Substitution of Eq. (C.4) in Eq. (C.3) gives

$$< \rho > \tilde{u} \frac{\partial \tilde{\phi}}{\partial x} = < \rho > \tilde{u} \frac{\partial}{\partial\Psi} \left[r^2 < \rho > \tilde{u} \Gamma_\phi \frac{\partial \tilde{\phi}}{\partial\Psi} \right] + < \rho > \tilde{S}_\phi. \quad (\text{C.5})$$

Eq. (C.5) is the conservation differential equation in terms of Von Mises coordinates x and Ψ . Now considering planar ($r = 1$) unsteady flows, divide by $< \rho >$ and assume that $\tilde{u} = 1$ everywhere to transform [163] Eq. (C.5) into a one-dimensional transient equation

$$\frac{\partial \tilde{\phi}}{\partial t} = \frac{\partial}{\partial\Psi} \left[< \rho > \Gamma_\phi \frac{\partial \tilde{\phi}}{\partial\Psi} \right] + \tilde{S}_\phi. \quad (\text{C.6})$$

Spalding [163] proposed to use a normalized, dimensionless cross-stream variable ω due to various problems with the rectangular $x - y$ coordinates and the Von Mises coordinates $x - \Psi$. ω is defined as

$$\omega = \frac{\Psi - \Psi_I}{\Psi_E - \Psi_I} \quad (\text{C.7})$$

where Ψ_I and Ψ_E are the values of Ψ at the I and E boundary, respectively. It follows from the above definition that

$$\left(\frac{\partial}{\partial\Psi} \right)_x = \frac{1}{\Psi_E - \Psi_I} \left(\frac{\partial}{\partial\omega} \right)_x. \quad (\text{C.8})$$

The transformation formulae from the $x - \Psi$ to the $x - \omega$ coordinate system reads

$$\left(\frac{\partial}{\partial x} \right)_\Psi = \left(\frac{\partial}{\partial x} \right)_\omega + \left(\frac{\partial}{\partial\omega} \right)_x \left(\frac{\partial\omega}{\partial x} \right)_\Psi \quad (\text{C.9})$$

where the subscript is indicating what is held constant during the differentiation. Substitution of Eq. (C.8) into Eq. (C.6) (e.g. Eq. (C.5)) and application of Eq. (C.9) results in a general equation that describes conservation and transport of mass and momentum [160]

$$\frac{\partial \phi}{\partial t} + (a + b\omega) \frac{\partial \phi}{\partial \omega} = \frac{\partial}{\partial \omega} \left[c \frac{\partial \phi}{\partial \omega} \right] + d \quad (\text{C.10})$$

where

$$a = \frac{\dot{m}_I''}{\Psi_E - \Psi_I} \quad b = \frac{\dot{m}_E'' - \dot{m}_I''}{\Psi_E - \Psi_I} \quad c = \frac{\langle \rho \rangle \Gamma_\phi}{(\Psi_E - \Psi_I)^2} \quad d = \tilde{S}_\phi. \quad (\text{C.11})$$

$\dot{m}_I''$ and $\dot{m}_E''$ represent the rate of mass transfer across the I and E boundary, respectively, and are related to Ψ through the corresponding entrainment laws

$$\frac{\partial \Psi_I}{\partial t} = -\dot{m}_I'' \quad \frac{\partial \Psi_E}{\partial t} = -\dot{m}_E''. \quad (\text{C.12})$$

For a steady propagating turbulent flame, the rate of mass transfer across the boundaries are given by the simple expression

$$\dot{m}_I'' = \dot{m}_E'' = -\rho_u u_u = -\rho_b u_b = -\rho_u u_T \quad (\text{C.13})$$

where subscripts u and b refers to unburned and burned gases, respectively. The turbulent burning velocity, u_T , is obtained from the reaction rate integral. Consider Eq. (1.43)

$$\rho_u u_T \frac{d\tilde{\phi}}{dx} = -\frac{d \langle \rho \rangle \widetilde{u''\phi''}}{dx} + \langle \rho \rangle \tilde{S}_\phi. \quad (\text{C.14})$$

Integration over entire physical space yields

$$\rho_u u_T (\tilde{\phi}|_\infty - \tilde{\phi}|_0) = - \left(\underbrace{\langle \rho \rangle \widetilde{u''\phi''}|_\infty}_{=0} - \underbrace{\langle \rho \rangle \widetilde{u''\phi''}|_0}_{=0} \right) + \int_0^\infty \langle \rho \rangle \tilde{S}_\phi dx \quad (\text{C.15})$$

and the turbulent burning velocity is given by

$$u_T = \frac{\int_0^\infty \langle \rho \rangle \tilde{S}_\phi dx}{\rho_u (\tilde{\phi}|_\infty - \tilde{\phi}|_0)}. \quad (\text{C.16})$$

The methodology described above was applied by Spalding & Stephenson [160] in the context of propagating laminar premixed flames.

