

**PREDICTION OF FLOW,
COMBUSTION AND HEAT TRANSFER
IN COAL FIRED CEMENT KILNS**

by

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a la memoria de Juan
para la familia Martinez

à Edith

*" The most beautiful thing we can
experience is the mysterious"*

Albert Einstein

ABSTRACT

The available models written for the cement industry are few and although they describe accurately the chemical reactions occurring in the material, they tend to simplify considerably the gas phase, especially in the flame zone. A new computer code has been developed for the prediction of flow, combustion and heat transfer in a pulverised fuel fired two dimensional furnace. Its aim is to provide the cement industry with a tool capable of predicting the performance of cement rotary kilns fired with pulverised fuel (P.F.). The program has therefore been developed for industrial utilisation. It has also been validated by comparing the predictions with experimental data measured on furnace geometries similar to those of cement kilns.

The mathematical formulation applies the eulerian conservation equations for the gaseous carrier-phase. A finite difference method is used for the numerical resolution of these equations. A lagrangian approach is used for the prediction of P.F. particles trajectories and burnout. Several mathematical models describing the different physical phenomena occurring in the combustor, such as devolatilisation, char combustion, volatile combustion and radiation, are examined and selected according to their performance.

The predictions are validated using two different sets of experimental data. Firstly a 1/20th scale water model of a Cement Kiln has been build. Flow visualisation was performed using a Laser Sheet technique and compared with the predicted flow pattern. Secondly, predictions were compared with experimental data measured on the International Flame Research Foundation n° 1 furnace. The correlations between measurement and predictions are examined.

Finally, the code is run on a full size cement kiln case, giving satisfactory results.

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GLOSSARY OF SYMBOLS**R o m a n S y m b o l s**

$(F_{Ox})_{\infty}$	Molar fraction of oxygen
$(P_{Ox})_{\infty}$	Oxygen partial pressure
A	Area. Pre-exponential factor in section 3.5
a	Finite volume equation coefficient
C	Constant
C_D	Drag coefficient
C_p	Specific heat
CS	Control surface
CV	Control Volume
D, d	Diameter
D_c	Diffusion coefficient
D_o	Binary diffusion coefficient
E	A quantitative measure of the wall roughness function. Activation energy in section 3.5
F	Boundary function (section 2.3.3)
f	scattering factor
$\vec{F}$	Force applied to a particle
f_{co}	Particle combustion factor
E_R	Radiation flux
G	Generation term of turbulent energy
g	Acceleration due to gravity
h	Gas enthalpy. Heat transfer coefficient (section 3.4.1)
H_c	Calorific value of Carbon for complete combustion
H_{fu}	Calorific value of fuel

I	Radiation intensity
K	Conductivity
k	Turbulent kinetic energy. Devolatilisation rate constant in section 3.5
k_c	Chemical reaction rate coefficient
k_d	Diffusion reaction rate coefficient
K_e	Equivalent absorption coefficient
k_t	Overall reaction rate coefficient
L_v	Latent heat coefficient
m	Mass
$\dot{m}$	Mass flow rate
n	Number of particle size groups
Nu	Nusselt number
P	Pressure
$P()$	Probability (chapter 4)
Pe	Peclet number
Pr	Prandtl number
Q	Heat exchange. Ratio of volatile contents in section 3.5.3
$\dot{q}$	Sum of the convective and diffusive fluxes across the boundaries of a cell
R	Gas constant
r	Space coordinate in the radial direction
R_c	Particle burning rate
Re	Reynolds number
R_{esor}	Residual source
R_f	Rate of volatile combustion
$r_{m e}$	Rate of mass efflux from the particle surface (section 3.3)
S	Source term. Stoichiometric oxygen in section 3.7

S_m	Source of mass from the particulate phase into the gas phase
T	Temperature
t	Time
T_R	Radiation temperature
U	Velocity component parallel to a wall
u, v, w	Components of the velocity in the axial, radial and tangential directions
u_i	Component of the gas velocity in direction i
U_R	Under-relaxation factor
V	Cumulative amount of volatiles at time 't'
$\vec{v}$	Velocity of a gas in relation to the control surface of the gas-particle mixture
V^*	Effective volatile content of coal
VM	Measured coal volatile content
$\vec{w}$	Velocity of a gas in relation to the control surface related to the particle phase
x	Space coordinate in the direction of the axis of symmetry
x_i	Space coordinate in direction i
X_{ub}	Fraction of original char mass remaining unburnt at any time
y	Normal distance from a wall surface

Greek Symbols

α	Velocity factor (see section 3.2)
δ	Dirac delta function ($\delta_{i=j} = 1, \delta_{i \neq j} = 0$)
ϵ	Dissipation rate of the turbulent kinetic energy. Emissivity
ϕ	Any dependent variable
Γ	Exchange coefficient or diffusion coefficient when related to the momentum equation
κ	Von Karman's constant

λ	Wavelength of monochromatic radiant energy
μ	Dynamic viscosity
π	Pi constant
θ	Angular coordinate
ρ	Density of gas. Reflectivity in chapter 4.
σ	Stefan-Boltzman constant. Prandtl/Schmidt number in chapter 2. Standard deviation of activation energy in chapter 4.
τ	Shear stress
$\underline{\Omega}, \underline{\Omega}'$	Direction of radiation
ω, ω'	Solid angle
$\vec{\nabla}$	The spatial gradient (nabla)

S u b s c r i p t s

a	Related to absorption
b	Related to combustion in chapter 3. Related to black body in chapter 4.
c	Related to convection
D	Related to drag
diff	Related to diffusion velocity
eff	Effective value
fu	Related to fuel
G	Related to gravity
g	Related to the gas phase
i, j	Can take the values 1,2 or 3, denoting the three space coordinates in the Cartesian-tensor form (see the definition in section 2.2.2)
m	Related to the gas-particle mixture
o	Related to reference temperature and pressure
ox	Related to oxygen

p	Related to the particulate phase, or to the central location of a cell (section 2.3.3)
pr	Related to combustion products
ps	Related to particle size
r	Related to radiation
s	Related to scattering
sl	Related to starting location
SW	Related to swirl
T	Related to a total value
t	Related to turbulence.
u	Related to the momentum
W	Related to the wall in section 2.3.5
W, E, S, N	Central locations of West, East, South, North neighboring cells
w, e, s, n, b	West, East, South, North boundaries of a cell, b denotes one of them

Superscripts

—	Time average
->	Vector
m	Related to m th iteration
+, -	Incident, reflected in chapter 4.
+	Related to the Couette flow analysis for velocity distribution near to a wall in chapter 2.
*, **, ***	Intermediate field values obtained through splitting operations in PISO algorythm
'	Fluctuating component of a property

CHAPTER 1**INTRODUCTION****1.1 PREAMBLE**

Following the seventies price rises of both fuel oil and natural gas coupled with doubts regarding the long term availability of these fuels, many industries have started to consider coal as an alternative energy source. This applies in particular to the cement industry as clinker production is a relatively high energy consuming process.

During the eighties, most of cement rotary kilns in Europe and America were gradually converted to coal firing, and although many cement manufacturers had, at first, some reservations regarding the technical feasibility of coal firing (Moye 1980) it was soon considered as the most cost effective fuel for use in cement production. (see also Bonet et al 1985). However, coal is a variable fuel compared with both oil and natural gas, containing many impurities such as ash and sulphur. Being a solid material, a combustion system to handle coal is much more complex than a similar system for oil or natural gas (Mullinger 1984). The probable future use of a variety of solid fuels such as industrial wastes will only be possible if cement manufacturers have a complete mastery of pulverised fuel flame. Therefore it is now indispensable that cement manufacturers are able to understand and predict the behaviour of their pulverised fuel fired cement kilns.

The objective of this work is to provide the cement industry with a tool capable of predicting and thus optimising the performance of cement rotary kilns fired with pulverised fuel (P.F.)

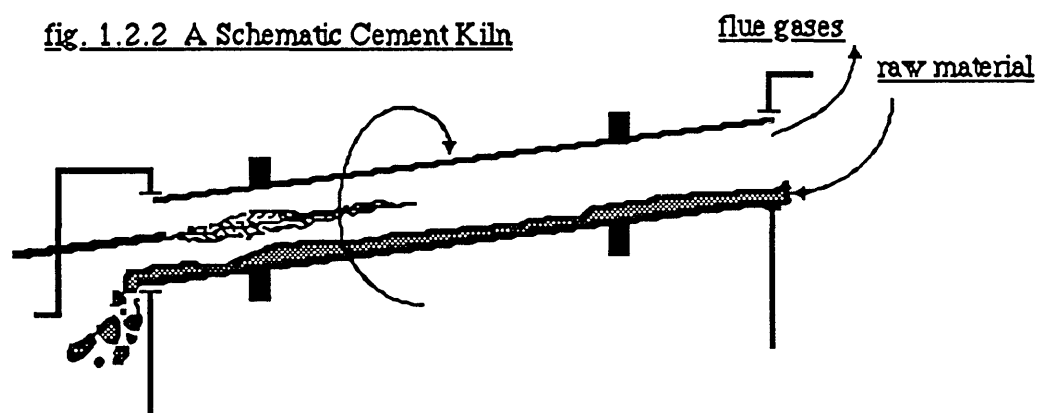
We need first to consider what a cement kiln is. It is not necessary to give a thorough description of a cement plant, a short description of a typical cement kiln will suffice and is provided here in the next section.

In section 1.3 an overview of the existing predictive procedures will be given.

The contribution of this work to the field will be discussed in section 1.4 and finally the layout of this thesis will be presented in section 1.5.

1.2 THE CEMENT KILN

The typical cement rotary kiln is a steel tube with an internal brickwork lining resting on several pairs of grinding rollers (fig. 1.2.1). Its length ranges from 50 to 150m, its diameter from 3 to 6 m according to the process. It lies at a shallow angle of a few degrees and is fed at its top with a mixture of clay and limestone as the kiln rotates. The material slowly travels down the tube towards the flame zone at the lower extremity of the furnace. By then, it has attained the necessary temperature (1450 °C) for the reactions of clinkerisation to occur. The cooked material, called clinker, exits into a cooler where its heat is used to preheat the combustion air. The coal is introduced into the kiln by a burner, axially positioned (fig. 1.2.2), by means of primary air acting as a carrying agent. The rest of the required combustion air is preheated secondary air.



The burner is one of the most critical components of the kiln system. It is only in recent years that the real importance of burner design has been recognized (Mullinger 1984). The geometry of the burner for PF flames can vary considerably depending on the process and on the firing system. In a direct firing system the coal is brought into the burner immediately from the mill. In an indirect firing system, an intermediate hopper is placed in between the milling process and the burner feeding system. For a long time the burner has simply been a straight pipe (Ruhland 1967). According to Lowes et al. (1986) two basic types of flame exist related to two types of burner: axial flames are produced by simple non swirling burners and are prevalent in direct coal firing systems; divergent flames are produced by burners which generate a swirl induced reverse flow zone. Other burner designs involving several concentric pipes such as the three way burner or the more recently designed PYROJET (Vollan and Klingbeil 1988) or ROTAFLAM (see Jacques and Gillouin 1990 or Pillard 1990) attempt to integrate both axial and swirling flow effects.

1.3 BACKGROUND

Two types of approach may be used in order to predict the behaviour of cement kilns. The first one, described as synthetic, may be called the 'macro approach'. In this approach, cement manufacturers have tried to correlate the quality and cost of the product, the clinker, with the input variables such as mass flows of air and fuel, temperatures, fuel requirement, diameters of kiln and burner etc... This first approach is based on experimental measurements, including full scale furnaces and scaled water or air models, and provides us now with empirical or semi-empirical formulae which can be very useful as long as they are used within their limits of application. Different correlation models obtained in this way are presented in section 1.3.1

The second approach, which can be described as an analytical or 'micro approach', is based on the analysis of the different physical phenomena occurring in coal flames. 'Physical models' are written in the form of partial differential equations that describe the many complex physical processes involved. These models are validated on specifically designed experiments. The resulting governing partial differential equations are then solved using numerical solution techniques. It is this approach, also known as 'Mathematical Modelling' or MM (see Lockwood 1990), which has been adopted in this work. An overview of the available MM for prediction of P.F. is presented in section 1.3.2.

1.3.1 Cement Kilns Correlation Models.

1.3.1.1 Experiments on Full Scale Furnaces

As early as 1936, during his investigations of the thermodynamics of rotary cement kilns, Gigy (1936) made measurements on an individual pulverised fuel flame. Ruhland (1967) pointed out the fact that since the number of input variables is quite large, functional relationships between these variables and flame properties can only be traced if a considerable number of different flame settings are covered.

The size of the flame and of the furnace, as well as the continuous rotation of the latter, considerably complicate flame measurements in rotary kilns. Such measurements have been performed using different techniques such as attaching the whole measurement system to the kiln shell (see for example Ruhland 1967) or introducing a long probe at one end of the kiln (see for example Bonet et al. 1985) or using a 'hot' or a 'cold' stopped kiln (see Moles et al. 1973)

In most cases, there is no possibility of observing the influence of an individual input variable in a rotary kiln in operation, at least this would not be possible over a large range of values and it would take a large amount of time (many years) and money.

One of the solutions to these problems consist of experimenting on scale models of kilns.

1.3.1.2 Experiments on Scaled Models

Three types of experimental settings can be found in the literature: air and water models, and experimental furnaces.

In the first two the visualisation of the flow pattern is the main objective. Flow visualisation in the water model can be produced using a polystyrene bead technique coupled with high-speed cinematography and still photography. Air model flow patterns can be obtained using a pitot-static tube. The disadvantage of air model tests compared to water is that there are difficulties in reaching the turbulence levels found in cement kilns (usually only very low Reynolds numbers can be reached in air models). Similarity errors are therefore much higher with air models than with water.

Water models have also been used to measure the length of the mixing zone between the primary flow (combustible) and the secondary flow (combustion air) by using an acid/alkali mixing technique. The primary flow is represented by dilute caustic soda solution containing a phenolphthalein indicator, whilst the secondary flow is represented by dilute hydrochloric acid. The substance in the primary jet is of a blue colour on account of the phenolphthalein. It becomes colourless as it mixes with the hydrochloric acid contained in the secondary flow. Thus the flame envelope is defined by the coloured region (see Ruhland 1967 and Mullinger and Jenkins 1987).

The third type of experimental setting consists of laboratory coal fired furnaces such as that of the International Flame Research Foundation (IFRF), using cement kiln burners (see for example Shreier and Flament 1981). It is clear that those furnaces are not only used for cement industry research, and that their geometry is far from being comparable to a cement kiln one. In fact they are used more for research into specific physical phenomena than for 'macro modelling'.

1.3.1.3 Available Correlation Models

The scale models described above have been used in one way or another for the study of the aerodynamics of axially symmetric turbulent jets in confined combustion chambers (that is not only cement kiln ones). Apart from the authors cited in the previous section further studies may be found in Thring and Newby 1964, Craya and Curtet 1955, Becker et al. 1963, Barchilon and Curtet 1964 or Chedaille et al. 1966.

These authors put forward mathematical relations based on their experimental work. The formulae generally relate the length of the flame to input conditions and geometrical considerations. It is not our objective here to describe these empirical relations and to discuss their validity and qualities. We simply observe that practically the theory of Craya and Curtet is the most commonly used among designers in the cement industry (see 'anonymous' 1974). It appears to provide a reasonable tool for the designing of simple burners.

Another type of predictive model is described by in Frisch and Jeschar (1983). Here the cement kiln is sliced into sections along its axis, and the heat and matter transferred between the material and the gas is calculated for each section. This kind of model is very good in predicting the evolution of the material inside the kiln, but because it is a one dimensional approach, the predictions regarding the flame and the gas temperature are poor.

1.3.2 Pulverised Fuel Mathematical Models

A review of the work on modelling of coal combustion and gasification processes may be found in Smoot (1981), Beer et al. (1984) and Smoot and Smith (1985).

The first general Two-Dimensional predictive study for pulverised coal combustion was reported as recently as 1970 by Gibson and Morgan. In this work the stream function-vorticity ($\psi - \omega$) solution procedure of Gosman et al. (1969) was employed, in conjunction with the Eulerian treatment of Spalding (1971) for the coal particles. The performance of the BCURA (British Coal Utilisation Association) cylindrical furnace for a swirling bituminous flame was successfully predicted using this method along with a two-flux radiation model and a simple algebraic specification for the turbulent transport. Later, Richter and Quack (1974) presented a set of calculations employing the above solution technique and using an improved turbulence model based on the turbulence kinetic energy and its dissipation rate ($k - \epsilon$). The resulting numerical procedure was used to predict the low-volatile flames of the IFRF, (Beer 1962), with reasonable success.

Lockwood and Syed (1977) reported calculations for pulverised coal flames in a two-dimensional axially symmetric furnace using a Lagrangian approach for the particulate phase originally formulated by Migdal and Agosta (1967). The above procedure for handling the flow/particle interaction was termed the particle-source-in-cell (PSIC) method. The two-equation $k-\epsilon$ model was used for gas-phase turbulence modelling, and included a 'drift velocity' concept for the particle diffusion calculations. Radiation exchanges were estimated using the procedure of Gibb (1977).

Lockwood et al. (1978) presented exploratory calculations of the flow and combustion in a cement kiln using the techniques of Lockwood and Syed (1977). Further predictions for combustion and heat transfer were reported for flames in cement kilns by

Lockwood and Salooja (1979), Lockwood and Salooja (1980) and in a hypothetical furnace by Lockwood et al. (1980)

Smith et al. (1981) reported predictions for a two-dimensional coal flame. The various model components employed in this study were: a 'k- ϵ ' turbulence model, the Lagrangian approach for particles, a two-step devolatilisation model of Ubhayakar et al. (1976), diffusion and kinetic heterogeneous rates for char combustion, a gaseous fast chemistry combustion model with the scalar fluctuations described by a probability density function for the mixture fraction, and the radiation exchange calculated using the flux model (see Gosman and Lockwood 1973). This research team had earlier reported one-dimensional modelling of P.F. flames (See Smoot and Pratt (1979) and Smith and Smoot (1980)).

Lockwood and Salooja (1983) applied the procedure developed for a cement kiln to the 'long flame' trials of the IFRF (Michel and Payne (1980)) and obtained quite good agreement with the data. Dixon et al. (1983) successfully examined the aerodynamics and mixing of a brown coal swirl-stabilised burner by means of modelling and experiments in an air model. Truelove et al. (1982) and Truelove (1984) studied flow, mixing and combustion in swirled pulverised coal burners using experimental data from 'C-14 Trials' of the IFRF (Hein and Leuckel 1969). This prediction procedure is based on the Lagrangian particle approach using a rectangular shape probability density function for the mixture. The thermal radiation is described by a discrete ordinate method, and a single reaction model is used to describe devolatilisation, diffusion and kinetic heterogeneous rates model for char combustion. The limited comparison presented for the axial gas temperature shows reasonable agreement with the data.

Lockwood and Rizvi (1983) used a faster particle tracking procedure compared with the previous studies by the same research group (see for example Lockwood and Salooja 1983). This resulted in a major improvement in computing economy for equivalent

accuracy. The calculation procedure was further used in a hypothetical furnace by Lockwood et al. (1983) for predicting the heat transfer behaviour of two coals. In work by Lockwood et al. (1984) a further improved computational procedure has been applied to explore the ability of available physical models, particularly those of devolatilisation and char combustion.

Rizvi (1985) used a novel 'recurrence relation' type solution technique for the particle motion and temperature. He also introduced the PISO (Pressure-Implicit-Split-Operator) algorithm for the gas-phase calculations, and included the calculation of swirl for gas and particle phases.

To conclude this overview let us quote Lockwood and Mahmud (1988):

"Pulverised coal prediction codes embody an especially large number of submodels to describe the many relevant physical processes. Some systematic validation work has been effected, but it is probably fair to say that code development has now outstripped code validation by an unacceptably large margin."

The aim of much of today's research effort in PF modelling is to improve the available physical models on the basis of ever more detailed experimental data in order to reduce this margin. Examples of such research can be found in Visser et al. (1990), Costa et al. (1990), or Truelove and Holcombe (1990).

1.4 OBJECTIVES AND PRESENT CONTRIBUTION

In the present work a computer program has been developed on the basis of some of the models described above. As seen previously, the goal is to be able to predict and optimise industrial cement kilns.

Instead of applying the existing codes to the specific case of cement rotary kilns, it was decided to write a generalised program which could be used on different kinds of geometries, including rotary kilns. The advantages of this procedure are threefold:

Firstly the new program can be validated on geometries others than those of the cement kiln type, for which there is not enough experimental data available. Secondly this 'generalisation' facilitates any geometrical modification a user might wish. Finally the creation of a 'standard' program allows any modification or improvement to be spread rapidly among the users, independently of the problem they are solving.

The new code, called FAFNIR, has the following characteristics:

- Any kind of axially symmetrical furnace can be specified,
- Any burner geometry can be specified,
- Any kind of P.F. can be burnt (eg. Petroleum Coke),
- The user is not required to modify the program itself, thanks to an interactive pre-processor,
- The program runs on many different computer systems.

(CDC/NOS, IBM/MVS, VAX/VMS, VAX/ULTRIX, CRAY/COS...)

In the present thesis a validation study relevant to cement kilns geometries has been carried out in two steps. Firstly, gas-phase isothermal predictions have been compared with flow visualisation experiments made on a water scaled model of a cement kiln. Secondly, combustion predictions have been compared with available experimental data (Bortz 1983) for a burner geometry similar to the ones used in the cement industry.

1.5 LAYOUT OF THE THESIS

This thesis has 7 chapters including this first one, the Introduction. In Chapters 2 and 3 a description of the physical and chemical phenomena of the gas and particulate

phases respectively are presented. Chapter 2 commences with a description of the Reynolds Transport Theorem, on the basis of which the governing equations for the gas phase are developed. The mathematical models used to calculate the latter are introduced together with their numerical solutions. In chapter 3 a similar development process is followed for each of the physical models concerning particle trajectories and combustion.

Chapter 4 is dedicated to the modelling of the radiative heat transfer between gas, particles and the walls. Different radiation models are described and the choice of one of them justified. The calculations for the optical properties of a furnace are detailed.

The code FAFNIR is presented in chapter 5. Its structure is described and computational details concerning convergence are presented.

Isothermal and combustion validation studies carried out on the code are reported in chapter 6. The water model apparatus is described and the results are presented. Special attention is paid to the combustion runs by comparing them with experimental data from the IFRF. Results of cement kiln predictions are shown.

Finally an assessment of the extent to which the objectives of this study are fulfilled is presented in the last chapter, chapter 7. Concluding remarks together with suggestions for future work are drawn.

CHAPTER 2

THE GAS PHASE

2.1 THE REYNOLDS TRANSPORT THEOREM

Euler introduced in the 18th century two different concepts to describe fluid motion. From the first one, later called the Lagrangian point of view, the flow field is regarded as the motion of numerous small contiguous fluid elements. Each one is 'labelled' and their position, velocities, temperature etc... are studied as a function of time. This approach is generally impracticable to describe the flow of a continuum because of the large amount of mass elements needed to achieve a reasonably accurate description of the flow field. On the other hand, it is suitable for the description of discrete phase, particularly to simulate the effects of drag, heat transfer and particle sizes.

In the second approach, called Eulerian approach, fluid quantities are considered on a given point as all fluid elements pass it for all time. Flow field solutions are obtained by integrating the governing equations over all points. This approach is only valid when the studied phase is a continuum.

The relationship between the two approaches is provided by the Reynolds Transport Theorem.(R.T.T.). Let us consider a system of mass m (Lagrangian approach) passing through a control volume (Eulerian approach). The theorem states that the rate of change of some property ϕ of the system is equal to the rate of change of the property within the control volume (CV) plus the net efflux of the property across the control surface (CS) at the very instant the mass occupies the control volume.

$$\frac{dm \phi}{dt} = \frac{d}{dt} \int_{CV} \rho \phi dV + \int_{CS} \rho \phi \vec{v} \cdot d\vec{A} \quad (2.1.1)$$

where m is the mass of the fluid element, ρ is the density, $\vec{v}$ is the velocity with respect to the control surface and the differential area vector $d\vec{A}$ is normal outward from the control surface.

In this chapter, the mathematical equations governing the gaseous carrier-phase will be derived from the Reynolds Transport Theorem (2.1.1) and then their numerical solution will be developed. The mathematical formulation can be found in Crowe (1976) and also in Smoot and Pratt (1979).

2.2 GOVERNING EQUATIONS OF THE GAS PHASE.

We want to be able to calculate the velocities, the concentrations, the temperature and the pressure of the gas at all points. For this we will divide the field into Control Volumes and apply the Reynolds Transport Theorem. In each of these Control Volumes, we include the two phases: particulate and gaseous. In order to study the gas phase alone we will separate it from the particles included in the volume. (fig. 2.1)

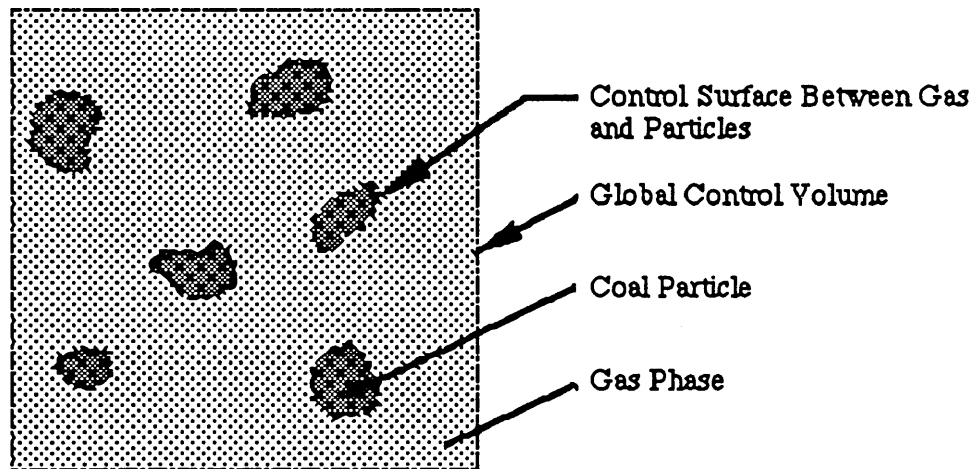


fig. 2.1
Control surfaces

The void left by the particles can be neglected in terms of volume for pf flames (Smoot and Pratt 1979) so we can write

$$\rho_m = \rho \quad (2.2.1)$$

where ρ_m is the density of the gas-particle mixture and ρ the density of the gas. The surface of the Control Volume can be written as:

$$CS_g = CS_p + CS \quad (2.2.2)$$

where CS_g is the control surface of the gas alone, CS_p the control surface between the particulate and the gas phase, and CS the control surface of the bulk.

The Reynolds Transport Theorem can then be written as:

$$\frac{dm \phi}{dt} = \frac{d}{dt} \int_{CV} \rho \phi dV + \int_{CS} \rho \phi \vec{v} \cdot d\vec{A} + \int_{CS_p} \rho \phi \vec{w} \cdot d\vec{A} \quad (2.2.3)$$

where $\vec{v}$ is the velocity of gas in relation to the control surface CS , and $\vec{w}$ the gas velocity in relation to the control surface CS_p .

2.2.1 Continuity Equation.

If we set the intensive property ϕ to 1, the R.T.T. gives the equation for conservation of mass with $\frac{dm}{dt} = 0$

$$0 = \frac{d}{dt} \int_{CV} \rho dV + \int_{CS} \rho \vec{v} \cdot d\vec{A} + \int_{CS_p} \rho \vec{w} \cdot d\vec{A} \quad (2.2.4)$$

We define S_m as the source of mass coming from the particulate phase:

$$\int_{CS_p} \rho \vec{u} \cdot d\vec{A} = - \int_{CV} S_m dV \quad (2.2.5)$$

By applying the Gauss theorem of divergence to these integral of volume, we obtain: (the integrand is constant since the control volume is arbitrary)

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \rho \vec{u} = S_m \quad (2.2.6)$$

where $\vec{\nabla}$ is the spatial gradient (nabla). This is the differential form of the continuity equation.

2.2.2 General Differential Equation

A similar procedure may be followed for all the dependent variables of interest. A general differential equation can be written:

$$\frac{\partial \rho \phi}{\partial t} + \vec{\nabla} \cdot (\rho \phi \vec{u}) = \vec{\nabla} \cdot (\Gamma_\phi \vec{\nabla} \phi) + S_\phi \quad (2.2.7)$$

where Γ_ϕ is the diffusion coefficient. S_ϕ is the source or sink defined as:

$$S_\phi = S_{g,\phi} + S_{p,\phi} \quad (2.2.8)$$

The quantities Γ_ϕ and $S_{g,\phi}$ are specific to a particular meaning of ϕ (see Patankar 1980). As not all diffusion fluxes are governed by the gradient of the relevant variable, whatever cannot be fitted into the diffusion term can always be expressed as part of the source term. $S_{p,\phi}$ embodies the exchange of the property ϕ between the particulate and the carrier phase.

We can write equation (2.2.7) in the Cartesian-tensor form :

$$\frac{\partial}{\partial t}(\rho \phi) + \frac{\partial}{\partial x_i}(\rho u_i \phi) = \frac{\partial}{\partial x_i} \left(\Gamma \frac{\partial \phi}{\partial x_i} \right) + S_\phi \quad (2.2.9)$$

where the subscript i can take the values 1, 2 or 3, denoting the three space coordinates.

NB: in this notation, when a subscript is repeated in a term, a summation of three terms is implied. For example: $\frac{\partial}{\partial x_i}(\rho u_i) = \frac{\partial}{\partial x_1}(\rho u_1) + \frac{\partial}{\partial x_2}(\rho u_2) + \frac{\partial}{\partial x_3}(\rho u_3)$

2.2.3 Momentum Equations

To illustrate the use of the General Differential Equation, let us write the differential equation for the fluid momentum in a direction j by replacing ϕ by the velocity. As the velocity has three components, a vectorial equation is now found. Therefore it will be necessary to solve three equations for components u_1 , u_2 and u_3 . (or u_i with $i=1,2,3$)

$$\frac{\partial}{\partial t}(\rho u_j) + \frac{\partial}{\partial x_i}(\rho u_i u_j) = \frac{\partial}{\partial x_i} \left(\mu \frac{\partial u_j}{\partial x_i} \right) - \frac{\partial p}{\partial x_i} + S_{uj} \quad (2.2.10)$$

The diffusion coefficient for momentum is the dynamic viscosity μ , the pressure stress

$\frac{\partial p}{\partial x_i}$ appears as a source, and S_{uj} is the momentum exchange rate between the

particles and the gas phase per unit of volume.

2.2.4 The Modelling of Turbulence

Turbulence is a three dimensional time-dependent motion in which vortex stretching causes velocity fluctuations to spread to all wavelengths between a minimum determined by viscous forces and a maximum determined by the boundary conditions of the flow. It is the usual state of fluid motion except at low Reynolds numbers. (Bradshaw 1975)

The velocity of fluid in turbulent motion can be described as a random continuous function of position and time. We are thus faced with an essentially unpredictable sequence of widely differing dynamic states, as opposed to the comparatively well

ordered and predictable laminar flow condition. The size scale of the smallest vortices, before their individual identities are lost through viscous smearing, may be as small as 10^{-4} m with frequencies greater than 10^4 Hz. Solution of the exact equations in such detail is not possible for engineering purposes, even with the most powerful computer available. Fortunately we are interested mostly in the **time-averaged** behaviour of the motion rather than its time-dependent random properties. The problem is therefore reduced to the solution of the time averaged version of the exact equations. Then we will construct some kind of turbulence model in order to show the influence of the fluctuations on the time averaged quantities.

2.2.4.1 The Closure Problem

The velocity u_i , as well as any scalar ϕ , are now defined as the sum of their time-average value $\overline{u_i}$, and $\overline{\phi}$, and a fluctuating part u_i' , and ϕ' respectively:

$$\begin{cases} u_i = \overline{u_i} + u_i' \\ \phi = \overline{\phi} + \phi' \end{cases} \quad (2.2.11)$$

where the time-averaging of a variable is written as $\overline{\phi} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \phi(t) dt$

(we have of course $\overline{\phi'} = 0$)

The averaging of the Differential Equation (2.2.9) leads to the appearance of a new unknown $\overline{u_i' \phi'}$ since:

$$\overline{u_i \phi} = \overline{u_i} \overline{\phi} + \overline{u_i' \phi'} \quad (2.2.12)$$

In the case of the momentum equations, $\overline{u_i' u_j'}$ is called the Reynolds stress after Osborne Reynolds (1842-1912) who, together with Joseph Boussinesq (1842-1929) identified laminar and turbulent types of flow. This term is an additional unknown in the

resolution of the averaged equations and it requires special treatment. This difficulty is known as the **closure problem**. One way to solve it is to approximate the above correlation in terms of quantities we can evaluate. These approximations are provided by **Turbulence Models**.

Extensive literature is available to describe turbulence models, their classification, applications and limitations. (See for example Launder and Spalding (1972)). It is not considered necessary to describe, list and classify those models here. The Two-Equation 'k- ϵ ' turbulence model was chosen for this study since it has been shown (Launder et al. 1972) to offer the best performance among other models excepting the more complex 'Reynolds stress' models. (Launder and Spalding 1974).

2.2.4.2 The Two-Equation 'k- ϵ ' Turbulence Model

This model has been used extensively (see Khalil et al. (1976), Carvalho (1983), Chakravarty (1984), Stolakis (1984), Rizvi (1985), Lockwood and Mahmud (1988) etc). Nevertheless it is necessary to point out some shortcomings of this model. Firstly, it is formulated assuming a constant density in the flow field. Secondly, the equations involved are not valid for low Reynolds number (see § 2.2.4.3). Thirdly, the discrete phase is not taken into consideration, and finally, the values of the constants used in the model are empirical and their universality is questionable

In the 'k- ϵ ' Turbulence Model, the transport equations are solved for the turbulent kinetic energy k and its dissipation rate ϵ defined by:

$$\begin{cases} k = \frac{1}{2} \overline{u_i' u_i'} \\ \varepsilon = \mu \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial u_i}{\partial x_k}} \end{cases} \quad (2.2.13)$$

In order to resolve the closure problem, it is assumed that the following linear relations may be used to relate the Reynolds Stresses to the rate of strain (Hinze 1975) :

$$-\rho \overline{u_i' u_j'} = \mu_t \left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right) - \frac{2}{3} \rho k \delta_{ij} \quad (2.2.14)$$

where δ_{ij} is the Dirac delta function and μ_t is the turbulent viscosity defined by:

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon} \quad (2.2.15)$$

where C_μ is a constant of the model.

The scalar correlation is estimated using the following equation introduced by Boussinesq (1877):

$$-\rho \overline{u_i' \phi'} = \Gamma_{\phi, t} \left(\frac{\partial \overline{\phi'}}{\partial x_i} \right) \quad (2.2.16)$$

with:

$$\Gamma_{\phi, t} = \frac{\mu_t}{\sigma_\phi} \quad (2.2.17)$$

Where $\Gamma_{\phi, t}$ and σ_ϕ are respectively the turbulent exchange coefficient and the Prandtl number for a scalar ϕ .

2.2.4.3 Transport Equation for Turbulent Kinetic Energy

At high Reynolds number, the transport equation may be expressed by (Rodi 1970):

$$\frac{\partial \rho k}{\partial t} + \frac{\partial}{\partial x_i} (\rho \overline{u_i k}) = \frac{\partial}{\partial x_i} \left(\frac{\mu_{eff}}{\sigma_k} \frac{\partial k}{\partial x_i} \right) + G - \rho \mathcal{E} \quad (2.2.18)$$

where:

- σ_k is the Prandtl number for turbulent energy.

- G represents the generation of turbulent energy and is given by (with $\overline{u_i' u_j'}$ being modelled by equation 2.2.14):

$$G = -\rho \overline{u_i' u_j'} \frac{\partial u_i}{\partial x_j} \quad (2.2.19)$$

- μ_{eff} is the effective viscosity and is the sum of the turbulent viscosity μ_t and the molecular or laminar viscosity μ :

$$\mu_{eff} = \mu + \mu_t \quad (2.2.20)$$

2.2.4.3 Transport Equation for Rate of Dissipation of Turbulent

Energy

Similarly, the transport equation for $\mathcal{E}$ may be written as (Rizvi 1985):

$$\frac{\partial \rho \mathcal{E}}{\partial t} + \frac{\partial}{\partial x_i} (\rho \overline{u_i \mathcal{E}}) = \frac{\partial}{\partial x_i} \left(\frac{\mu_{eff}}{\sigma_{\mathcal{E}}} \frac{\partial \mathcal{E}}{\partial x_i} \right) + C_1 \frac{\mathcal{E}}{k} G - C_2 \rho \frac{\mathcal{E}^2}{k} \quad (2.2.21)$$

where C_1 and C_2 are constants of the model, and $\sigma_{\mathcal{E}}$ is Prandtl number for $\mathcal{E}$. In the present study, the values used for the model constants are the ones recommended by Launder and Spalding (1974) and Launder (1978). They are listed in table 2.1 below together with the Prandtl numbers.