Bibliography

- [1] Abdel-Gayed, R. G., Al-Khishali, K. J. and Bradley, D. Turbulent burning velocities and flame straining in explosions. *Proceedings of the Royal Society of London A* 391:393-414, 1984.
- [2] Aluri, N. K., Pantangi, P. K. G., Muppala, S. P. R. and Dinkelacker, F. A numerical study promoting algebraic models for the Lewis number effect in atmospheric turbulent premixed bunsen flames. *Flow, Turbulence and Combustion* 75:149-172, 2005.
- [3] Aluri, N. K., Muppala, S. P. R. and Dinkelacker, F. Substantiating a fractal-based algebraic reaction rate closure of premixed turbulent combustion for high pressure and the Lewis number effects. *Combustion and Flame* 145:663-674, 2006.
- [4] Anand, M. S. and Pope, S. B. Calculations of premixed turbulent flames by PDF methods. *Combustion and Flame* 67:127-142, 1987.
- [5] Anand, M. S., Hsu, A. T. and Pope, S. B. PDF calculations for swirl combustors. *AIAA paper* 96-0522, 1996.
- [6] Anand, M. S., Hsu, A. T. and Pope, S. B. Calculations of swirl combustors using the joint velocity-scalar probability density function method. *AIAA Journal* 35:1143-1150, 1997.
- [7] Bauer, W., Haag, O. and Hennecke, D. K. Accuracy and robustness of non-linear eddy viscosity models. *International Journal of Heat and Fluid Flow*, 21:312-319, 2000.

- [8] Bell, J. H. and Mehta, R. D. Contraction design for small low-speed wind tunnels. *NASA contractor report 177488*, Stanford University, California, 1988.
- [9] Bianchi, G. M., Cantore, G., Parmeggiani, P. and Michelassi, V. On application of nonlinear k- ϵ models for internal combustion engine flows. *Transactions of the ASME: Journal of Engineering for Gas Turbines and Power*, 124:668-677, 2002.
- [10] Bilger, R. W. Turbulent flows with nonpremixed reactants. In P. A. Libby and F. A. Williams, editors. *Turbulent Reacting Flows, Topics in Applied Physics*, volume 44, pp. 65-113, Springer-Verlag, 1980.
- [11] Bilger, R. W. The structure of turbulent non-premixed flames. *Proceedings of the Combustion Institute*, 22:475-488, 1988.
- [12] Bray, K. N. C. Turbulent flows with premixed reactants. In P. A. Libby and F. A. Williams, editors. *Turbulent Reacting Flows, Topics in Applied Physics*, volume 44, pp. 115-183, Springer-Verlag, 1980.
- [13] Bray, K. N. C., Libby, P. A., Masuya, G. and Moss, J. B. Turbulence production in premixed turbulent flames. *Combustion Science and Technology* 25:127-140, 1981.
- [14] Bray, K. N. C., Libby, P. A. and Moss, J. B. Unified modeling approach for premixed turbulent combustion-Part I: General formulation. *Combustion and Flame* 61:87-102, 1985.
- [15] Bray, K. N. C. Studies of the turbulent burning velocity. *Proceedings of the Royal Society of London A* 431:315-335, 1990.
- [16] Bray, K. N. C., Champion M., and Libby, P. A. Premixed flames in stagnating turbulence part III—The k- ϵ theory for reactants impinging on a wall. *Combustion and Flame* 91:165-186, 1992.
- [17] Bray, K. N. C. and Peters, N. Laminar flamelets in turbulent flames. *Turbulent Reacting Flows* pp. 63-113, Academic Press, London, 1994.

-
- [18] Bray, K. N. C., Champion, M. and Libby P. A. Flames in stagnating turbulence. *Turbulent Reacting Flows* pp. 573-608, Academic Press, London, 1994.
 - [19] Bray, K. N. C. The challenge of turbulent combustion. Hottel plenary lecture, *Proceedings of the Combustion Institute* 26:1-26, 1996.
 - [20] Bray, K. N. C., Champion M., and Libby, P. A. Premixed flames in stagnating turbulence part II. The mean velocities and pressure and the Damkhler number. *Combustion and Flame* 112:635-654, 1998.
 - [21] Bray, K. N. C., Champion M., and Libby, P. A. Premixed flames in stagnating turbulence part IV: A new theory for the Reynolds stresses and Reynolds fluxes applied to impinging flows. *Combustion and Flame* 120:1-18, 2000.
 - [22] Bray, K. N. C., Champion M., and Libby, P. A. Premixed flames in stagnating turbulence part V—Evaluation of models for the chemical source term. *Combustion and Flame* 127:2023-2040, 2001.
 - [23] Brewster, B. S., Cannon, S. M., Farmer, J. R. and Meng, F. Modeling of lean premixed combustion in stationary gas turbines. *Progress in Energy and Combustion Science* 25:353-385, 1999.
 - [24] Cannon, S. M., Brewster, B. S. and Smoot, L. D. PDF modelling of lean premixed combustion using *In Situ* Tabulated Chemistry. *Combustion and Flame* 119:233-252, 1999.
 - [25] Cant, R. S. and Mastorakos, E. *An Introduction to Turbulent Reacting Flows*. Imperial College Press, United Kingdom, 2008.
 - [26] Cao, R. R., Pope, S. B. and Masri, A. R. Turbulent lifted flames in a vitiated coflow investigated using joint PDF calculations. *Combustion and Flame* 142:438-453, 2005.
 - [27] Cao, R. R., Wang, H. and Pope, S. B. The effect of mixing models in PDF calculations of piloted jet flames. *Proceedings of the Combustion Institute* 31:1543-1550, 2007.