Table 2.1Values of constants for k- ϵ model.

(Launder and Spalding 1974 and Launder 1978)

C_μ	C_1	C_2	σ_k	σ_ϵ	σ_ϕ
0.09	1.44	1.92	0.9	1.3	0.9

2.2.5 Final form of the Equations for Gas-Phase

The final form of the transport equations describing the gas phase are shown in tables 2.2.1 and 2.2.2. They represent the actual equations that are solved in the present study. They are derived from the general differential equation (2.2.9) which has been time averaged, and to which the k- ϵ turbulence model has been introduced. They are written for an axi-symmetric flow. The set of coordinates is therefore cylindrical with 'x' located on the axis of symmetry, 'r' is the radial distance, and 'θ' is the angular coordinate.

The effective exchange coefficient $\Gamma_{\phi, \text{eff}}$ is defined, in the same way as the effective viscosity (cf. eq. (2.2.20)), as the sum of the molecular and the turbulent exchange coefficients:

$$\Gamma_{\phi, \text{eff}} = \Gamma_{\phi} + \Gamma_{\phi, t} = \frac{\mu}{\sigma_{\phi}} + \frac{\mu_t}{\sigma_{\phi, t}} \quad (2.2.22)$$

The source terms are defined in table 2.2.3

All the final equations are represented in table 2.2.1 and 2.2.2. Their similarity allows us to write them in the following generalised form:

$$\frac{\partial}{\partial x_i} (\rho \overline{u_i} \overline{\phi}) = \frac{\partial}{\partial x_i} \left(\Gamma_{\phi \text{ eff}} \frac{\partial \overline{\phi}}{\partial x_i} \right) + S_{\phi} \quad (2.2.23)$$

where $\overline{\phi}$ stands for the time-averaged value of any variable, $\Gamma_{\phi \text{ eff}}$ is the corresponding effective turbulent exchange coefficient as defined in equation (2.2.22) and S_{ϕ} is the sum of $S_{g \phi}$ and $S_{p \phi}$ the gas-phase and the particle source terms (see equation 2.2.8).

2.3 DISCRETISATION METHOD

2.3.1 Introduction

The complexity of the differential equations of tables 2.2.1-3 rules out the possibility of an analytical solution, and leaves us with no other choice but to employ a numerical method. This approach treats as its basic unknowns the values of the dependent variable ϕ at a finite number of locations called grid points. In the Finite-Difference method, which has been chosen for this study, the calculation domain is divided into a number of non-overlapping control volumes such that there is one control volume surrounding each grid point. In this method, only the grid-point values of the variable ϕ are considered to constitute the solution, with no account being taken as to how ϕ varies between the grid points. (see Patankar (1980))

An original code for the calculation of two dimensional recirculating flows was created at Imperial College with the name of TEACH-T (see Gosman and Ideriah (1976)). It is this procedure which, after being improved and expanded, is used in the present project. In this section, this procedure will be outlined and discussed.

2.3.2 Computing Grid and Layout of the Variables

The grid arrangement employed in the Finite Difference solution is shown in figures 2.2. to fig.2.4. The intersections of the solid lines • represent the locations where all the variables, except velocity components $\bar{u}$ and $\bar{v}$, are computed. The latter are stored at the points denoted by arrows ($\rightarrow$), mid-way between two scalar nodes (fig.2.2). This 'staggered grid' system has the advantage of having the variables u , v and p stored in such a way that the pressure gradients which drive the velocities are easy to evaluate. Moreover the velocities are readily available for the calculation of the convective fluxes across the boundaries of the scalar cells.

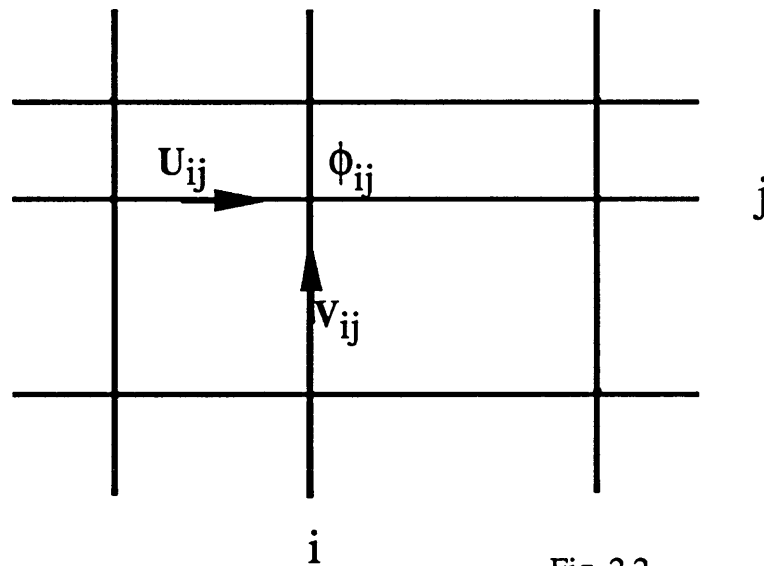


Fig. 2.2
The Staggered Grid System

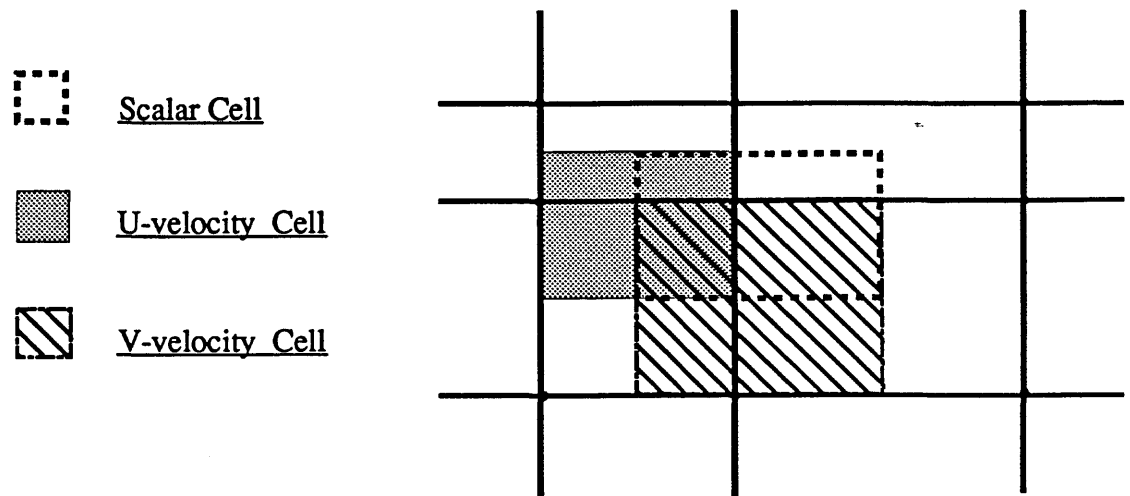


Fig. 2.3
The Control Volumes

The control volumes for scalars and velocities are depicted in fig.2.3. Note the convention for neighbouring cells shown in fig.2.4 : **N**, **S**, **E** and **W** stand for North, South , East and West respectively, whereas **P** represents the studied cell. Upper case symbols designate points whereas lower case designate control volume boundaries.

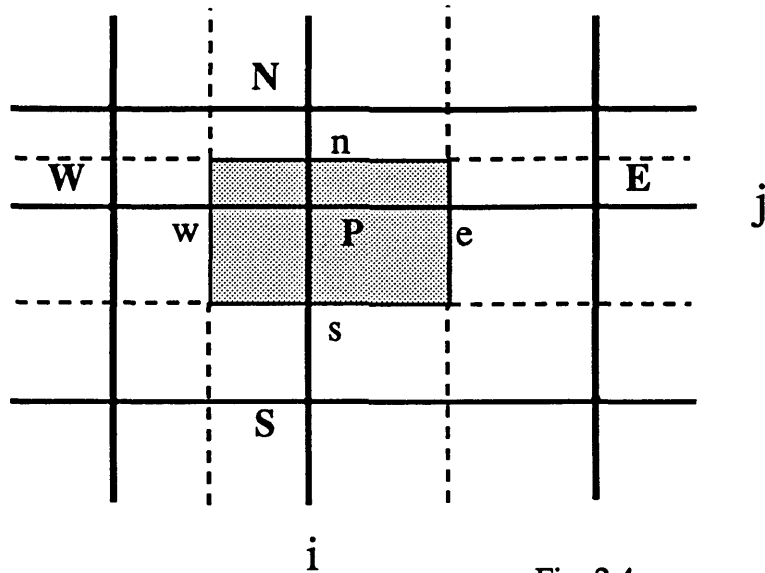


Fig. 2.4
Control Volume boundaries

2.3.3 Discretisation of the Differential Equations

The integration of equation (2.2.23) over the volume V_p of the cell shown in fig. 2.4 gives:

$$\sum_{\substack{4 \text{ boundaries} \\ \text{of cell}}} \left[\int_A \left(\rho \bar{u}_i \bar{\phi} - \Gamma_{\phi \text{ eff}} \frac{\partial \bar{\phi}}{\partial x_i} \right) dA \right] = \int_{V_p} S_{\phi} dV$$

(2.3.1)

where S_{ϕ} is the total source (gas and particle) per unit volume and A is the area of the considered cell boundary. The integration of the left hand side term over the cell gives:

$$-\dot{q}_w + \dot{q}_e - \dot{q}_s + \dot{q}_n = \int_{V_p} S_\phi dV \quad (2.3.2)$$

where $\dot{q}_b$ ($b = w, e, s, n$) is the sum of the convective and diffusive fluxes of $\bar{\phi}$ across the west, east, south and north boundaries:

$$\dot{q}_b = \rho_b u_b A_b (F_b \bar{\phi}_B + (1-F_b) \bar{\phi}_P) \quad (2.3.3)$$

In the 'exact' analytical solution of equation (2.3.1), the definition of F for a boundary b is:

$$F_b = \frac{\exp(Pe_b)}{\exp(Pe_b) - 1} \quad (2.3.4)$$

where Pe_b is the local Peclet number defined by:

$$\begin{cases} Pe_b = \frac{\rho_b u_b \delta x_i}{\Gamma_b} \\ \rho_b = \frac{\rho_B + \rho_P}{2} \\ \Gamma_b = \frac{\Gamma_B + \Gamma_P}{2} \end{cases} \quad (2.3.5)$$

In order to avoid time expensive calculations of exponential functions, a method using piece-wise linear fit is adopted to approximate the 'exact' $\dot{q}$ - Pe relation with little loss of accuracy (Gosman et al. 1969). In this method, the central and the upwind difference schemes (Patankar 1980) are combined. The resulting 'hybrid' scheme is defined by:

$$F_b \equiv \begin{cases} \frac{1}{2} \left[(1+2Pe_b^{-1}) \bar{\phi}_B + (1-2Pe_b^{-1}) \bar{\phi}_P \right] & \text{for } -2 < Pe_b < 2 \\ \bar{\phi}_W & \text{for } Pe_b \geq 2 \\ \bar{\phi}_P & \text{for } Pe_b \leq -2 \end{cases} \quad (2.3.6)$$

The integration of the source term of equation (2.3.2) gives:

$$\int_{V_p} S_\phi dV = S_g \phi + S_p \phi = (S_u + S_p \phi) + S_p \phi \quad (2.3.7)$$

Note that the gas term $S_g \phi$ is expressed as a linear function of $\bar{\phi}$.

The assembly of equations (2.3.6), (2.3.7), (2.3.3) and (2.3.2) finally gives the finite-volume equation:

$$(a_p - S_p) \bar{\phi}_P = \sum_b (a_b \bar{\phi}_B) + S_u + S_p \phi \quad (2.3.8)$$

where:
$$a_b = \rho_b u_b A_b F_b = (\rho u A F)_b \quad (2.3.9)$$

$$a_p = \sum_b a_b = a_n + a_e + a_w + a_s \quad (2.3.10)$$

and:

$$\sum_b a_b \bar{\phi}_P = a_n \bar{\phi}_N + a_e \bar{\phi}_E + a_w \bar{\phi}_E + a_s \bar{\phi}_S \quad (2.3.11)$$

This finite volume difference equation is an integral representation of the differential equation (2.2.23) over the control volume formed by each grid node for any property ϕ . It yields a closed set of algebraic equations which will be solved using a line-by-line (LBL) procedure (see § 2.4). As can be seen in equation (2.3.8), the solution of these equations needs the knowledge of a **given** flow field (i.e. velocities and density). The velocity components are governed by the momentum equations, which are particular cases of the general differential equation for ϕ .

2.3.4 The Pressure-Correction Algorithm

PISO

The real difficulty in the calculation of the flow field lies in the unknown pressure field, the gradient of which forms part of the source term of a momentum equation. The pressure field is not directly specified in any equation and it can only be indirectly calculated via the continuity equation. A special algorithm is therefore necessary to convert the indirect information in the continuity equation into a direct calculation of the pressure field. This algorithm will now be described.

In the procedure introduced by Patankar and Spalding (1972), the Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) the momentum equations are solved in the following way: Firstly the pressure field is estimated. Secondly, estimates of velocities are obtained. Finally the pressure field is corrected in order to bring the velocity field into conformity with the continuity equations. This procedure sometimes suffers from slow convergence for recirculating flows. (Benodekar et al. (1983))

Rizvi (1985) showed that the use of the two-stage predictor-corrector scheme PISO (Pressure Implicit Split Operator) (see Issa (1982)) improved the computational efficiency of the code. This is explained by the fact that at each cycle of iteration, the mass and momentum balance equations are more closely satisfied than with SIMPLE. The PISO algorithm involves splitting of operations to deal with the coupling between velocity and the pressure fields.

Let the superscripts *, ** and *** denote intermediate field values obtained during the splitting operations. The PISO procedure consists of the following sequential steps:

1.- Predictor Step. The discretised finite-volume momentum conservation equation (refer to table 2.2.1 and to Eq. (2.3.8)) is written as:

$$a_p \overline{u_i} = \sum_b (a_b \overline{u_{iB}}) - \Delta_i p + Su_i \quad (2.3.12)$$

where $\overline{u_i}$ stands for the velocity components $\overline{u}$ and $\overline{v}$ and Δ_i is the finite-difference equivalent of the gradient operating on the pressure p . Su_i is the cumulative associated source inclusive of the particle-gas interaction effects.

In this predictor step, the prevailing pressure field, at the m^{th} iteration, p^m , is used in the solution of equation (2.3.12) to obtain an intermediate velocity field u_i^* , thus:

$$a_p \overline{u_i^*} = \sum_b (a_b \overline{u_{iB}^*}) - \Delta_i p^m + Su_i \quad (2.3.13)$$

2.- First corrector step. A new velocity field u_i^{**} is sought together with a new pressure field p^* such that the divergence condition:

$$\nabla_i \overline{u_i^{**}} = S_{p\ m} \quad (2.3.14)$$

representing the continuity equation (2.2.6), is satisfied. The required finite-difference momentum equation is:

$$a_p \overline{u_i^{**}} = \sum_b (a_b \overline{u_{iB}^{**}}) - \Delta_i p^* + Su_i \quad (2.3.15)$$

The procedure is as follows. An incremental form of the momentum equation is obtained by subtracting Eq. (2.3.13) from Eq. (2.3.15) so that:

$$a_p (\overline{u_i^{**}} - \overline{u_i^*}) = - \Delta_i (p^* - p^m) \quad (2.3.16)$$

Taking the divergence of Eq. (2.3.16) and using the continuity equation (2.3.14), we obtain the following form of the pressure-correction equation:

$$\nabla_i \left(\frac{1}{a_p} \Delta_i p' \right) = \nabla_i \overline{u_i^*} - S_{p m} \quad (2.3.17)$$

where $p' = p^* - p^m$

The pressure-correction equation (2.3.17) is solved in terms of p' and the first corrector stage velocity field $\overline{u_i^{**}}$ is calculated using equation (2.3.16)

3.- Second corrector stage. An improved velocity field $\overline{u_i^{***}}$ with its corresponding pressure field p^{**} is obtained in the second corrector step such that:

$$\nabla_i \overline{u_i^{***}} = S_{p m} \quad (2.3.18)$$

The operative momentum equation for this case is represented as:

$$a_p \overline{u_i^{***}} = \sum_b (a_b \overline{u_{i B}^{**}}) - \Delta_i p^{**} + S_{u_i} \quad (2.3.19)$$

Subtracting Eq. (2.3.15) from Eq. (2.3.19) we get:

$$a_p (\overline{u_i^{***}} - \overline{u_i^{**}}) = \sum_b a_b (\overline{u_{i B}^{**}} - \overline{u_{i B}^*}) - \Delta_i (p^{**} - p^*) \quad (2.3.20)$$

A second stage pressure correction equation is obtained by combining the divergence of Eq.(2.3.20) with the continuity relations (2.3.14) and (2.3.18):

$$\nabla_i \left(\frac{1}{a_p} \Delta_i p'' \right) = \nabla_i \left(\frac{1}{a_p} \sum_b a_b (\overline{u_{i B}^{**}} - \overline{u_{i B}^*}) \right) \quad (2.3.21)$$

Equation (2.3.21) is solved for p'' which is then used in conjunction with Eq.(2.3.20) to calculate $\overline{u_i^{***}}$. This completes the two-stage splitting operations resulting in the improved velocity field $\overline{u_i^{***}}$ and the pressure field p^{**} for the $(m+1)^{th}$ iteration values, namely, $\overline{u_i^m}$ and p^{m+1} .

2.3.5 Boundary Conditions

The resolution of the finite difference equation for a property $\bar{\phi}$ is only possible if a condition is specified at the limits of the calculation domain. These are the Boundary Conditions. The grid is arranged in such a way that the flow boundaries coincide with the faces of the ϕ -cell at the periphery of the domain. Such a layout ensures conservation of the fluxes and simplifies the treatment at the boundary, which can be dealt with by manipulation of flux and source coefficients. The domain is outlined by two kinds of neighbouring cells: a 'wall' cell or a 'flow' cell. The latter might be located at the inlet, at the exit or on the axis of symmetry.

2.3.5.1 Boundary Conditions for 'flow' cells

Boundary conditions at the inlet.: At the inlet boundary, the distribution of all the variables is either known or can be estimated. The specified distribution of the flow variables is supplied at all grid nodes of the entry plane. k and $\mathcal{E}$ are estimated using the relations:

$$\begin{cases} k_{\text{inlet}} = 0.005 u_{\text{inlet}}^2 \\ \mathcal{E}_{\text{inlet}} = C_{\mu} \frac{k_{\text{inlet}}^{1.5}}{\rho} \end{cases} \quad (2.3.22)$$

Boundary conditions at the outlet.: At the exit, the flow is assumed to be parabolic and the values of the variables, with the exception of the velocity component normal to the outlet plane, are set equal to the ones at the previous location. They do not have any affect on the field values. The normal velocity at the outlet plane is estimated according to the consideration of global mass conservation.

Boundary conditions on the axis of symmetry: At the axis of symmetry, the convective and diffusive fluxes are set to zero which implies zero gradient for all the variables in the normal direction.

2.3.5.2 The Wall Function.

It has been seen in section 2.2.4 that the k - ϵ turbulence model is applicable only for fully turbulent flows. In the near-wall regions, the turbulence (measured by the Reynolds number) reaches such levels that the molecular viscosity, rather than the turbulent one, can influence the production, destruction and diffusion of turbulence energy. The present turbulence model is therefore inapplicable near the walls.

The first way out this problem would be to employ a model that accounts for low Reynolds numbers (Jones and Launder 1973). However, the importance of the flow property gradients encountered in the near-wall regions would require such an impracticably fine grid that another solution is required.

The chosen technique employs the 'wall function' method to bridge over the near-wall region. (see Patankar and Spalding (1972)). The main assumptions made in the application of this technique for the near-wall region are:

1.- The flow in the region is assumed to behave as a one-dimensional Couette flow. This means that the shear stress remains equal to its value at the wall, a reasonable assumption except when there are high pressure gradients or near separation / reattachment.

2.- Diffusion and convection in the region can be neglected (Hinze (1975)). Therefore the generation of the turbulence energy is balanced by its dissipation rate. i.e.,

$$-\overline{u'v'} \frac{\partial U}{\partial y} \approx \epsilon \quad (2.3.23)$$

With the above assumptions it is rather easy to obtain the relations which link the shear stress and heat flux at the wall to the values of velocity, turbulence energy, rate of dissipation and temperature at the first grid points located next to the wall. A brief outline of the application of the 'wall function' is given below. For a more detailed analysis, refer to Launder and Spalding (1974).

1.- Velocity Distribution Near the Wall:

A one-dimensional Couette flow analysis in the absence of significant pressure gradient gives the following logarithmic law for the velocity component U , parallel to the wall (Shlichting (1968)):

$$\frac{U}{U_\tau} = U^+ = \begin{cases} y^+ & \text{for } y^+ \leq 11.63 \\ \frac{1}{\kappa} \ln (E y^+) & \text{for } y^+ > 11.63 \end{cases} \quad (2.3.24)$$

where $y^+ = \frac{\rho U_\tau y}{\mu}$; and $U_\tau = \sqrt{\frac{\tau_w}{\rho}}$ is the friction velocity.

Here τ_w is the wall shear stress, y is the normal distance from the wall, κ is Von Karman's constant ($\kappa = 0.4187$) and E is a quantitative measure of the wall roughness function and is obtained by measurement ($E = 9.793$ see Patel(1965)). Equation (2.3.24) is used to obtain the source terms for the cells next to the wall, see Gosman and Ideriah (1976).

2. Distribution of k and ϵ near the wall.

The gradient transport hypothesis (2.2.14) for a one dimensional flow with uniform shear-stress gives:

$$\frac{\tau_w}{\rho} = - \overline{u'v'} = \frac{\mu_t}{\rho} \frac{\partial U}{\partial y} \quad (2.3.25)$$

A one-dimensional Couette flow analysis using Eq. (2.3.25) yields the following boundary conditions which are used to obtain the source terms for the near wall cells (see Rizvi (1985)):

$$\left\{ \begin{array}{l} k = C_{\mu}^{-1/2} \frac{\tau_w}{\rho} \\ \epsilon = \frac{C_{\mu}^{3/4} k^{-1/2}}{\kappa y} \end{array} \right. \quad (2.3.26)$$

3.- Scalar Distribution near the wall

The incorporation of the scalar variable wall boundary conditions is done in a similar manner to that of momentum conditions (eq. 2.3.24).

For example, the heat flux to the wall can be represented by:

$$q'' = \frac{\rho U_{\tau} (h_p - h_w)}{\sigma_{ht} (U^+ + P_j)} \quad (2.3.27)$$

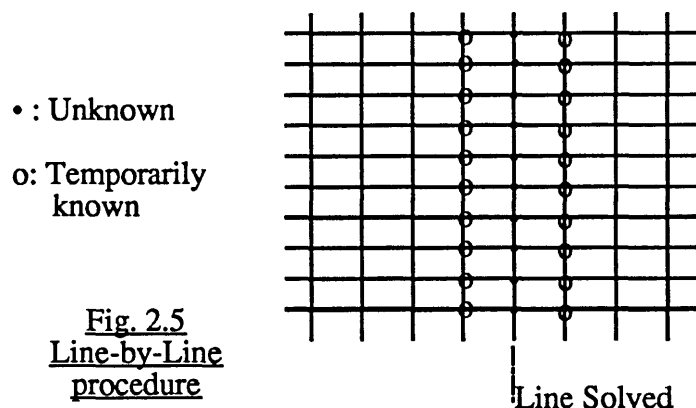
where P_j is a constant the value of which depends upon the ratio of the laminar to the turbulent Prandtl numbers. (see Salooja (1978))

2.4 SOLUTION OF THE FINITE DIFFERENCE EQUATIONS

The general finite difference equation introduced in section 2.3 represents the integration of the differential equations of table 2.2. over the control volume of a grid cell. There is one such equation to be solved for every cell of the domain, and for all the

properties ϕ to be calculated. The procedure to solve this set of equations will be discussed in this section.

The solution technique employed is iterative and line-by-line (LBL). An initial guess of values for the flow field is made, and these are improved upon one line to the next by sweeping in that direction over the entire domain (fig.2.5). For each point on each line five variables are unknown: ϕ_P , ϕ_N , ϕ_S , ϕ_W and ϕ_E . Values on neighbouring lines are assumed to be temporarily known (eg. ϕ_W and ϕ_E). The equations for each point then reduce to one where only three values are unknown (eg. ϕ_P , ϕ_N and ϕ_S). The set of equations for all points on the line (N-S in our example) then takes a particularly simple form in which the non-zero coefficient matrix is tri-diagonal. This matrix is solved by the Tri-Diagonal Matrix Algorithm (TDMA). (see Gosman and Ideriah (1976) or Patankar (1980))



Several sweeps can be applied for one variable. Alternatively different variants are possible: for example directions can be alternated. The number of sweeps as well as the direction used in the present study are described in chapter 5.

TIME AVERAGED FORM OF THE CONTINUITY EQUATION	
$\frac{1}{r} \left(\frac{\partial}{\partial r} (r \bar{\rho} \bar{v}) + \frac{\partial}{\partial z} (r \bar{\rho} \bar{u}) \right)$	$= S_{p,m}$
TIME AVERAGED FORM OF THE MOMENTUM EQUATION	
<u>r-direction:</u>	
$\frac{1}{r} \left(\frac{\partial}{\partial r} (r \bar{\rho} \bar{v} \bar{v}) + \frac{\partial}{\partial z} (r \bar{\rho} \bar{v} \bar{u}) \right)$	$= \frac{1}{r} \left\{ \frac{\partial}{\partial r} \left(r \mu_{\text{eff}} \frac{\partial \bar{v}}{\partial r} \right) + \frac{\partial}{\partial z} \left(r \mu_{\text{eff}} \frac{\partial \bar{v}}{\partial z} \right) \right\} - \frac{\partial \bar{p}}{\partial r} + \bar{\rho} g_r + S_v + S_{p,v}$
<u>z-direction:</u>	
$\frac{1}{r} \left(\frac{\partial}{\partial r} (r \bar{\rho} \bar{u} \bar{v}) + \frac{\partial}{\partial z} (r \bar{\rho} \bar{u} \bar{u}) \right)$	$= \frac{1}{r} \left\{ \frac{\partial}{\partial r} \left(r \mu_{\text{eff}} \frac{\partial \bar{u}}{\partial r} \right) + \frac{\partial}{\partial z} \left(r \mu_{\text{eff}} \frac{\partial \bar{u}}{\partial z} \right) \right\} - \frac{\partial \bar{p}}{\partial z} + \bar{\rho} g_z + S_u + S_{p,u}$
<u>θ-direction:</u>	
$\frac{1}{r} \left(\frac{\partial}{\partial r} (r \bar{\rho} \bar{v} \bar{w}) + \frac{\partial}{\partial z} (r \bar{\rho} \bar{u} \bar{w}) \right)$	$= \frac{1}{r} \left\{ \frac{\partial}{\partial r} \left(r \mu_{\text{eff}} \frac{\partial \bar{w}}{\partial r} \right) + \frac{\partial}{\partial z} \left(r \mu_{\text{eff}} \frac{\partial \bar{w}}{\partial z} \right) \right\} + S_w + S_{p,w}$

Table 2.2.1 The Final Form of the Transport Equations, Continuity and Momentum

Additional Source Terms associated with non uniform viscosity for Momentum Equations	
$S_v =$	$\frac{1}{r} \frac{\partial}{\partial r} \left(r \mu_{eff} \frac{\partial \bar{v}}{\partial r} \right) + \frac{\partial}{\partial z} \left(r \mu_{eff} \frac{\partial \bar{u}}{\partial r} \right) + \frac{\rho \bar{w}^2}{r} - 2 \mu_{eff} \frac{\bar{v}}{r^2} - \frac{\partial}{\partial r} \left(\frac{2}{3} \bar{\rho} k \right)$
$S_u =$	$\frac{1}{r} \frac{\partial}{\partial r} \left(r \mu_{eff} \frac{\partial \bar{v}}{\partial z} \right) + \frac{\partial}{\partial z} \left(r \mu_{eff} \frac{\partial \bar{u}}{\partial z} \right) - \frac{\partial}{\partial z} \left(\frac{2}{3} \bar{\rho} k \right)$
$S_w =$	$-\bar{w} \left(\frac{\bar{\rho} \bar{v}}{r} + \frac{\mu_{eff}}{r^2} + \frac{\partial \mu_{eff}}{r \partial r} \right)$

Table 2.2.2 The Final Form of the Transport Equations. Additional Sources

TIME AVERAGED FORM OF THE SCALAR TRANSPORT EQUATION	
$\frac{1}{r} \left(\frac{\partial}{\partial r} (r \bar{\rho} \bar{v} \bar{\phi}) + \frac{\partial}{\partial z} (r \bar{\rho} \bar{u} \bar{\phi}) \right)$	$= \frac{1}{r} \left\{ \frac{\partial}{\partial r} \left(r \Gamma_{\phi \text{ eff}} \frac{\partial \bar{\phi}}{\partial r} \right) + \frac{\partial}{\partial z} \left(r \Gamma_{\phi \text{ eff}} \frac{\partial \bar{\phi}}{\partial z} \right) \right\} + S_{g,\phi} + S_{p,\phi}$
TIME AVERAGED FORM OF THE TRANSPORT EQUATION FOR THE TURBULENCE MODEL	
<u>kinetic energy:</u>	
$\frac{1}{r} \left(\frac{\partial}{\partial r} (r \bar{\rho} \bar{v} k) + \frac{\partial}{\partial z} (r \bar{\rho} \bar{u} k) \right)$	$= \frac{1}{r} \left\{ \frac{\partial}{\partial r} \left(r \frac{\mu_{\text{eff}}}{\sigma_k} \frac{\partial k}{\partial r} \right) + \frac{\partial}{\partial z} \left(r \frac{\mu_{\text{eff}}}{\sigma_k} \frac{\partial k}{\partial z} \right) \right\} + G - \bar{\rho} \epsilon$
<u>dissipation:</u>	
$\frac{1}{r} \left(\frac{\partial}{\partial r} (r \bar{\rho} \bar{v} \epsilon) + \frac{\partial}{\partial z} (r \bar{\rho} \bar{u} \epsilon) \right)$	$= \frac{1}{r} \left\{ \frac{\partial}{\partial r} \left(r \frac{\mu_{\text{eff}}}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial r} \right) + \frac{\partial}{\partial z} \left(r \frac{\mu_{\text{eff}}}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial z} \right) \right\} + C_1 \frac{\epsilon}{k} G - C_2 \bar{\rho} \frac{\epsilon^2}{k}$

Table 2.2.3 The Final Form of the Transport Equations, Scalar and Turbulence Model

CHAPTER 3

PARTICULATE PHASE MODELLING

A concise description of the Lagrangian and the Eulerian approaches was presented in chapter 2. It was shown there how the gaseous carrier-phase of the flow is predicted by means of the Eulerian approach. In these calculations, the coal particles entrained by the gas were excluded from the control volumes, and considered only as sources or sinks of matter, momentum and energy (cf. section 2.3). In this chapter, the behaviour of the particulate or solid phase will be described, and its modelling introduced.

3.1 THE TRACKING OF THE PARTICLES

3.1.1 Choice of Method

The solid phase may be considered as a continuum, and therefore modelled by an Eulerian approach, or as a discrete phase characterised by its statistics. Previous attempts were made to use the Eulerian approach for the particulate phase. Spalding (1971) described the particle size distribution by a discretisation into uniform diameter groups with 'species-like' partial differential equations being solved for the mass fraction of particles in each group. An Eulerian particle treatment of this kind was employed to make general computations in pulverised coal combustors by Gibson and Morgan (1970) and later by Gosman et al. (1976). As expected, conceptual difficulties arise in defining the averages for the velocities and temperatures. The averaging procedure is further complicated by the fact that different-sized particles will have different temperatures and velocities and consequently the mass-averaged quantities will be different from the momentum averaged ones.

In the Lagrangian approach formulated by Migdal and Agosta (1967) and later used by Crowe (1974) for a spray cooling problem, the flights of statistically representative particles are tracked from the point of entry through to the combustor exit. The

information regarding the presence of particles to the gas flow is provided by means of the source coupling parameters in the Reynolds Transport Theorem.

Comparisons between discrete and continuum models carried out by Lockwood and Syed (1977) and by Abbas et al. (1981) showed that Eulerian based models required greater computer storage due to its dependence on the number of size groups. They also made it more difficult to apply physical laws such as drag, heat transfer, particle devolatilisation and char combustion, and were not as computationally economical as Lagrangian methods (Abbas 1982)

Unfortunately the interaction of Lagrangian based computations with the gas field (determined using the Eulerian approach) may be a source of instability. Another shortcoming of the Lagrangian approach is the difficulty in handling the dispersion of particles due to turbulence.

On the basis of these arguments, preference was given to the discrete Lagrangian procedure for the computation of the particulate phase. The present treatment has been employed in various studies by for example Abbas et al. (1981) for spray combustion, and by Lockwood et al (1978), Lockwood et al (1984), Rizvi (1985), Lockwood and Mahmud (1988) for Coal flames.

3.1.2 Description of the Method.

It is necessary to assume the following hypotheses in order to predict the courses that coal particles follow inside the combustor:

- First, it is assumed that the particles are spherical.
- Then that they are distributed into a finite number n_{ps} of size groups, each one representing a certain number of mono-sized identical particles having the same mass, momentum and temperature.
- Finally, it is assumed that they enter the computational region of the combustor from a discrete number n_{sl} of 'starting locations' in the plane of the burner exit.

On the basis of these premises, it is possible to reduce the considerable amount of coal particles to be studied into a smaller number of samples n_p , each representing a size group and a starting location:

$$n_p = n_{sl} \times n_{ps} \quad (3.1.1)$$

with n_{sl} and n_{ps} being the number of starting locations and the number of particle sizes respectively. In the example shown in fig. 3.1, the bulk of particles have been divided into 2 size groups and 2 starting locations, therefore only four particle histories need to be calculated. It is clear that the quality of the prediction is proportional to the number of samples computed. Experiments have shown that satisfactory results can be obtained by sampling the particle flow in 4 size groups and calculating from 4 starting locations ($n_p = 16$).

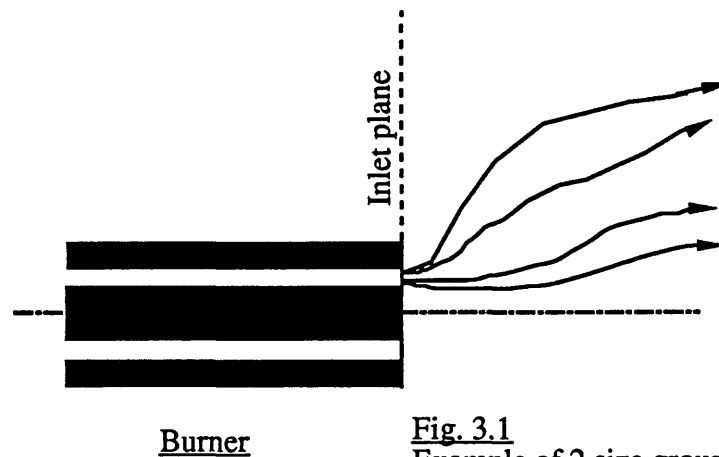


Fig. 3.1
Example of 2 size groups
starting from to 2 locations.

To simplify the situation, it is assumed that the effect of the particle to particle interaction is small. Also, the effect of the presence of particles on the gas turbulence is ignored. It is further assumed that the effect of particle collisions is small compared to the effect of gas-particle coupling occurring between two collisions. (see Crowe (1976) and Smoot and Pratt (1979))

3.1.3 Particle History.

It has been described how the tracking of a small number of particles will be used to predict the behaviour of a pulverised fuel flame. In the following sections, the models used in order to calculate the history of one particle are presented. The objective is to determine the physical and chemical responses of the particle to the environment of the furnace.

First, the particle trajectory will be calculated by taking into account its initial momentum and the gas velocities (see section 3.2). Then, the heat transfers will be dealt with in order to determine its temperature (see section 3.4). Finally, the knowledge of the temperature will enable the chemical reactions to be predicted. When coal is heated to a sufficiently high temperature it begins to decompose into volatiles. This step is called devolatilisation or pyrolysis (see section 3.5). The released volatiles consist of a mixture of combustible gases and water vapour. These gases will react with the oxygen contained in the gas phase (see section 3.7). The char remaining after devolatilisation consists primarily of carbon together with the ash components and some remaining volatiles. The carbon contained in the char will now react in a heterogeneous reaction. (see section 3.6)

3.2 PARTICLE TRAJECTORY.

In this section, the mathematical formulation leading to the calculation of the trajectory of the n_p particles will be presented.