- [28] Catlin, C. A. and Lindstedt, R. P. Premixed turbulent burning velocities derived from mixing controlled reaction models with cold front quenching. *Combustion and Flame* 85:427-439, 1991.
- [29] Cheng, R. K. and Shepherd, I. G. The influence of burner geometry on premixed turbulent flame propagation. *Combustion and Flame* 85:7-26, 1991.
- [30] Cho, P., Law, C. K., Cheng, R. K. and Shepherd, I. G. Velocity and scalar fields of turbulent premixed flames in stagnation flow. *Proceedings of the Combustion Institute* 22:739-745, 1988.
- [31] Chou, C.-P., Chen, J.-Y., Janicka, J. and Mastorakos, E. Modeling of turbulent opposed-jet mixing flows with k- ϵ model and second-order closure. *International Journal of Heat and Mass Transfer* 47:1023-1035, 2004.
- [32] Correa, S. M. A direct comparison of Pair-Exchange and IEM models in premixed combustion. *Combustion and Flame* 103:194-206, 1995.
- [33] Craft, T. J., Graham, J. W. and Launder, B. E. Impinging jet studies for turbulence model assessment—II. An examination of the performance of four turbulence models. *International Journal of Heat and Mass Transfer* 36(10):2685-2697, 1993.
- [34] Craft, T. J., Launder, B. E. and Suga, K. Development and application of a cubic eddy-viscosity model of turbulence. *International Journal of Heat and Fluid Flow* 17:108-115, 1996.
- [35] Daly, B. J. and Harlow, F. H. Transport equations in turbulence. *The Physics of Fluids* 13(11):2634-2649, 1970.
- [36] Daou, J. and Liñán, A. Triple flames in mixing layers with nonunity Lewis numbers. *Proceedings of the Combustion Institute* 27:667-674, 1998.
- [37] Darbyshire, O. R., Swaminathan, N. and Hochgreb, S. Mixing models for the simulation of stratified combustion. *4th European Combustion Meeting*, Vienna, Austria, 2009.

-
- [38] Dianat, M., Fairweather, M. and Jones W. P. Predictions of axisymmetric and two-dimensional impinging turbulent jets. *International Journal of Heat and Fluid Flow* 17:530-538, 1996.
- [39] Domingo, P. and Bray, K. N. C. Laminar flamelet expressions for pressure fluctuation terms in second moment models of premixed turbulent combustion. *Combustion and Flame* 121:555-574, 2000.
- [40] Dopazo, C. Probability density function approach for a turbulent axisymmetric heated jet. Centerline evolution. *Physics of Fluids* 18(4):397-404, 1975.
- [41] Dopazo, C. Relaxation of initial probability density functions in the turbulent convection of scalar fields. *Physics of Fluids* 22(1):20-30, 1979.
- [42] Dowling, A. P. and Morgans, A. S. Feedback control of combustion oscillations. *Annual Review of Fluid Mechanics* 37:151-182, 2005.
- [43] Dryer, F. and Glassman, I. High temperature oxidation of CO and CH_4 . *Proceedings of the Combustion Institute* 14:987-1003, 1972.
- [44] Egolfopoulos, F. N. and Law, C. K. Chain Mechanisms in the overall reaction orders in laminar flame propagation. *Combustion and Flame* 80:7-16, 1990.
- [45] Egolfopoulos, F. N. and Law, C. K. An experimental and computational study of the burning rates of ultra-lean to moderately-rich $H_2/O_2/N_2$ laminar flames with pressure variations. *Proceedings of the Combustion Institute* 23:333-340, 1990.
- [46] Eswaran, V. and Pope, S. B. Direct numerical simulations of the turbulent mixing of a passive scalar. *Physics of Fluids* 31(3):506-520, 1988.
- [47] Fairweather, M., Ormsby, M. P., Sheppard, C. G. W. and Woolley, R. Turbulent burning rates of methane and methane-hydrogen mixtures. *Combustion and Flame* 156:780-790, 2009.