It is assumed that a non-rotating particle moving in a carrier phase is subjected only to the following forces:

- the gravitational force $\vec{F}_G$
- the drag force $\vec{F}_D$ (which includes turbulent diffusion)
- the forces due to the swirl, or tangential velocities of the carrier phase $\vec{F}_{sw}$

Newton's second law is written as:

$$m_p \frac{d\vec{V}_p}{dt} = \vec{F}_G + \vec{F}_D + \vec{F}_{sw} \quad (3.2.1)$$

where $\vec{V}_p$ is the particle velocity and m_p its mass.

The effect of gravity is generally small compared with the drag forces (see Ioannides and Gosman (1978)), and can therefore be ignored in most cases.

$$\vec{F}_G = m_p \vec{G} \quad (3.2.2)$$

The drag force is a function of particle relative velocity and may be expressed as:

$$\vec{F}_D = \frac{1}{2} \rho_g C_D A_p |\vec{V}_g - (\vec{V}_p + \vec{V}_{diff})| (\vec{V}_g - (\vec{V}_p + \vec{V}_{diff})) \quad (3.2.3)$$

where $\vec{V}_p$ is the particle velocity, $\vec{V}_g$ the local gas velocity, $\vec{V}_{diff}$ represents the effect of turbulent diffusion on the particle velocity and is calculated separately in section 3.2.1. C_D is the drag coefficient, ρ_g the local gas density, and A_p the area of the particle.

An expression for the drag coefficient of a solid sphere in a carrier phase is given by Wallis (1969):

$$C_D = \frac{1 + 0.15 Re_p^{0.687}}{Re_p / 24} \quad (3.2.4)$$

where Re_p is the particle Reynolds number defined by:

$$Re_p = \frac{\rho_p D_p |\vec{V}_g - (\vec{V}_p + \vec{V}_{diff})|}{\mu} \quad (3.2.5.)$$

where D_p is the particle diameter, ρ_p its density, and μ the viscosity.

Finally, the forces due to the swirl are written as:

$$\vec{F}_{SW} = \frac{m_p}{r} \begin{pmatrix} 0 \\ w_p w_p \\ v_p w_p \end{pmatrix} \quad (3.2.6)$$

where $(w_p w_p)$ is the radial component due to the centrifugal force and $(v_p w_p)$ is the angular component due to the Coriolis force.

Equation (3.2.1) combined with equation (3.2.2) to (3.2.6) gives:

$$\begin{cases} \frac{du_p}{dt} = -\alpha [(u_p + u_{diff}) - u_g] + g_u \\ \frac{dv_p}{dt} = -\alpha [(v_p + v_{diff}) - v_g] + g_v + \frac{w_p^2}{r} \\ \frac{dw_p}{dt} = -\alpha [w_p - w_g] - \frac{v_p w_p}{r} \end{cases} \quad (3.2.7)$$

where α is defined by:

$$\alpha = \frac{18 \mu (1 + 0.15 Re_p^{0.687})}{\rho_p D_p^2} \quad (3.2.8)$$

Equation (3.2.7) is integrated over a time step Δt . This is performed by assuming that gas velocities u_g , v_g , w_g , and turbulence diffusion velocities u_{diff} , v_{diff} , and α are constant during the time step:

$$\begin{cases} u_{p2} = u^* - (u^* - u_{p1}) e^{-\alpha \Delta t} \\ v_{p2} = v^* - (v^* - v_{p1}) e^{-\alpha \Delta t} \\ w_{p2} = \frac{w_g \alpha r}{\alpha r + v_p} - \left[\frac{w_g \alpha r}{\alpha r + v_p} - w_{p1} \right] e^{-\left(\frac{\alpha r + v_p}{r}\right) \Delta t} \end{cases} \quad (3.2.9)$$

where 1 and 2 stand for the velocities at time "t" and "t + Δt " respectively, and u^* and v^* are defined below:

$$\begin{cases} u^* = -u_{diff} + u_g + \frac{1}{\alpha} g_u \\ v^* = -v_{diff} + v_g + \frac{1}{\alpha} g_v + \frac{w_p^2}{\alpha r} \end{cases} \quad (3.2.10)$$

Computational restrictions at boundaries do not allow further integration of equations (3.2.10). The position of the particles is therefore calculated using an averaged particle velocity during the time step.

$$\begin{cases} x_{p2} = 0.5 (u_{p2} + u_{p1}) \Delta t + x_{p1} \\ y_{p2} = 0.5 (v_{p2} + v_{p1}) \Delta t + y_{p1} \end{cases} \quad (3.2.11)$$

With these equations, it is now possible to calculate the trajectory of a particle starting from the inlet plane up to the end of the combustor.

3.2.1 Dispersion due to Turbulence

The particle dispersion is the result of the gas-phase turbulence. It is due to the fluctuating part of the gas velocity. Lockwood et al. (1980) related the particle diffusion velocity in the axial and radial direction with the gas turbulence as follows:

$$\begin{cases} u_{diff p} = C_1 \sqrt{\overline{u'^2}} \\ v_{diff p} = C_2 \sqrt{\overline{v'^2}} \end{cases} \quad (3.2.12)$$

where C_1 and C_2 are empirical constant generally taken equal to 1.

In order to calculate the gas velocity fluctuations, the relation between the Reynolds Stresses and the rate of strain of section 2.2.4 is used as follows (equation 2.2.14):

$$-\rho \overline{u_i' u_j'} = \mu_t \left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right) - \frac{2}{3} \rho k \delta_{ij} \quad (2.2.14)$$

If we write the the axial and radial components for $i=j$ we obtain the Boussinesq hypothesis:

$$\begin{cases} \overline{u'^2} = -\frac{2 \mu_t}{\rho} \left(\frac{\partial \overline{u}}{\partial x} \right) + \frac{2}{3} k \\ \overline{v'^2} = -\frac{2 \mu_t}{\rho} \left(\frac{\partial \overline{v}}{\partial y} \right) + \frac{2}{3} k \end{cases} \quad (3.2.13)$$

The particle drift velocity can now be written as:

$$\begin{cases} u_{\text{diff } p} = C_1 \sqrt{\left| \frac{-2 \mu_t}{\rho} \left(\frac{\partial \bar{u}}{\partial x} \right) + \frac{2}{3} k \right|} \\ v_{\text{diff } p} = C_2 \sqrt{\left| \frac{-2 \mu_t}{\rho} \left(\frac{\partial \bar{v}}{\partial y} \right) + \frac{2}{3} k \right|} \end{cases} \quad (3.2.14)$$

Unfortunately these calculations do not give us the sign of the diffusion velocities $U_{\text{diff } p}$ and $V_{\text{diff } p}$. As the direction taken by the drift is random, there is no deterministic way to calculate it. An attempt was made to give to these diffusion velocities a randomly determined sign. The result of this attempt is given in chapter 6, section 6.2.3.3. It will be seen there that this attempt did not result in an improvement of the prediction.

3.3 THE PARTICLE MASS BALANCE.

During the history of the particles inside the combustors, they experience changes in mass. These are due to chemical reactions such as devolatilisation, and char combustion. The amount of matter the particles lose or gain is accounted for as sinks and sources of mass in the gas phase:

$$\frac{d m_p}{dt} = r_{me} \quad (3.3.1)$$

where r_{me} is the rate of mass efflux from the particle surface. It is a complicated function of the thermodynamic and aerodynamic states of the particle and the gas, and it is estimated using special models which are described in sections 3.6 and 3.7.

3.4 THE PARTICLE HEAT BALANCE.

In order to calculate the temperature of the particle, it is necessary to solve its energy balance. The total rate of heat Q_T gained or lost by the particle per unit of mass is composed of the contributions due to convection Q_C , radiation Q_R and combustion Q_B :

$$Q_T = Q_c + Q_r + Q_b \quad (3.4.1)$$

Latent heat is also lost by mass transfer due to devolatilisation, and this heat rate is written as $L_v \frac{d m_p}{dt}$ where L_v is the latent heat coefficient. Similarly sensible heat is lost by mass transfer due to combustion, the heat rate being written as $C_p T_p (-\frac{d}{dt} m_p)$.

The first law of thermodynamics is therefore written as:

$$\frac{d}{dt} (m_p C_p T_p) = m_p Q_t - C_p T_p (-\frac{d}{dt} m_p) - L_v \frac{d m_p}{dt} \quad (3.4.2)$$

where m_p , C_p and T_p are the particle mass, specific heat and temperature respectively, and L_v is the latent heat of devolatilisation.

By assuming that $\frac{d C_p}{dt} = 0$, we have:

$$C_p \frac{d T_p}{dt} = Q_t - \frac{L_v}{m_p} \frac{d m_p}{dt} \quad (3.4.3)$$

This equation is used to calculate the particle temperature using small time increments δt . The amounts of heat gain or loss are calculated as follows.

3.4.1 Convection.

The heat transfer due to convection is calculated using (see Baum and Street (1971)):

$$Q_c = \pi d_p^2 h \frac{T_g - T_p}{m_p} \quad (3.4.4)$$

where h is the heat transfer coefficient given by the Nusselt number Nu and the gas thermal conductivity K_g :

$$h = Nu \frac{K_g}{d_p} \quad (3.4.5)$$

$$Nu = 2 + 0.6 Re_p^{1/2} Pr^{1/3} \quad (3.4.6)$$

where Pr is the Prandtl number. For the conductivity, the following relation suggested by Baum and Street (1971) is used:

$$K_g = 6.739 \times 10^{-5} T_g + 6.446 \times 10^{-3} \quad (3.4.7)$$

It is assumed here that the particle surface temperature is uniform.

3.4.2 Radiation.

The heat exchange due to radiation between the particle and the surroundings may be expressed as:

$$Q_r = \pi \sigma \epsilon_p d_p^2 \frac{T_R^4 - T_p^4}{m_p} \quad (3.4.8)$$

where σ is Stefan-Boltzman constant ($\sigma = 5.67 \times 10^{-8} \text{ J / m}^2 \text{ s K}^4$), T_R is the radiation temperature, and ϵ_p is the particle emissivity.

3.4.3 Combustion.

The char combustion process is described in section 3.6 together with the numerical model. The latter calculates the char burning rate in terms of mass (see equation 3.6.7) Therefore the heat release is calculated as a function of the burning rate. It is first assumed that the reaction of carbon dioxide and water with carbon are small and can be ignored. It is further presumed that the char is composed of pure carbon together with the ash components. The heat release is written as:

$$Q_b = \frac{f_{CO} H_c}{m_p} - \frac{d m_p}{dt} \quad (3.4.9)$$

where m_p is the particle mass and H_c is the calorific value of Carbon for complete combustion ($C + O_2 \rightarrow CO_2$)

Two different schemes of char combustion can be considered depending on whether the product of combustion transported away from the surface of the particle is assumed to be carbon monoxide or carbon dioxide. The factor f_{CO} depends on the adopted scheme. It depends also on whether the heat generated by the char combustion is supposed to be given to the bulk gas or to the particle. In this study, it is the latter which is adopted together with a complete combustion hypothesis. The value of f_{CO} is therefore 1.

3.5 DEVOLATILISATION

The rate and extent of the thermal decomposition of coal particles plays an important part in the processes occurring in a pulverised fuel flame, where as much as 50 % by weight of the feed coal may volatilise and burn in the gas phase. (Badzioch and Hawksley 1970).

It is generally accepted that the variables which influence significantly the pyrolysis process and the composition of the volatiles released are: the characteristics of the coal dust such as concentration, particle size and distribution; the thermal history of the particles, including heating rate, final temperature, duration of heating; and the composition and pressure of the ambient gas. (See Anthony and Howard (1976), Smoot and Pratt (1979) and Howard (1981)).

It is important to identify the conditions in pulverised fuel flames relevant to rapid pyrolysis. The parameters of interest include particle size of 100 μm or less, heating rates of at least 10 000 K/s, final temperatures of 1000 °K or greater, total decomposition times of less than 1 second (see Field et al. (1967) for example).

3.5.1 General Observation

It has generally been supposed that the devolatilisation of coal is a chemical decomposition reaction, (see Anthony and Howard (1976) and Howard (1981)). However, evidence also indicates control by the mass transport processes (see Gray et al. (1974), Jost et al. (1984) and Simons (1984)), and heat transfer to the particle (See Peters (1960), Maloney and Jenkins (1984) and Tsai and Scaroni (1984)) during the rapid pyrolysis of coal. Measurable devolatilisation does not start until temperatures of 350° to 400° C are reached. It is generally agreed that rapid heating influences not only the amount of volatiles generated, but also the product composition, see for example Field et al. (1967).

It has been shown that high heating rates and final temperatures generate an increasing amount of volatiles V^* that can considerably surpass, and in some cases double or triple, the amount VM observed during proximate analysis (Field et al. (1967), Eddinger et al. (1966), Menster et al. (1974) and Anthony et al. (1975)). Interestingly, Anthony et al (1975) concluded that the volatiles gain depends only on final temperature (not on the heating rate) and that an increase in the final temperature produces an increased yield. It was further argued that the increased yield attributed to heating rate was probably due to conditions employed to achieve faster heating, such as well dispersed small particles, which suppress some of the secondary reactions like cracking and repolymerisation.

Secondary reactions have also been attributed as responsible for the decrease in the yield and as influencing the volatile composition with increase in particle size and pressure, see Howard (1963) and Suuberg (1977).

3.5.2 Experimental Results

Due to the extremely complex nature of the pyrolysis process, heavy reliance on experimental data is necessary. The experimental conditions comparable to those expected in full-scale p.f. operation, with attendant sampling and analysis requirements, are difficult to achieve. The phenomena are so complex that it is difficult to isolate properly the data from significant influences of the equipment itself. Detailed descriptions of the way the experimental techniques are employed and the critical assessment of the published data may be found in the reviews of Badzioch (1967), Badzioch and Hawksley (1970) Essenhigh and Howard (1971), Anthony and Howard (1976) and Howard (1981).

3.5.3 Devolatilisation Models

Several proposals have been made to describe the release of volatiles when a coal particle is heated. A complete pyrolysis model should be able to describe, at all stages of devolatilisation, the composition and physical state of the coal dust as well as the composition and evolution rate of the volatiles. The theoretical formulation must be sufficiently versatile to accommodate the coal type, particle size, and local conditions of the surroundings. In the case where the solid phase reacts with the volatile products, these secondary reactions and their reaction rates should also be defined. Clearly, the quest for the universal model formulation is a difficult one. The hope is that the predictions will not be critically dependent on the detailed features and parametric prescription of the model.

A complete review of the available models can be found in Anthony and Howard (1976) and Smoot and Pratt (1979). In the following sections, some of the most commonly used devolatilisation models are examined.

3.5.3.1 Single Reaction Model

The overall pyrolysis process is approximated as a first-order decomposition occurring uniformly throughout the particle. Thus, the rate of devolatilisation is expressed as:

$$\frac{dV}{dt} = k(V^* - V) \quad (3.5.1)$$

where V is the cumulative amount of volatiles released up to time ' t ' expressed as a weight fraction of the initial coal and k is the rate constant. We have:

$$\lim_{t \rightarrow \infty} V(t) = V^* \quad (3.5.2)$$

V^* is the effective volatile content of the coal which, as seen before, is not necessarily equal to the volatile content VM obtained from proximate analysis. The ratio

$$Q = \frac{V^*}{VM} \quad (3.5.3)$$

can vary from 1.0 to 2.0. (see Badzioch and Hawksley (1970) , Anthony and Howard (1976)).

The rate constant k is typically correlated to the temperature by an Arrhenius expression:

$$K = A \exp\left(\frac{-E}{RT}\right) \quad (3.5.4)$$

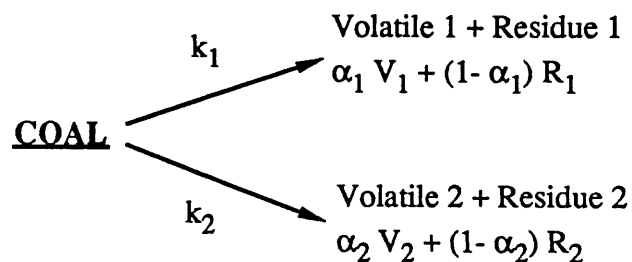
where A is the pre-exponential factor, E is the activation energy, R the gas constant and T is the absolute temperature of the particle.

There is little agreement on pyrolysis rate constants between different investigators, with several orders of magnitude discrepancy at a given temperature. These discrepancies are due to coal type, differences in equipment and experimental procedures. (see Howard (1981)). The apparent requirement of different A and E values for each set of experimental conditions is the main weakness of this model.

The main advantage of the model is its simplicity.

3.5.3.2 Two-Competing Reactions Scheme

An alternative model accounting for the increase in volatile yield with the increase in temperature is that the coal decomposition is governed by competing reactions having different volatile yields. The reaction having the higher yield has the higher activation energy. (See Kobayashi et al. 1976)



The rate constants are of the Arrhenius form:

$$\begin{cases} k_1 = A_1 \exp \frac{-E_1}{RT} \\ k_2 = A_2 \exp \frac{-E_2}{RT} \end{cases} \quad (3.5.5)$$

where A_1 and A_2 are the pre-exponential factors, and E_1 and E_2 the activation energies.

The first reaction is assumed to be dominant at relatively low temperatures leading to the asymptotic yield α_1 . At high temperatures the second reaction is assumed to become faster than the first one, which amounts to requiring that E_2 be much higher than E_1 , resulting in larger volatile yields.

The overall weight loss is given by:

$$V = \int_0^t \left[(\alpha_1 k_1 + \alpha_2 k_2) \exp \left(- \int_0^t (k_1 + k_2) dt \right) \right] dt \quad (3.5.6)$$

The major drawback of this model is the necessity to determine six empirical coefficients (α_1 , α_2 , A_1 , A_2 , E_1 and E_2). Insufficient data exists to determine these parameters making the use of the model often impossible. (see Truelove and Williams (1988))

3.5.3.3 Multiple Parallel Reactions Model

This proposal from Anthony et al. (1975) represents a further attempt to find a convenient chemical scheme of sufficient generality to fit the data. It is assumed that the pyrolysis process is described by a large number of independent chemical reactions. The decomposition of one particular reaction 'i' is expressed as:

$$\frac{d V_i}{dt} = k_i (V_i^* - V_i) \quad (3.5.7)$$

where k_i is of the Arrhenius form $k_i = A_i \exp (-E_i / RT)$ and $(V_i^* - V_i)$ is the amount of volatiles yet to be released at time t .