- [48] Ferziger, J. H. and Perić, M. *Computational Methods for Fluid Dynamics*, Second edition, Springer-Verlag Berlin Heidelberg, 1999.
- [49] Fox, R. O. *Computational Models for Turbulent Reacting Flows*. Cambridge University Press, United Kingdom, 2003.
- [50] Freitag, M. and Janicka, J. Investigation of a strongly swirled unconfined premixed flame using LES. *Proceedings of the Combustion Institute* 31:1477-1485, 2007.
- [51] Geipel, P. Personal communication July 2010.
- [52] Geipel, P. *Experimental Research on Turbulent Reacting Flows using Gaseous and Liquid Fuels*. PhD thesis, Department of Mechanical Engineering, Imperial College, London, 2010.
- [53] Geipel, P., Goh, K. H. H. and Lindstedt, R. P. Fractal-generated turbulence in opposed jet flows. *Flow, Turbulence and Combustion* article in press, 2010.
- [54] Geyer, D., Kempf, A., Dreizler, A. and Janicka, J. Scalar dissipation rates in isothermal and reactive turbulent opposed-jets: 1-D-Raman/Rayleigh experiments supported by LES. *Proceedings of the Combustion Institute* 30:681-689, 2005.
- [55] Geyer, D., Dreizler, A., Janicka, J., Permana, A. D. and Chen, J. Y. Finite-rate chemistry effects in turbulent opposed flows: comparison of Raman/Rayleigh measurements and Monte Carlo PDF simulations. *Proceedings of the Combustion Institute* 30:711-718, 2005.
- [56] Geyer, D., Kempf, A., Dreizler, A. and Janicka, J. Turbulent opposed-jet flames: A critical benchmark experiment for combustion LES. *Combustion and Flame* 143:524-548, 2005.
- [57] Gibson, M. M. and Launder, B. E. On the calculation of horizontal, turbulent, free shear flows under gravitational influence. *ASME Journal of Heat Transfer* 98C:81-87, 1976.

-
- [58] Gkagkas, K. and Lindstedt R. P. Transported PDF modelling with detailed chemistry of pre- and auto-ignition in CH_4 /air mixtures. *Proceedings of the Combustion Institute* 31:1559-1566, 2007.
- [59] Gouldin, F. C. An application of fractals to modeling premixed turbulent flames. *Combustion and Flame* 68:249-266, 1987.
- [60] Guin, C. and Trichet, P. Optimisation of a two-head lean prevaporised premixed combustor. *Aerospace Science and Technology* 8:35-46, 2004.
- [61] Gulati, A. and Driscoll, J. F. Velocity-density correlations and Favre averages Measured in a premixed turbulent flame. *Combustion Science and Technology* 48:285-307, 1986.
- [62] Hakberg, B. and Gosman, A. D. Analytical determination of turbulent flame speed from combustion models. *Proceedings of the Combustion Institute* 20:225-232, 1984.
- [63] Hanjalić, K. and Launder B. E. Sensitizing the dissipation equation to irrotational strains. *ASME Journal of Fluids Engineering* 102:34-40, 1980.
- [64] Hanjalić, K. Advanced turbulence closure models: a view of the current status and future prospects. *International Journal of Heat and Fluid Flow* 15:178-203, 1994.
- [65] Hanjalić, K., Jakirlić, S. and Hadžić, I. Expanding the limits of “equilibrium” second-moment turbulence closures. *Fluid Dynamics Research* 20:25-41, 1997.
- [66] Haworth, D.C. and Pope, S. B. A generalized Langevin model for turbulent flows. *Physics of Fluids* 29(2):387-405, 1986.
- [67] Haworth, D.C. and Pope, S. B. A pdf modelling study of self-similar turbulent free shear flows. *Physics of Fluids* 30(4):1026-1044, 1987.
- [68] Haworth, D.C. Progress in probability density function methods for turbulent reacting flows. *Progress in Energy and Combustion Science* 36:168-259, 2010.

- [69] Hůlek, T. and Lindstedt, R. P. Computations of steady-state and transient premixed turbulent flames using PDF methods. *Combustion and Flame* 104:481-504, 1996.
- [70] Hůlek, T. *Modelling of turbulent combustion using transported probability density function methods*. PhD thesis, Department of Mechanical Engineering, Imperial College, London, 1996.
- [71] Incropera, F. P. and DeWitt, D. P. Diffusion mass transfer. *Fundamentals of Heat and Mass Transfer* pp. 783-824, Fourth edition, John Wiley & Sons, Inc., 1996.
- [72] IPCC Intergovernmental Panel on Climate Change, *Climate change 2001: The scientific basis*, Cambridge University Press, Cambridge, 2001.
- [73] Issa, R. I. Solution of the implicitly discretised fluid flow equations by operator-splitting. *Journal of Computational Physics* 62:40-65, 1986.
- [74] James, S., Anand, M. S., Razdan, M. K. and Pope, S. B. In situ detailed chemistry calculations in combustor flow analyses. *Journal of Engineering for Gas Turbines and Power* 123:747-756, 2001.
- [75] James, S., Zhu, J. and Anand, M. S. Simulations of gas turbine combustor flows using the node-based PDF transport method. *AIAA* 2002-4013, 2002.
- [76] James, S., Anand, M. S. and Pope, S. B. The lagrangian PDF transport method for simulations of gas turbine combustor flows. *AIAA* 2002-4017, 2002.
- [77] Janicka, J., Kolbe, W. and Kollmann, W. J. Closure of the transport equation for the probability density function of scalar fields. *Journal of Non-equilibrium Thermodynamics*, 4(1):47-66, 1979.
- [78] Jiang, X., Zhao, H. and Luo, K. H. Direct computation of perturbed impinging hot jets. *Computers & Fluids* 36:259-272, 2007.