The problem is simplified if it is assumed that the k_i 's differ only in activation energy (i.e. $A_i = A_0$ for all i) and that the number of reactions is large enough to permit E to be expressed as a continuous Gaussian distribution $f(E)$, about a mean value E_0 , with $F(E) dE$ representing the fraction of the potential volatile V^* which has an activation energy between E and $E+dE$. Then the volatile content can be expressed as:

$$V = V^* \frac{1}{\sigma \sqrt{2\pi}} \int_0^{\infty} \left\{ 1 - \exp \left[- \int_0^t A_0 \exp \left(\frac{-E_0}{RT} \right) dt \right] \right\} \times \exp \left(\frac{-(E-E_0)^2}{2\sigma^2} \right) dE$$

(3.5.8)

where σ is the standard deviation of E .

3.5.3.4 Choice of model

The single-reaction model has been found by many authors to be inadequate for high temperatures and high volatile coals, because it does not account for the increase of volatile yield with increasing temperature. Truelove and Williams (1988) even calculated a devolatilisation rate an order of magnitude greater, using the two-reaction model, than that obtained using the single-reaction model at a particle temperature of 1000°C. In Lockwood and Mahmud (1988) a greater and more accurate rate of devolatilisation was found using the multiple parallel reaction model than that found using the single-reaction model.

Despite the short-comings of the single-reaction model, its use is much simpler than the others. It only needs the knowledge of three quantities: the Q-factor (equation 3.5.3), the pre-exponential factor A and the activation energy E which have been determined for a considerable amount of coals (see Badzioch and Hawksley (1970) and the review by Anthony and Howard (1976)). The Two-Competing Reaction Model needs six empirical constants and the Multiple-Reaction Model also introduces another unknown quantity (the

standard deviation σ). For this reason, and as one of the objectives of the present work was to increase the generality of the code and to simplify its use, preference was given to the single reaction model.

3.6 CHAR COMBUSTION

Historical aspects of coal and carbon combustion have been outlined by Essenhigh (1961) and Mulcahy (1978). Field (1967) and Smoot and Pratt (1979) have given comprehensive accounts of pulverised coal combustion. Specific reviews on the mechanics involved in the coal-oxygen and related reactions have been given by Thring and Essenhigh (1963), Mulcahy and Smith (1969) and Essenhigh (1981). Smith reviewed factors controlling the reactivity of pulverised coal chars.

The char remaining after devolatilisation is considered to be pure carbon together with the ash components. The heterogeneous reaction between oxygen and a single char particle is governed by the external (near the particle surface) and internal (within the porous char matrix) diffusion of oxygen, and the chemical reaction with the particle surface matrix. However, for computational purposes a simplified description of heterogeneous char reaction is used where the reaction rate is controlled by the external diffusion of oxygen and the chemical reaction at the surface of the particle which is assumed to be spherical.

3.6.1 Mass Transfer of Oxygen to the Particle Surface

Mass balance considerations give the particle burning rate R_c as

$$R_c = k_d [(P_{Ox})_{\infty} - (P_{Ox})_0] \quad (3.6.1)$$

where $(P_{Ox})_{\infty}$ is the oxygen partial pressure in the bulk gas and k_d is the diffusion reaction rate coefficient defined by (Field et al. (1967)):

$$k_d = \frac{D_c M_c \phi}{\left[R \frac{d}{2} \left(\frac{T_p + T_g}{2} \right) \right]} \quad (3.6.2)$$

where M_c is the atomic weight of Carbon. ϕ is a mechanism factor and its value is 2 if CO is the main product being driven away from the particle boundary layer, 1 if it is CO₂, T_p and T_g are the particle and gas temperatures respectively, R is the gas constant and D_c is the diffusion coefficient defined by:

$$D_c = D_o \left(\frac{p_o}{p} \right) \left(\frac{T_g}{T_o} \right)^{1.75} \quad (3.6.3)$$

where the subscript _o designates reference temperature and pressure. D_o is the binary diffusion coefficient for an oxygen-nitrogen mixture. D_o is taken as 3.13×10^{-4} m²/s at a reference temperature $T_o = 1500$ K and reference pressure $p_o = 1.013 \times 10^5$ Pa.

3.6.2 Chemical Kinetics

The rate of reaction of a char particle with oxygen may be expressed as:

$$R_c = k_c (P_{ox})_o^n \quad (3.6.4)$$

where k_c is the chemical reaction rate coefficient of order n and $(P_{ox})_o$ is the oxygen partial pressure at the surface. k_c may be expressed by an Arrhenius relation:

$$k_c = A \exp \left(\frac{-E}{RT_p} \right)^n \quad (3.6.5)$$

where A is the frequency factor and E the apparent activation energy. T_p is the particle temperature. In general K_c combines the separate effects of the intrinsic reactivity of the carbon and the pore diffusion. Experimental studies have been carried out to determine the reaction rate coefficient K_c for different types of coals, see for example Field et al. (1967), Smith (1971) and Wall et al. (1982).

3.6.3 Overall Rate Coefficient

Field et al. (1967) recommended the use of an overall rate coefficient k_t , which is formed by combining the two rate coefficients:

$$k_t = \frac{1}{\frac{1}{k_d} + \frac{1}{k_c}} \quad (3.6.6)$$

where k_d and k_c are the diffusion and chemical rate coefficients defined above.

The char burning rate is finally written as:

$$\frac{d m_p}{dt} = - k_t \pi d^2 p (F_{ox})_\infty \quad (3.6.7)$$

where p is the gas pressure and $(F_{ox})_\infty$ the molar fraction of oxygen in the combustion gas.

3.7 VOLATILE COMBUSTION

The pyrolysis process and different ways of modelling it have been treated in section 3.5. The released volatiles react with the oxygen contained in the gas phase. The 'eddy dissipation model' proposed by Magnussen and Hjertager (1976) is a simple and computationally economical combustion model similar to the 'eddy break-up' approach of Spalding (1971). The essential feature of this model is that it is applicable to premixed as well as diffusion flames. The main features of the combustion model can be described as follows. In diffusion flames fuel and oxygen occur in separate eddies. Because the chemical reactions in most cases are very fast, it can be assumed that the rate of combustion will be determined by the rate of dissipation of the eddies. This dissipation rate is proportional to the time scale of the large-scale eddies (ϵ / k). It is further assumed that the reaction rate of dissipation is proportional to the smallest of the fuel, oxygen or products concentrations. The rate of combustion of fuel is then written as:

$$R_f = A \bar{\rho} \frac{\epsilon}{k} \min \left(m_{fu} ; \frac{m_{ox}}{S} ; \frac{m_{pr}}{B(1+S)} \right) \quad (3.7.1)$$

where $A=4$ and $B=2$ are empirical constants, ρ is the gas density, k the turbulence kinetic energy, ϵ the dissipation rate of kinetic energy, S the stoichiometric oxygen requirement and m_{fu} , m_{ox} and m_{pr} are the mass concentrations of fuel, oxygen and combustion products respectively.

CHAPTER 4

THERMAL RADIATION TRANSFERS

Radiation heat transfer plays a dominant role in most industry combustors and furnaces, especially oil and coal-fired ones. Calculation of the radiation exchange at any point in the furnace, whether on a surface or within the gas, is a very complex task. The energy emitted by a small volume of gas within a combustor is not difficult to estimate provided one knows the gas composition and mean temperature. The problem arises in estimating the radiation arriving at this volume, see Johnson (1971). The reason is that the radiant energy received by the volume is attenuated by absorption in the intervening medium, or by scattering away from the line travel, and it is enhanced by scattering into the considered direction. Therefore estimating the radiation exchange by the given small volume is strongly influenced by the combustor geometry and the local values of the radiation properties such as emissivity, absorptivity, reflectivity and scattering coefficients of the radiating medium.

4.1 THE TRANSPORT EQUATION

The radiation transport equation is derived in terms of a transport property known as the radiation intensity I_λ , defined as the amount of monochromatic radiant energy Q transported in a given direction per unit of area normal to the direction, per unit of solid angle and per unit of time:

$$I_\lambda \equiv \lim_{(d\lambda, dA, d\omega, dt) \rightarrow 0} \left(\frac{dQ}{d\lambda, dA, d\omega, dt} \right) \quad (4.1.1)$$

where λ represents the wavelength of the monochromatic radiant energy, dA is an element of area normal to the specified direction $\underline{\Omega}$, and $d\omega$ is the element of solid angle about that direction. The balance of radiant energy transfer in a specified direction $\underline{\Omega}$ through a small volume in an emitting-absorbing-scattering medium, taken along a pencil

of rays within an elemental solid angle $d\omega$, can be written as (see for example Lowes et al. (1973):

$$(\underline{\Omega} \cdot \nabla) I_{\lambda} = \underbrace{- (K_{\lambda a} + K_{\lambda s}) I_{\lambda}}_{(I)} + \underbrace{K_{\lambda a} I_{b\lambda}}_{(II)} + \underbrace{\frac{K_{\lambda s}}{4\pi}}_{(III)} \int_{4\pi} P_{\lambda}(\underline{\Omega}, \underline{\Omega}') I_{\lambda}(\underline{\Omega}') d\omega' \quad (4.1.2)$$

where $K_{\lambda a}$ and $K_{\lambda s}$ are the monochromatic absorption and scattering coefficients, $I_{b\lambda}$ is the intensity of black body radiation at wavelength λ . $P_{\lambda}(\underline{\Omega}, \underline{\Omega}')$ is the probability that incident radiation of wavelength λ in the direction $\underline{\Omega}'$ confined in the element of solid angle $d\omega'$ will be scattered into the increment of solid angle $d\omega$ in the $\underline{\Omega}$ direction.

In equation (4.1.2):

term (I) represents the gradient of radiation intensity in the $\underline{\Omega}$ direction,

term (II) is attenuation of intensity due to absorption within the volume and the scattering into other directions;

term (III) gives the intensity augmentation due to the emission from the volume,

term (IV) estimates the intensity enhancement due to scattering into the considered $\underline{\Omega}$ direction from all the other directions.

Details of the development of this equation may be found in Viskanta (1966)

Equation (4.1.2) can be integrated over all possible wavelengths and over the solid angle of 4π to obtain the net radiative heat flux per unit time. Integrating equation (4.1.2) gives:

$$\begin{aligned}
& \int_{\lambda=0}^{\infty} \int_{\omega=0}^{4\pi} (\underline{\Omega} \cdot \nabla) I_{\lambda} d\omega d\lambda = - \int_{\lambda=0}^{\infty} \int_{\omega=0}^{4\pi} (K_{\lambda a} + K_{\lambda s}) I_{\lambda} d\omega d\lambda \\
& + \int_{\lambda=0}^{\infty} \int_{\omega=0}^{4\pi} K_{\lambda a} I_{b\lambda} d\omega d\lambda \\
& + \int_{\lambda=0}^{\infty} \int_{\omega=0}^{4\pi} \frac{K_{\lambda s}}{4\pi} \int_{\omega'=0}^{4\pi} P_{\lambda}(\underline{\Omega}, \underline{\Omega}') I_{\lambda}(\underline{\Omega}') d\omega' d\omega d\lambda \quad (4.1.3)
\end{aligned}$$

Equations of the above form can be written for surfaces, which will provide us with the necessary boundary conditions for equation (4.1.3). The integration will be performed over a solid angle of 2π on the surface. The result represents the radiant flux leaving (q^-) or reaching (q^+), the considered surface:

$$q^- = \int_{\lambda=0}^{\infty} \int_{\omega=0}^{2\pi} (\underline{\Omega} \cdot \nabla) I_{\lambda}^- d\omega d\lambda \quad (4.1.4)$$

and

$$q^+ = \int_{\lambda=0}^{\infty} \int_{\omega=0}^{2\pi} (\underline{\Omega} \cdot \nabla) I_{\lambda}^+ d\omega d\lambda \quad (4.1.5)$$

where I_{λ}^- and I_{λ}^+ are the intensity of radiation leaving or reaching the surface. As the surface is a wall, a portion of the incident radiation is absorbed while the rest is reflected. The departing flux q^- is the resultant of the reflected flux and the flux emitted from the surface, so that:

$$q^- = (1-\epsilon) q^+ + \sigma \epsilon T_w^4 \quad (4.1.6)$$

where ϵ and T_w the wall emissivity and temperature respectively and σ is the Stefan-Boltzmann constant. Here the surface is assumed to be opaque to thermal radiation, and therefore the transmitted component of q^+ is zero and the reflected flux is equal to $(1-\epsilon)$ times the incident flux q^+ .

Ideally, equation (4.1.3) will have to be solved for every point within the combustor in conjunction with equations (4.1.4) and (4.1.5) for every point at the combustor wall as boundary conditions. The analytical solution for this set of integro-differential equations is very complex even for very simple geometries. In the following section some of the available numerical solution procedures for the radiation calculation are briefly described.

4.2 RADIATION SOLUTION PROCEDURES

The existing radiation models are generally classified into three groups commonly referred to as: 'Monte Carlo Methods', the 'Zone Method', and 'Flux Models'. Some of the radiation solution procedures are summarised below.

4.2.1 The Monte Carlo Method

In the Monte Carlo methods (Howell (1968) and Stewart and Cannon (1971)) statistical studies are made to obtain the history of emitted energy bundles. The relationships between radiative transfers of the energy are obtained in terms of the probability of occurrence of different events. This method solves the exact radiation transport equation and its accuracy depends upon the number of rays along which the emission history is determined. By taking enough rays any degree of accuracy is achievable, but the computing time is considerable.

4.2.2 The Zone Method

In the zone method, (Hottel and Cohen (1958)), the combustion space and the boundary walls are divided into finite zones in which gas thermal radiation and other properties are assumed to be uniform. Radiation exchange is estimated between zone pairs. Consequently, if n is the total number of zones, n simultaneous equations will be obtained. This method requires excessive storage and is expensive in terms of computational economy.

4.2.3 Flux Models

In the flux method a suitable spatial intensity distribution is assumed. The basic idea is to separate the directional dependence from the spatial dependence of the intensity. In a 'discrete flux' method, De Marco and Lockwood (1975) and Lockwood and Shah (1976) used a truncated Taylor's series to represent the directional dependence of intensity. This series is substituted into the transfer equation (4.1.2) which is then integrated over selected angles to yield a set of simultaneous first-order equations. The angles of integration are made dependent on the local intensity distribution. The first-order equations are recast into a set of second-order equations of the diffusion kind and are solved by the numerical algorithm employed for flow calculations (see chapter 2). Flux methods are adequate and economical but are not easily adapted to new coordinate systems.

4.2.4 Discrete Transfer Method

Shah (1979) and Lockwood and Shah (1981) proposed and applied a method which they termed the 'Discrete Transfer Method'. It combines features and advantages of the Zone, Monte Carlo and flux models for solving radiation problems. It is based on the solution of representatively directed beams of radiation within the enclosure between the

known wall boundary conditions, and on the subsequent computing of the radiation sources which arise within the finited difference control volumes of the flow procedure due to the passage of the beams. This method is exact and applicable to complex geometries but demands larger computational times.

4.3 NON-EQUILIBRIUM DIFFUSION MODEL

Gibb (1973) proposed a simple and computationally economical radiation model which is an adaptation of non-equilibrium diffusion theory to suit the radiation calculations in furnaces: he refers to it as 'Non-Equilibrium Diffusion Radiation Model'. This method reduces what is essentially an integral equation describing a non-local field problem to a local field problem, the latter being written as a diffusion type second-order differential equation. Though approximate, this method is capable of generating satisfactory solutions to a permitted degree of accuracy (see Gibb (1973)). It has also been used for radiation calculation by Arscott et al. (1973)

Gibb (1977) developped the model further for the absorbing-emitting-scattering particulate-gas medium and employed it for radiation calculations in Pulverised Fuel (PF) combustors. Gibb (1977) and Lockwood et al. (1984) reported predictions of the incident radiation wall fluxes and succesfully compared the results with the measured data in PF combustors. Since then, the model has been succesfully used by Rizvi (1985), Lockwood and Rizvi (1985), Lockwood and Mahmud (1988) , Costa el al. (1990) for the calculation of radiation transfer in PF flames.

On the basis of simplicity, ease of application and computational economy, it was decided to select this model for the present study. A brief formulation method is described below.

4.3.1 Mathematical Formulation

For the absorbing-emitting-scattering medium of a PF space, the radiation transfer equation (4.1.2) can be rewritten separating radiation effects of the gas and particles as (see Gibb 1977)):

$$\underline{\Omega} \cdot \nabla I_{\lambda} = K_{\lambda a g} (B_{\lambda}(T_g) - I_{\lambda}) + E_{\lambda p} - A_{\lambda p} - S_{\lambda}^O + S_{\lambda}^i \quad (4.3.1)$$

where the first term on the right hand side is the intensity augmentation by the combined effects of emission and absorption of the gas medium at temperature T_g ; $K_{\lambda a g}$ is the gas absorption coefficient for wavelength λ and $B_{\lambda}(T_g)$ is the Planck function at temperature T_g and wavelength λ such that the gas emission per unit volume is:

$$E_{\lambda g} = \int_0^{4\pi} K_{\lambda a g} d\omega \quad (4.3.2)$$

The rest of the terms in equation (4.3.1) are defined below.

1.- Total particulate emission rate per unit path length and solid angle:

$$E_{\lambda p} = \int_0^{\infty} dr \int_0^{\infty} n(r, T_p) K_{\lambda a p}(r, T_p) B_{\lambda}(T_p) dT_p \quad (4.3.3)$$

2.- Total particulate absorption rate per unit path length and solid angle:

$$A_{\lambda p} = I_{\lambda} \int_0^{\infty} dr \int_0^{\infty} n(r, T_p) K_{\lambda a p}(r, T_p) dT_p \quad (4.3.4)$$

3.- Total particulate out-scattering rate per unit path length and solid angle:

$$S_{\lambda}^O = I_{\lambda} \int_0^{\infty} dr \int_0^{\infty} n(r, T_p) K_{\lambda s p}(r, T_p) dT_p \quad (4.3.5)$$

4.- Total particulate in-scattering rate:

$$S_{\lambda}^i = \frac{1}{4\pi} \int_0^{\infty} dr \int_0^{\infty} n(r, T_p) K_{\lambda s p}(r, T_p) dT_p \int_{4\pi} P_{\lambda}(\underline{\Omega}, \underline{\Omega}') I_{\lambda}(\underline{\Omega}') d\omega' \quad (4.3.6)$$

where $n(r, T_p) \cdot dr \cdot dT_p$ are the number of particles of radius between r and $(r+dr)$ and of temperature between T_p and (T_p+dT_p) in a unit chamber volume. Subscripts g and p here denote gas and particulate phase respectively. $K_{\lambda a p}(r, T_p)$ and $K_{\lambda s p}(r, T_p)$ are the radiation absorption and scattering cross sections for a particle of section r and temperature T_p .