-
- [79] Jones, W. P. and Launder, B. E. The prediction of laminarization with a two-equation model of turbulence. *International Journal of Heat and Mass Transfer* 15:301-314, 1972.
- [80] Jones, W. P. Models for turbulent flows with variable density and combustion. *Prediction Methods for Turbulent Flows* pp. 379-421, VKI-Lecture Series, Hemisphere, 1980.
- [81] Jones, W. P. and Lindstedt, R. P. Global reaction schemes in hydrocarbon combustion. *Combustion and Flame* 73:233-249, 1988.
- [82] Jones, W. P. and Lindstedt, R. P. The calculation of the structure of laminar counterflow diffusion flames using a global reaction mechanism. *Combustion Science and Technology* 61:31-49, 1988.
- [83] Jones, W. P. and Musonge, P. Closure of the Reynolds stress and scalar flux equations. *Physics of Fluids* 31(12):3589-3604, 1988.
- [84] Jones, W. P. and Pascau, A. Calculation of confined swirling flows with a second moment closure. *Transactions of the ASME, Journal of Fluids Engineering* 111:248-255, 1989.
- [85] Jones, W. P. Turbulence modelling and numerical solution methods for variable density and combustng flows. *Turbulent Reacting Flows* pp. 309-374, Academic Press, London, 1994.
- [86] Kempf, A., Forkel, H., Chen, J.-Y., Sadiki, A. and Janicka, J. Large-eddy simulation of a counterflow configuration with and without combustion. *Proceedings of the Combustion Institute* 28:35-40, 2000.
- [87] Kim, W. W., Menon, S. and Mongia, H. C. Large-eddy simulation of a gas turbine combustor flow. *Combustion Science and Technology* 143:25-62, 1999.
- [88] Kolla, H., Rogerson, J. W., Chakraborty, N. and Swaminathan, N. Scalar dissipation rate modeling and its validation. *Combustion Science and Technology* 181:518535, 2009.

- [89] Kolla, H. and Swaminathan, N. Strained flamelets for turbulent premixed flames II: Laboratory flame results. *Combustion and Flame* 157:1274-1289, 2010.
- [90] Kostiuk, L. W., Bray, K. N. C. and Cheng, R. K. Experimental study of premixed turbulent combustion in opposed streams. Part I—Nonreacting flow field. *Combustion and Flame* 92:377-395, 1993.
- [91] Kostiuk, L. W., Bray, K. N. C. and Cheng, R. K. Experimental study of premixed turbulent combustion in opposed streams. Part II—Reacting flow field and extinction. *Combustion and Flame* 92:396-409, 1993.
- [92] Kostiuk, L. W., Shepard, I. G. and Bray, K. N. C. Experimental study of premixed turbulent combustion in opposed streams. Part III—Spatial structure of flames. *Combustion and Flame* 118:129-139, 1999.
- [93] Korusoy, E. and Whitelaw, J. H. Opposed jets with small separations and their implications for the extinction of opposed flames. *Experiments in Fluids* 31:111-117, 2001.
- [94] Korusoy, E. and Whitelaw, J. H. Extinction and relight in opposed flames. *Experiments in Fluids* 33:75-89, 2002.
- [95] Kuan, T. S. *Prediction methods for steady and transient turbulent flames* PhD thesis, Department of Mechanical Engineering, Imperial College London, 2003.
- [96] Kuan, T. S. and Lindstedt, R. P. Transported probability density function modeling of a bluff body stabilized turbulent flame. *Proceedings of the Combustion Institute* 30:767-774, 2005.
- [97] Kundu, P. K. *Fluid Mechanics*, Academic Press, United Kingdom, 1990.
- [98] Launder, B. E. and Spalding, D. B. Turbulence models and their application to the prediction of internal flows. *Heat and Fluid Flow* 2(1):43-54, 1972.

-
- [99] Launder, B. E. and Sharma, B. I. Application of the energy-dissipation model of turbulence to the calculation of flow near a spinning disc. *Letters in Heat and Mass Transfer* 1:131-138, 1974.
- [100] Launder, B. E. An introduction to single-point closure methodology. In Gatski, T. B., Hussaini, M. Y. and Lumley, J. L. (Eds.) *Simulation and modelling of turbulent flows* ch. 6, pp. 243-310, New York, Oxford University Press, 1996.
- [101] Lawn, C. J. and Schefer, R. W. Scaling of premixed turbulent flames in the corrugated regime. *Combustion and Flame* 146:180-199, 2006.
- [102] Leung, K. M. and Lindstedt, R. P. Detailed kinetic modeling of $C_1 - C_3$ alkane diffusion flames. *Combustion and Flame* 102:129-160, 1995.
- [103] Libby, P. A. and Williams, F. A. Fundamental aspects. In P. A. Libby and F. A. Williams, editors. *Turbulent Reacting Flows, Topics in Applied Physics*, volume 44, pp. 1-43, Springer-Verlag, 1980.
- [104] Libby, P. A. and Williams, F. A. Fundamental aspects and a review. *Turbulent Reacting Flows* pp. 1-61, Academic Press, London, 1994.
- [105] Lindstedt, R. P. Personal communication September 2009.
- [106] Lindstedt, R. P. and Sakthitharan, V. Modelling of transient compressible turbulent reacting flows. *8th Symposium on Turbulent Shear Flows*, Technical University of Munich, 1991.
- [107] Lindstedt, R. P. and Város, E. M. Second moment modeling of premixed turbulent flames stabilized in impinging jet geometries. *Proceedings of the Combustion Institute* 27:957-962, 1998.
- [108] Lindstedt, R. P. and Város, E. M. Modeling of premixed turbulent flames with second moment methods. *Combustion and Flame* 116:461-485, 1999.
- [109] Lindstedt, R. P., Louloudi, S. A. and Város, E. M. Joint scalar probability density function modelling of pollutant formation in piloted turbulent jet dif-