The complexity of equation (4.3.1) can be reduced by assuming all materials to be grey and by defining:

$$\begin{cases} K_{\lambda a p} = \epsilon_p \pi r^2 \\ K_{\lambda s p} = \rho_p \pi r^2 \end{cases} \quad (4.3.7)$$

where ϵ_p and ρ_p are the emissivity and reflectivity of frequency and size independent particle material respectively. Also let:

$$K_p' = \int_0^{\infty} \pi r^2 n(r, T_p) dr dT_p \quad (4.3.8)$$

$$\overline{\rho_p} = \int_0^\infty \rho_p \pi r^2 n(r, T_p) dr \frac{dT_p}{K_p} \quad (4.3.9)$$

$$\overline{\epsilon_p} = \int_0^\infty \epsilon_p \pi r^2 n(r, T_p) dr \frac{dT_p}{K_p} \quad (4.3.10)$$

$$\frac{\sigma}{\pi} \overline{T_p^4} = \frac{\sigma}{\pi} \int_0^\infty \epsilon_p \pi r^2 n(r, T_p) T_p^4 dr \frac{dT_p}{(\overline{\epsilon_p} K_p)} \quad (4.3.11)$$

where $\overline{T_p}$ is a particle mean emission temperature.

The grey system assumption and the definitions (4.3.8) to (4.3.11) can be used to rewrite equation (4.3.1) in the frequency integrated form as: (see Gibb (1977))

$$\begin{aligned} \underline{\Omega} \cdot \nabla I &= K \left(\frac{\sigma}{\pi} T_g^4 - I \right) + \overline{\epsilon_p} K_p \left(\frac{\sigma}{\pi} \overline{T_p^4} - I \right) \\ &+ \overline{\tau_p} K_p \left\{ \frac{1}{4\pi} \int_{4\pi} p(\underline{\Omega}, \underline{\Omega}') I(\underline{\Omega}') d\omega' - I \right\} \end{aligned} \quad (4.3.12)$$

The appropriate boundary condition for a grey Lambert surface is expressed in the form:

$$I(\underline{\Omega}) = \frac{1}{\pi} \left\{ \epsilon_w T_w^4 + \tau_w \underline{E}_R^+ \cdot \underline{n}^> \right\} \quad (4.3.13)$$

where

$$\underline{E}_R^+ \cdot \underline{n}^> = \int_{2\pi} I(\underline{\Omega}^+) \underline{\Omega}^+ \cdot \underline{n}^> d\omega \quad (4.3.14)$$

is the flux incident in the wall, $\underline{n}^>$ the outward normal to the wall, $\underline{\Omega}^-$ and $\underline{\Omega}^+$ are respectively the directions of the reflected and incident radiation at the surface. Subscript w denotes the conditions at the wall. Also (+) denotes the incident direction. The radiation field variable $\underline{E}_R^+$, the radiation flux at any point within the gas, and T_R the 'radiation temperature', are defined as:

$$\underline{E}_R = \int_0^{\infty} d\lambda \int_0^{4\pi} I_{\lambda} \underline{\Omega} d\omega \quad (4.3.15)$$

$$4 \sigma T_R^4 = \int_{4\pi} I d\omega \quad (4.3.16)$$

Though somewhat simpler than equation (4.3.1), equation (4.3.12) and equation (4.2.13) still present formidable computational problems. Gibb (1973) employed a technique of truncated moment expansion to simplify the equations further. This technique offers a means of reducing the dimensionality of the problem by eliminating directional dependence $\underline{\Omega}$ from equation (4.3.12) and allows the derivation of the following two equations (see Gibb (1973) and Gibb (1977)):

$$\nabla \cdot \underline{E}_R = 4 \sigma K_g (T_g^4 - T_R^4) + 4 \sigma \overline{\epsilon_p} K'_p (\overline{T_p^4} - T_R^4) \quad (4.3.17)$$

$$\underline{E}_R = -\frac{4}{3} \frac{\sigma}{K_e} \nabla T_R^4 \quad (4.3.18)$$

where K_e is the 'equivalent absorption coefficient' and is defined as:

$$K_e = K_g + K'_p (\overline{\epsilon_p} + \overline{r} (1-f)) \quad (4.3.19)$$

where f is a 'scattering factor given by:

$$f = \frac{1}{(4\pi)^2} \int_0^{4\pi} d\omega \int_0^{4\pi} p(\underline{\Omega}, \underline{\Omega}') \underline{\Omega} \cdot \underline{\Omega}' d\omega' \quad (4.3.20)$$

The boundary condition equation (4.3.12) can be expressed as:

$$-\frac{1}{3K_e} \frac{\partial T_R^4}{\partial n} = \frac{1}{2} \frac{(1-r_w) T_R^4 - \epsilon_w T_w^4}{1 + r_w} \quad (4.3.21)$$

4.3.2 Model Governing Equations

The non-equilibrium diffusion radiation model may be summarised as follows: To estimate the radiation behaviour for a small volume in the combustion space, a single second-order elliptic equation is obtained from equations (4.3.17) and (4.3.18):

$$\nabla \cdot \left(\frac{1}{3 K_e} \nabla T_R^4 \right) = (K_g + \overline{\epsilon_p} K'_p) T_R^4 - K_g T_g^4 - \overline{\epsilon_p} K'_p \overline{T_p}^4 \quad (4.3.22)$$

It is solved using the boundary conditions of equation (4.3.21). Here K_g is the gas absorption coefficient, $\overline{T_p}^4$ is the particle mean emission temperature, $\overline{\epsilon_p}$ is the mean particle emissivity and $\overline{\epsilon_p} K'_p$ is the total absorption coefficient for the particle phase.

The radiation flux may then be calculated from equation (4.3.18)

4.3.3 Calculation of Source Terms

The net gas and particle radiation absorption rates per unit volume are the estimates of the radiation energy sources $S_{g h}$ and $S_{p h}$ of the gas energy balance equation (see equations of table 2.2.3 for $\phi = h$, the gas enthalpy). They can be expressed as:

$$S_{g h} = 4 \sigma K_g (T_R^4 - T_g^4) \quad (4.3.23)$$

and

$$S_{p h} = 4 \sigma \overline{\epsilon_p} K'_p (T_R^4 - \overline{T_p}^4) \quad (4.3.24)$$

T_R^4 is all that is required from the present radiation model for the calculation of radiation sources $S_{g h}$ and $S_{p h}$ and it is obtained solving equation (4.3.22)

4.4 OPTICAL PROPERTIES OF THE COMBUSTOR

The radiation properties of the materials within the combustion space need to be set for radiation heat exchange calculations. The properties for the particulate-gas medium and for the enclosing surface will be considered separately.

The main components of the medium inside a PF combustor contributing to radiation heat exchanges are: absorption due to carbon dioxide and water vapour; absorption by the micro size particles (soot); absorption and scattering by the larger particles (coal particles).

4.4.1 Absorption Coefficient for Combustion gases

The absorption coefficient K_g in equation (4.3.22) is an 'equivalent grey' absorption coefficient of the component real gases which are not grey and exhibit a wavelength variation in absorption coefficient. Truelove (1976) used a mixed grey-gas representation for estimating the total absorption coefficient. The value for the equivalent grey system gas absorption coefficient K_g , recommended by Gibb (1977) for PF flames in combustors and furnaces, is equal to 0.1 m^{-1} . This value is the one used in the present study.

4.4.2 Absorption Coefficient for Soot

No reliable data on the soot absorption coefficient for PF flames appears to be available. Soot measurements for oil flames indicate a maximum soot absorption coefficient value of 1.0 m^{-1} within 10 burner diameters (Gibb and Joyner (1979)). Field et al. (1967) and Csaba and Legett (1964) have given theoretical estimates for the soot absorption coefficient for PF flames. These theoretical values appear to be high ($\approx 2.0 \text{ m}^{-1}$) since it is difficult to believe that the higher excess air and lower volatile evolution rate in PF flames could lead to more vapour phase cracking than in an oil flame. In the absence of favourable experimental evidence these values are not credible. Gibb (1977) and Gibb and Joyner (1979) have recommended a typical volume mean value for soot absorption coefficient of 0.4 m^{-1} . This value has been adopted for radiation calculations.

4.4.3 Particle Absorption and Scattering Coefficients

The theory proposed by Mie can be used to obtain the absorption and the scattering coefficients of the larger particles, see for example Smoot and Pratt (1979). For the present study, however, geometrical concepts are employed to estimate these properties following the lead of Gibb and Joyner (1979). Treating the particles as opaque spheres with surface emissivity $\epsilon_p (= \overline{\epsilon_p})$ and reflectivity $\rho_p (= 1 - \overline{\epsilon_p})$, the absorption coefficient is given by:

$$K_p = \epsilon_p K'_p \quad (4.4.1)$$

and the scattering coefficient by:

$$K_p = (1 - \epsilon_p) K'_p \quad (4.4.2)$$

where K'_p is the cumulative projected area of particles of all sizes at all temperatures in a small volume.

4.4.4 Particle Emissivity

Experimental evidence indicates that the particle emissivity ϵ_p varies between 1 and 0.6 for unburnt coal particles and residual ash, (see Street and Twamley 1971). This recommendation has been adopted here and ϵ_p is estimated from the following approximate relationship (see Gibb and Joyner (1979)):

$$\epsilon_p = X_{uB} + 0.6 (1 - X_{uB}) \quad (4.4.3)$$

where X_{uB} is the fraction of the original char mass remaining unburnt at any point in the chamber.

4.4.5 Scattering Factor

The scattering factor 'f' of equation (4.3.20) is the overall effect of in-scattering. In the present study $f=0$ is used following the recommendation of Gibb (1977). However

Rizvi (1985) examined the influence of higher values ($f = 0.9$). He found no significant effect on incident wall radiation flux due to the in-scattering.

4.4.6 Wall Radiation Properties

The boundary condition equation (4.3.14) is based on the assumption that the enclosing wall is opaque to radiation (transmissivity = 0) and is a grey Lambert surface.

It follows that:

$$\varepsilon_w + \rho_w = 1 \quad (4.4.4)$$

The recommendation of Gibb (1977) and Gibb and Joyner (1979) was followed by assuming a wall emissivity of 0.6 for a fouled wall and 0.8 for a clean wall. Studies by Rizvi (1985) found the influence of varying wall emissivity significant only in the upstream region of the combustor where the flame temperatures are high.

CHAPTER 5

DESCRIPTION OF THE CODE: F A F N I R

In chapter 2 the differential equations governing a gas flow over a given domain were presented. A method to discretise those equations using a staggered grid was described in section 2.3, and the procedure to solve the set of such discretised equations was explained in section 2.4.

In chapter 3, the equations used to calculate the history of coal particles injected into a combustor were introduced. The mass and heat balance of the particles were treated, and it was shown how small time steps could be used to predict their trajectories (see section 3.2).

The radiation model and the discretisation of its equations has been described in the previous chapter .

The objective of the present chapter is to show how all those procedures are put together into routines forming a computer code. An overview of the code is first presented (section 5.1). Then the main routines will be analysed in detail (section 5.2). Finally computational and programming details will be given special attention with respect to the problems of convergence and the constants used to improve it. (section 5.3)

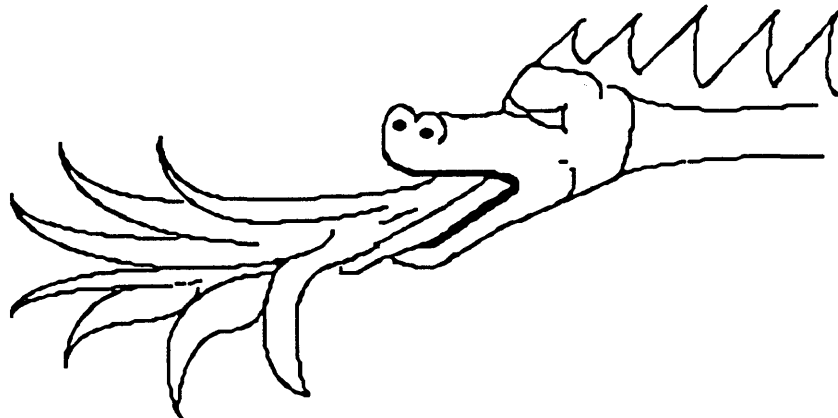
5.1 AN OVERVIEW OF THE PROGRAM

A complete code including radiation and coal combustion was first developed by Lockwood et al. (1980) and Lockwood and Salooja (1983). Rizvi (1985) improved it considerably making modifications to several of the models especially the tracking routine (see Lockwood and Rizvi (1983)). The present program is based on the latter. However, programming techniques were used to improve the performance and the ease of use of the

code. A better and more consistent structure was introduced and all the variables were re-defined in a more rational way. The program was translated from FORTRAN 4 to FORTRAN 5 (or 77). The particle tracking routine was completely revised and re-written. A principal improvement was achieved by creating a pre-processor whose function is to provide an interface between the user and the code, allowing several different types of geometries and settings to be solved with no need to tamper with the main program directly. A post-processor was also created giving the user several options for output.

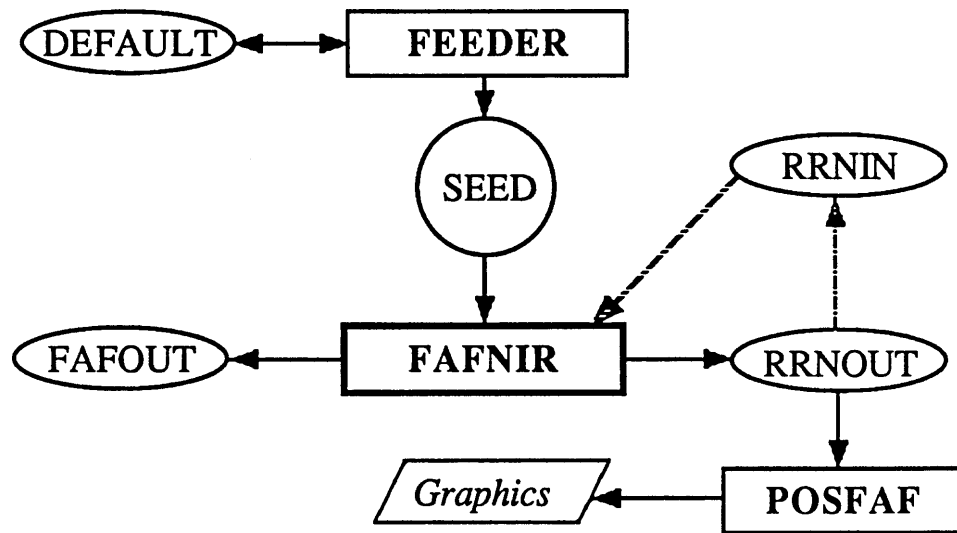
Finally the complete package was tested on several machines and systems: a VAX 8600 and a VAXstation 3200 (both under VMS), a DECstation 3100 (under UNIX), a Cyber 960 and a Cyber 930 (under Nos-Ve), a Cray I (under COS) and an IBM mainframe (under MVS). These runs proved that the package was not machine dependent.

The name given to the package is 'FAFNIR'. The name, in Norse mythology, of the son of Hreidmar who he killed to gain the cursed treasure of Andvari. He became a **Dragon** (!) and was slain by Sigurd while guarding the treasure. (Sigurd is also known as Siegfried in German mythology, see the song of Niebelung and the Gold of the Rhine)



5.1.1 The Structure of the Package

As explained in the previous section a pre-processor and a post-processor have been added to the code in order to help the input and output of the data and results. The layout of the package is shown in figure 5.1.1



Programs are shown in rectangles and files in ovals

Figure 5.1.1: Layout of the FAFNIR package

The pre-processor (FEEDER) gives the user the possibility to introduce the data into the program in a set of different simple ways. For example the input flow for each inlet can be given as a mass flow rate in kg/s or as a measured axial velocity in m/s. The pre-processor will then translate the data into a standard format (SEED) that the main program will understand. The pre-processor is interactive. It generates two files: the SEED and a default file. The latter is used as an input for subsequent runs of the pre-processor. It remembers the options taken when running FEEDER.

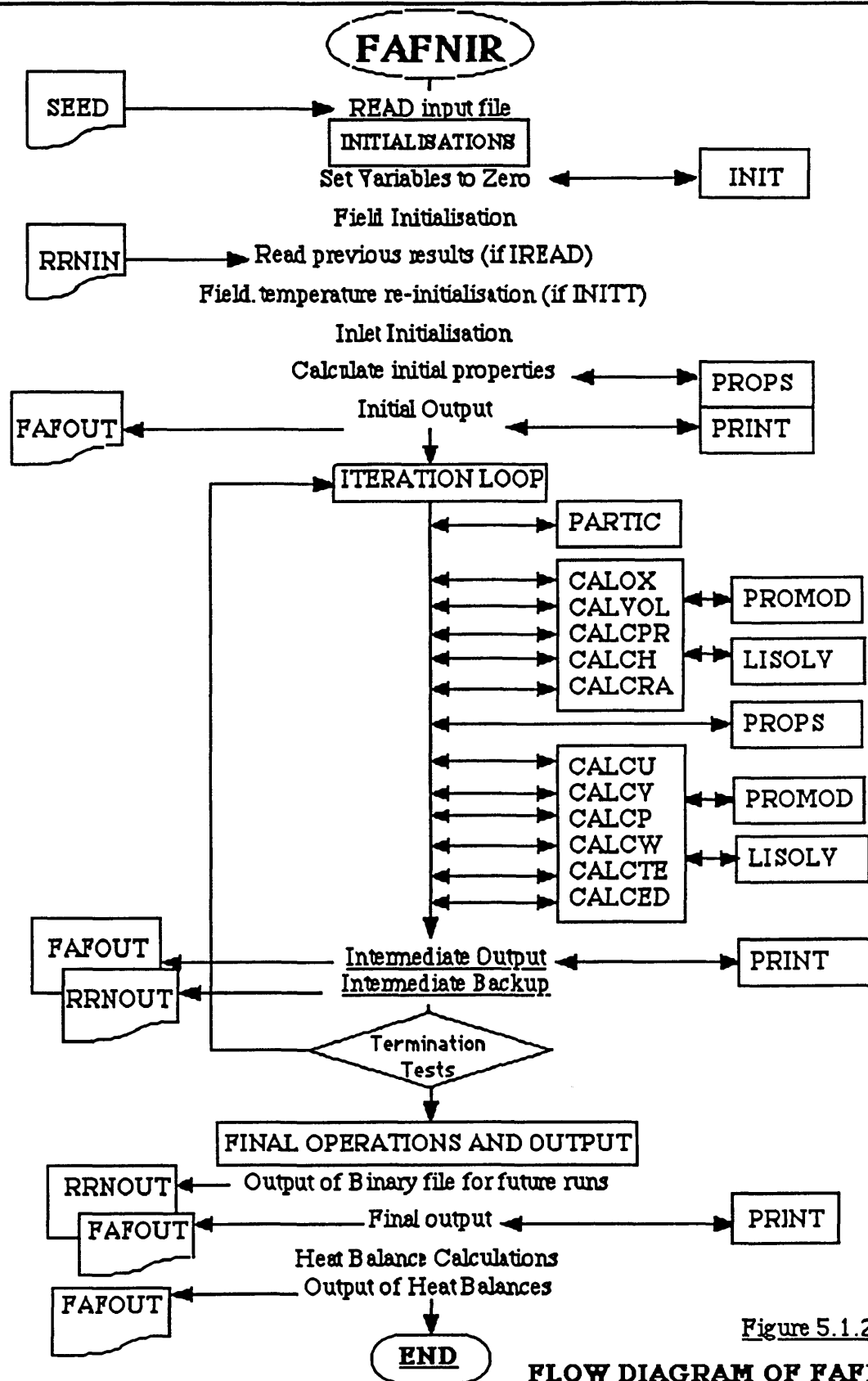
The file SEED is written in ASCII. Therefore it can be read and edited for minor modifications such as the number of iterations, or the under-relaxation factors. It is the input file for the main program FAFNIR.