- fusion flames with comprehensive chemistry. *Proceedings of the Combustion Institute* 28:149-156, 2000.
- [110] Lindstedt, R. P. and Város, E. M. Modeling of mixing processes in non-isothermal and combusting flows. *Advances in turbulence VIII. Proceedings of the Eighth European Turbulence Conference* 493-496, 2000.
- [111] Lindstedt, R. P. and Louloudi, S. A. Joint scalar transported probability density function modeling of turbulent methanol jet diffusion flames. *Proceedings of the Combustion Institute* 29:2147-2154, 2002.
- [112] Lindstedt, R. P., Luff, D. and Whitelaw, J. H. Velocity and strain-rate characteristics of opposed isothermal flows. *Flow, Turbulence and Combustion* 74(2):169-194, 2005.
- [113] Lindstedt, R. P. and Ozarovsky H. C. Joint scalar transported pdf modelling of non-piloted turbulent diffusion flames. *Combustion and Flame* 143:471-490, 2005.
- [114] Lindstedt, R. P., Milosavljevic, V. D., Ozarovsky H. C., Persson, M. and Város, E. M. Modelling technique for flameless combustion. *Flameless Combustion Workshop*, Lund University of Technology, 2005.
- [115] Lindstedt, R. P. and Város, E. M. Transported pdf modelling of high Reynolds number premixed turbulent flames. *Combustion and Flame* 145:495-511, 2006.
- [116] Lindstedt, R. P., Luff, D. S. and Whitelaw, J. H. Velocity fields of fuel lean premixed turbulent opposed jet flames. *Proceedings of the Combustion Institute* 31:1459-1466, 2007.
- [117] Lindstedt, R. P., Ozarovsky, H. C., Barlow, R. S. and Karpetis, A. N. Progression of localized extinction in high Reynolds number turbulent jet flames. *Proceedings of the Combustion Institute* 31:1551-1558, 2007.

-
- [118] Lindstedt, R. P., Milosavljevic, V. D. and Persson, M. Turbulent burning velocity predictions using transported PDF methods. *Proceedings of the Combustion Institute* 33:1277-1284, 2011.
- [119] Lipatnikov, A. N. and Chomiak, J. Molecular transport effects on turbulent flame propagation and structure. *Progress in Energy and Combustion Science* 31:1-73, 2005.
- [120] Lipatnikov, A. N. and Chomiak, J. Effects of premixed flames on turbulence and turbulent scalar transport. *Progress in Energy and Combustion Science* 36:1-102, 2010.
- [121] Luff, D. S. *Experiments and Calculations of Opposed and Ducted Flows*. PhD thesis, Department of Mechanical Engineering, Imperial College, London, 2005.
- [122] Lumley, J. L. Pressure-strain correlation. *The Physics of Fluids* 18(6):750, 1975.
- [123] Lumley, J. L. and Newman, G. R. The return to isotropy of homogeneous turbulence. *Journal of Fluid Mechanics* 82(1):161-178, 1977.
- [124] Lumley, J. L. Computational modeling of turbulent flows. *Advances in Applied Mechanics* 18:123-176, 1978.
- [125] Mastorakos, E. *Turbulent combustion in opposed jet flows*. PhD thesis, Department of Mechanical Engineering, Imperial College, London, 1993.
- [126] McDermott, R. and Pope, S. B. A particle formulation for treating differential diffusion effects in filtered density function methods. *Journal of Computational Physics* 226:947-993, 2007.
- [127] Merci, B., Roekaerts, D., Naud, B. and Pope, S. B. Comparative study of micromixing models in transported scalar PDF simulations of turbulent non-premixed bluff body flames. *Combustion and Flame* 146: 109-130, 2006.

- [128] Meyer, D. W. and Jenny, P. A mixing model for turbulent flows based on parameterized scalar profiles. *Physics of Fluids* 18(3), 2006.
- [129] Milosavljevic, V. D., Persson, M., Lindstedt, R. P. and Váos, E. M. Evaluation of the thermoacoustic performance of an industrial gas turbine combustion chamber with a second moment method. *Combustion and Noise Control*, Cranfield University Press, pp. 72-77, 2003.
- [130] Mohamed, M. S. and LaRue, J. C. The decay power law in grid-generated turbulence. *Journal of Fluid Mechanics* 219:195-214, 1990.
- [131] Nogenmyr, K.-J., Petersson, P., Bai, X. S., Nauert, A., Olofsson, J., Brackman, C., Seyfried, H., Zetterberg, J., Li, Z. S., Richter, M., Dreizler, A., Linne, M. and Aldén, M. Large eddy simulation and experiments of stratified lean premixed methane/air turbulent flames. *Proceedings of the Combustion Institute* 31:1467-1475, 2007.
- [132] Nottin, C., Knikker, R., Boger, M. and Veynante, D. Large eddy simulation of an acoustically excited turbulent premixed flame. *Proceedings of the Combustion Institute* 28:67-73, 2000.
- [133] Peters, N. Laminar flamelet concepts in turbulent combustion. *Proceedings of the Combustion Institute* 21:1231-1250, 1986.
- [134] Peters, N. *Turbulent Combustion*, Cambridge University Press, United Kingdom, 2002.
- [135] Pitsch, H. Large-eddy simulation of turbulent combustion. *The Annual Review of Fluid Mechanics* 38:453-482, 2006.
- [136] Poinso, T. and Veynante, D. *Theoretical and Numerical Combustion*, Edwards, 2001.
- [137] Pope, S. B. An explanation of the turbulent round-jet/plane-jet anomaly. *AIAA Journal* 16:279-281, 1978.

-
- [138] Pope, S. B. An improved mixing model. *Combustion Science and Technology* 28:131-145, 1982.
- [139] Pope, S. B. and Anand, M. S. Flamelet and distributed combustion in premixed turbulent flames. *Proceedings of the Combustion Institute* 20:403-410, 1984.
- [140] Pope, S. B. PDF methods for turbulent reactive flows. *Progress in Energy and Combustion Science* 11:119-192, 1985.
- [141] Pope, S. B. Mapping closures for turbulent mixing and reaction. *Theoretical and Computational Fluid Dynamics* 2:255-270, 1991.
- [142] Pope, S. B. On the relationship between stochastic Lagrangian models of turbulence and second-moment closures. *Physics of Fluids* 6(2):973-985, 1994.
- [143] Pope, S. B. *Turbulent Flows*. Cambridge University Press, United Kingdom, 2000.
- [144] Pope, S. B. Ten questions concerning the large-eddy simulation of turbulent flows. *New Journal of Physics* 6:35, 2004.
- [145] O'Brien, E. E. The probability density function (pdf) approach to reacting turbulent flows. *Turbulent reacting Flows*, Topics in Applied Physics Volume 44, chapter 5, pp. 185-218, Springer-Verlag, 1980.
- [146] Ren, Z. and Pope, S. B. An investigation of the performance of turbulent mixing models. *Combustion and Flame* 136:208-216, 2004.
- [147] Roekaerts, D. Use of a Monte Carlo PDF method in a study of the influence of turbulent fluctuations on selectivity in a jet stirred reactor. *Applied Scientific Research* 48:271-300, 1991.
- [148] Roekaerts, D. Monte Carlo PDF method for turbulent reacting flow in a jet stirred reactor. *Computers and Fluids* 21:97-108, 1992.

- [149] Sardi, K., Taylor, A. M. K. P and Whitelaw, J. H. Conditional scalar dissipation statistics in a turbulent counterflow. *Journal of Fluid Mechanics* 361:1-24, 1998.
- [150] Sardi, K. and Whitelaw, J. H. Extinction timescales of periodically strained, lean counterflow flames. *Experiments in Fluids* 27:199-209, 1999.
- [151] Sarkar, S., Erlebacher, G., Hussaini M. Y. and Kreiss, H. O. The analysis and modelling of dilatational terms in compressible turbulence. *Journal of Fluid Mechanics* 227:473-493, 1991.
- [152] Sarkar, S. The pressure-dilatation correlation in compressible flows. *Physics of Fluids A* 4(12):2674-2682, 1992.
- [153] Savarianandam, V. R. and Lawn, C. J. Burning velocity of premixed turbulent flames in the weakly wrinkled regime. *Combustion and Flame* 146:1-18, 2006.
- [154] Saxena, V. and Pope, S. B. PDF simulations of turbulent combustion incorporating detailed chemistry. *Combustion and Flame* 117:340-350, 1999.
- [155] Schumann, U. Realizability of Reynolds-stress turbulence models. *The Physics of Fluids* 20(5):721-725, 1977.
- [156] Selle, L., Lartigue, G., Poinso, T., Koch, R., Schildmacher, K.-U., Krebs, W., Prade, B., Kaufmann, P. and Veynante, D. Compressible large eddy simulation of turbulent combustion in complex geometry on unstructured meshes. *Combustion and Flame* 137:489-505, 2004.
- [157] Sengissen, A. X., Giauque, A. V., Staffelbach, G. S., Porta, M., Krebs, W., Kaufmann, P. and Poinso, T. J. Large eddy simulation of piloting effects on turbulent swirling flames. *Proceedings of the Combustion Institute* 31:1729-1736, 2007.
- [158] Shepherd, J. E. Chemical kinetics of hydrogen-air-diluent detonations. 10th ICDERS, Berkley, California, 263-293, 1985.

-
- [159] Sommerer, Y., Galley, D., Poinso, T., Ducruix, S., Lacas, F. and Veynante, D. Large eddy simulation and experimental study of flashback and blow-off in a lean partially premixed swirled burner. *Journal of Turbulence* 5:037, 2004.
- [160] Spalding, D. B. and Stephenson, P. I. Laminar flame propagation in hydrogen-bromine mixtures. Technical report BL/TN/C/43, Mechanical Engineering Department, Imperial College of Science and Technology, 1971.
- [161] Spalding, D. B. Mixing and chemical reaction in steady confined turbulent flames. *Proceedings of the Combustion Institute* 13:649-657, 1971.
- [162] Spalding, D. B. Development of the Eddy-Break-Up model of turbulent combustion. *Proceedings of the Combustion Institute* 16:1657-1663, 1976.
- [163] Spalding, D. B. *GENMIX — A General Computer Program for Two-Dimensional Parabolic Phenomena* volume 1. HMT Pergamon Press, 1977.
- [164] Speziale, C. G., Sarkar, S. and Gatski, T. B. Modelling the pressure-strain correlation of turbulence: an invariant dynamical systems approach. *Journal of Fluid Mechanics* 227:245-272, 1991.
- [165] Stein, O. *Large Eddy Simulation of Combustion in Swirling and Opposed Jet Flows*. PhD thesis, Department of Mechanical Engineering, Imperial College, London, 2009.
- [166] Subramaniam, S. and Pope, S. B. A mixing model for turbulent reactive flows based on Euclidean minimum spanning trees. *Combustion and Flame* 115:487-514, 1998.
- [167] Swaminathan, N. and Bray, K. N. C. Effect of dilatation on scalar dissipation in turbulent premixed flames. *Combustion and Flame* 143:549-565, 2005.
- [168] Valiño, L. and Dopazo C. A binomial sampling model for scalar turbulent mixing. *Physics of Fluids A* 2(7):1204-1212, 1990.

- [169] Valiño, L. and Dopazo C. A binomial Langevin model for turbulent mixing. *Physics of Fluids A* 3(12):3034-3037, 1991.
- [170] Váos, E. M. *Second moment methods for turbulent flows with reacting scalars*. PhD thesis, Department of Mechanical Engineering, Imperial College, London, 1998.
- [171] Versteeg, H. K. and Malalasekera, W. *An introduction to Computational Fluid Dynamics. The Finite Volume Method*, Pearson Education Limited, England, 1995.
- [172] Viswanathan, S. and Pope, S. B. Turbulent dispersion from line sources in grid turbulence. *Physics of Fluids* 20:101514, 2008.
- [173] Wandel, A. P. and Lindstedt, R. P. Hybrid binomial Langevin-multiple mapping conditioning modeling of a reacting mixing layer. *Physics of Fluids* 21:015103, 2009.
- [174] Wang, P. and Bai, X. S. Large-eddy simulation of turbulent premixed flames using level-set G-equation. *Proceedings of the Combustion Institute* 30:583-591, 2005.
- [175] Warnatz, J. Maas, U. and Dibble, R. W. *Combustion*. Fourth edition, Springer-Verlag Berlin Heidelberg, 2006.
- [176] Wilcox, D. C. *Turbulence Modeling for CFD*, DCW Industries, Inc., La Cañada, California, United States, 1994.
- [177] Wu, A. S. and Bray, K. N. C. Application of a coherent flame model to premixed turbulent combustion impinging on a wall. *Combustion Science and Technology* 113-114:367-392, 1996.
- [178] Wu, A. S. and Bray, K. N. C. A coherent flame model of premixed turbulent combustion in a counterflow geometry. *Combustion and Flame* 109:43-64, 1997.

- [179] Xu, J. and Pope, S. B. PDF calculations of turbulent nonpremixed flames with local extinction. *Combustion and Flame* 123:281-307, 2000.
- [180] Yilmaz, S. L., Nik, M. B., Givi, P. and Strakey, P. A. Scalar filtered density function for large eddy simulation of a bunsen burner. *Journal of Propulsion and Power* 26(1):84-93, 2010.
- [181] Zhang, S. and Rutland, C. J. Premixed flame effects on turbulence and pressure-related terms. *Combustion and Flame* 102:447-461, 1995.
- [182] Zhang, Y. Z. and Haworth, D. C. A general mass consistency algorithm for hybrid particle/finite-volume PDF methods. *Journal of Computational Physics* 194:156-193, 2004.
- [183] Zimont, V., Polifke, W., Bettelini, M. and Weisenstein, W. An efficient computational model for premixed turbulent combustion at high Reynolds numbers based on a turbulent flame speed closure. Presented at the *International Gas Turbine & Aeroengine Congress & Exhibition*, Orlando, Florida, 1997.
- [184] Combustion theory, *ANSYS CFX-Solver Theory Guide*, ANSYS CFX Release 11.0, ANSYS Inc., 2006.
- [185] Modeling premixed combustion, *FLUENT 6.3 User's Guide*, Fluent Inc., 2006.