FAFNIR generates three files. The first one, FAFOUT, is an ASCII file that recalls some input data, it also shows the evolution of the residuals during the run and it writes the final values of some variables over the field. It finally prints out the results of the heat and mass balance calculations which are used as a test for convergence (see section 5.3). The second one, PACL, is also an ASCII file giving the trajectory and history of the particles. The last one, RRNOUT, is a binary file that can be used as input (RRNIN) for posterior runs of similar cases. It is also used as input by the post-processor POSFAF for graphical outputs.

5.1.2 The Layout of the Main Program

The main program will now be overviewed. The layout of FAFNIR is shown in figure 5.1.2. It is divided into three parts. After **initialisation** of the variables (INIT), the physical properties (PROPS) and the setting of the boundary conditions (based on the reading of the input files) the program enters the **iteration loop**. It is in this loop that the main calculations are made. The program calls one by one the particle tracking routine (PARTIC) for the calculation of the particulate phase, and all the ϕ -routines (CALC...) for the calculations regarding the gas phase and radiation. The exit of the iteration loop is controlled by a test on the residuals and on the maximum number of iterations set by the user. The program ends with some **balance calculations** and with the **output** of the final data.

For information, the running of 1000 iterations on a 119 x 59 cell grid takes around 20 000 seconds CPU on a DECstation 3100 or 1000 seconds CPU on a CRAY I.



5.2 AN INTERNAL DESCRIPTION OF THE CODE

The most important routines will now be analysed. These are firstly the ϕ -routines that calculate the gas field quantities. Secondly the particle tracking routines will be described in sub-section 5.2.2. In the last sub-section 5.2.3 the interaction between particulate and gas phase will be described.

5.2.1 The Calc- ϕ Routines

The line-by-line (LBL) procedure to solve the finite-volume equation of section 2.3 (equations 2.3.8 to 2.3.11) was presented in section 2.4. It was shown how the same equation could be used for momentum as well as for scalar equations. Only the calculation of the coefficients and the sources differs from one problem to another. These calculations are performed in the CALC- ϕ routines. They can then each call the LISOLV routine where the LBL procedure will be applied several times (sweeps). The number of sweeps depends on the variable, and is determined experimentally in order to improve the convergence without increasing the computation time (see section 5.3).

CALC- ϕ routines are divided in chapters giving the following structure:

Chapter 1.- Calculates and assembles the coefficient a_b ($b = n, s, e, w$ -- see equation 2.3.9 in section 2.3.3--) and the source terms S_U and S_P (see also table 2.2.2) over the entire field. The sources from the particulate phase and radiation are then added using the Gas-Particle interaction technique (see section 5.2.3)

Chapter 2.- Modifies the sources and the boundary coefficients according to the particularities of the treated problems. This is done by calling the subroutine PROMOD. PROMOD plays a very important role in the program as it is the major area where the

sources and boundary conditions are modified to suit individual problems (e.g. the position of sudden enlargement etc...). It is here where most of the data introduced by the pre-processor through the input file SEED is dealt with.

Chapter 3.- Determines coefficient a_p (equation. 2.3.10) and residual sources using the values of ϕ calculated during the previous iteration. The residual source is the error that exists in the equality of equation 2.3.8. Therefore it is given by:

$$R_{\text{esor}} = \sum_b (a_b \overline{\phi_B}) + S_U - a_p \overline{\phi_P} \quad (5.2.1)$$

The residual source term is calculated in order to control the convergence of the prediction as this is attained when the sum of the residuals over the entire field for U and V velocity and for pressure is smaller than a given value (see section 5.3). The sum of the residuals is normalised by the momentum at the inlet for U and V and by the global mass flow rate for P, in order to have a non-dimensional value.

Finally in this chapter, the coefficient a_p and the source term S_U are under-relaxed as follows:

$$a_p := \frac{a_p}{U_{R\phi}} \quad (5.2.2)$$

$$S_U := S_U + (1 - U_{R\phi}) \cdot a_p \overline{\phi_P} \quad (5.2.3)$$

where $U_{R\phi}$ is the under-relaxation factor for ϕ . This factor is set between 0 (but not equal to 0) and 1. When set to 1, the result of the previous iteration ($\overline{\phi_P}$) is not taken into consideration in the calculation of the current iteration. This can lead to divergence or to oscillations of the residuals. If $U_{R\phi}$ is too small, the convergence will be slowed considerably. For most variables a value of 0.5 to 0.7 is generally chosen. (see section 5.3)

Chapter 4.- Calls LISOLV for the application of the Line-By-Line procedure. The number of sweeps is given as a parameter of the call.

The values used for the number of sweeps and the under-relaxation factors will be detailed in section 5.3 along with the levels of residual sources.

5.2.2 Particle Tracking and Coal Combustion

One of the most important improvements brought to the program during the present work was the re-writing of the particle tracking routine. Its completely revised structure is designed in a modular way leaving the door open to future implementation of other kinds of combustion (e.g oil combustion).

The method used to calculate the history of the particles was described in section 3.1.2. It was shown that only a small number of particles n_p need to be treated. Then the different models used in the procedure were described in sections 3.2 to 3.7. A description of how these models are gathered in the program will now be presented.

The layout of the procedure is shown in figure 5.2.2. First the loop on the particle sizes and starting locations can be seen. Inside this loop another one iterates on time steps, calculating the history of the particle from its entry into the combustor at the burner.

For every time step the velocity and trajectory are first calculated. A call to DIFVEL calculates the effect of turbulence diffusion (see section 3.2.1). SECLOC gives the location of the particle on the eulerian grid. BOUNCE and DOMAIN treat the boundary conditions (the particle is reflected if it strikes a wall or the axis of symmetry and stopped if it reaches the outlet). BNDCRS calculates which sectors the particle crosses during the considered time step. A sector is defined by a region of the grid where both velocities and

scalars are constant. There are therefore four sectors in a scalar cell (see figure 5.2.1). It is important to know which sectors of the eulerian gas phase grid a particle crosses in order to distribute mass and momentum sources in the corresponding cells for gas-particle iteration treatment (see section 5.2.3)

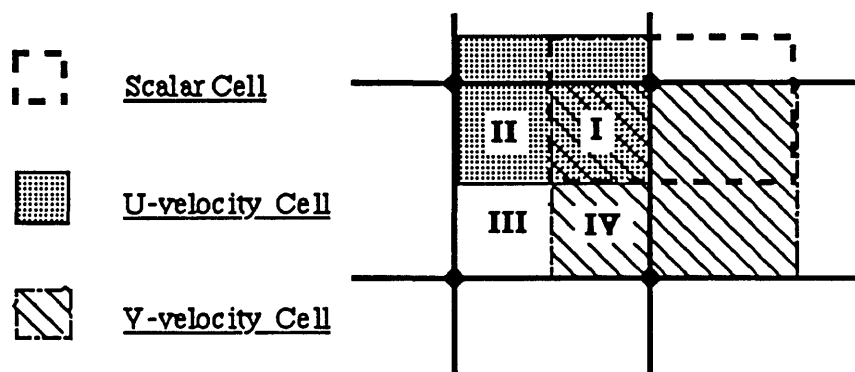


Fig 5.2.1
A Scalar Cell Contains Four Sectors

Finally the combustion routines are called to calculate the particle temperature and its devolatilisation and char combustion rates for the time step. These routines will return the sources of oxygen (< 0), volatiles (> 0) and heat (> 0 or < 0). These sources, along with the momentum sources, will be distributed over the sectors according to the time they have spent in each.

The time step iterations will end if the considered particle:

- 1.- is completely evolved (devolatilisation and char combustion have been completed),
- 2.- has reached an outlet of the furnace, or
- 3.- is in a loop, or is stopped.

The program then exits the 'particle tracking' loop and chooses the next particle. When the n_p particles have been treated the program adds the sources from all the particles to the source terms of the CALC- ϕ routines:

$$S_{p,\phi} := S_{p,\phi \text{ new}} + (1-U_{Rp}) \cdot S_{p,\phi \text{ old}} \quad (5.2.4)$$

where $S_{p,\phi}$ is the sum of sources (or sinks) of the property ϕ from the particles to the carrier phase. $S_{p,\phi \text{ new}}$ is the newly calculated source term and $S_{p,\phi \text{ old}}$ the source term calculated during the previous call to the particle tracking routine. U_{Rp} is an under-relaxation factor. In a similar way to the gas phase relaxation factors, this one is set between 0 and 1. It is generally set to a very small value (≈ 0.05) because the fluctuations of the trajectories between one call of the routine and another are an important source of oscillation or divergence of the program. The interaction between these sources and the gas field are described in the next section.

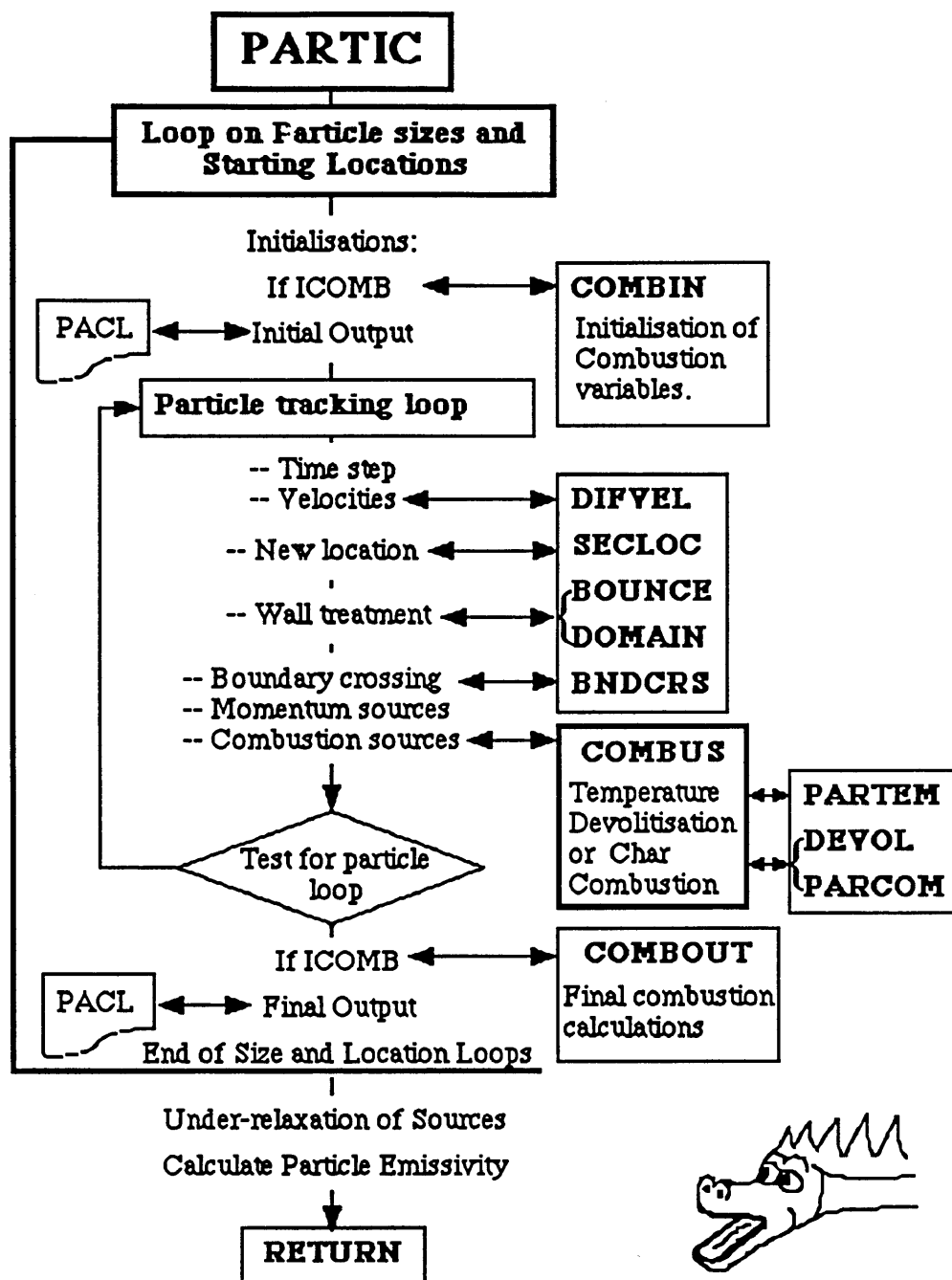


Figure 5.2.2: Layout of the particle Tracking Routine

5.2.3 Handling of the Gas-Particle Interaction

The procedure for handling the gas-particle interaction is termed the Particle Source in Cell (PSIC) technique and was originally proposed by Migdal and Agosta (1967). This method has since been extensively used for various particulate research problems, see for example and Lockwood et al. (1984).

The presence of a coal particle in the finite-difference control volume (cell) of the gas-phase is made known through the application of source terms to the mean flow equations. The processes that a coal particle entering the combustion space of a furnace undergoes, such as devolatilisation and burning, result in an exchange of mass between the phases. The exchange of momentum and energy between the two phases also occurs due to the particle drag and the gas-particle convective and radiative heat transfer. The PSIC model for the gas-phase results in a mass source being appended to the gas-phase continuity equation; the drag force on the particle is reflected in the gas-phase calculations as a source of momentum; heat transfer is identified as an enthalpy source, while particle burning and devolatilisation results in sources being applied to the species conservation equations.

By way of illustration, we may write the mass conservation equation for a control volume surrounding a grid node as:

$$-\dot{m}_w + \dot{m}_e - \dot{m}_s + \dot{m}_n - \Delta \dot{m}_p = 0 \quad (5.2.5)$$

where $\dot{m}_w$, $\dot{m}_e$ etc... are the gas mass flow rates across 'west', 'east'... faces of the control volume, and $\Delta \dot{m}_p$ is the net mass efflux rate of the coal particles in the gas-phase into the above control volume.

5.3 COMPUTATIONAL DETAILS

5.3.1 Computational Parameters

Parameters related to computational performance will be treated in this section. The main objectives of these parameters are to help the program to converge. Unfortunately the factors that avoid divergence or oscillations will tend to lengthen the execution time. The values of these parameters used in this work are shown in table 5.3.1. These values were chosen in order to insure a good convergence, they are therefore probably not the optimal ones in respect of code performance indicators.

When two values are shown this means that the first one is replaced by the second when convergence is on its way (after 1000 or 2000 iterations). The number of sweeps for the pressure equation is variable. A test is made on the sum of the pressure residual sources over the field. If the ratio between the result of this sum before and after a sweep is smaller than a given value, that is if the residuals have not improved sufficiently, then another sweep is made until a maximum of 35 sweeps is reached. This procedure causes the pressure equation to be swept more at the beginning of run than towards its end.

Some other computational details are listed below:

The particle tracking routine was called every 10 iterations of the gas field routines.

The particle tracking routine was not called before an isothermal converged gas-field was obtained.

Convergence is more difficult to obtain when the aspect ratio of the grid (the maximum ratio between the length and the height of a cell) is too large (≈ 70)

Variable	Number of Sweeps	Under-relaxation
U-Velocity	3	0.5 then 0.6
V-Velocity	3	0.5 then 0.6
W-Velocity	3	0.6
Pressure	1	up to 35
Turbulence Energy	2	0.4 then 0.5
Dissipation Energy	2	0.4 then 0.5
Oxygen	3 to 5	0.5
Volatiles	2	0.5
Products	2	0.5
Enthalpy	3 to 5	0.5
Particle tracking	-----	0.05

Table 5.3.1 Computational Parameters

5.3.2 Convergence Criteria

Three conditions had to be followed in order to consider a run to be converged:

- 1.- The normalised residual sources for U and V velocity equations as well as for the Pressure equation had to be less than $5 \cdot 10^{-3}$.
- 2.- The results monitored on a chosen location had to remain steady from one iteration to another.
- 3.- The global Mass Balance had to be 100 % correct.
- 4.- The global Heat Balance calculated at the end of the program, had to show a difference between inlet and outlet of less than 5 %.

The information necessary to check these conditions are printed out in the output file FAFOUT.

5.3.2 Concluding Remarks

This chapter completes the description of the computer program FAFNIR and its contents. It is now necessary to test the program, in order to reach the final objective, which is to provide the cement industry with a tool capable of predicting the performance of its rotary kilns. Therefore a validation study has been carried out, which is presented in the next Chapter.

CHAPTER 6

CALCULATIONS AND VALIDATION STUDIES

In chapters 2 to 4 of this work different physical and mathematical models were chosen in order to predict the phenomena occurring in a confined pulverised coal flame. It was shown in chapter 5 how these models were solved using numerical methods. The accuracy of the resulting solution procedure depends on the validity of the physical models, and on the rounding and discrete errors of the numerical method.

Therefore, it is necessary to evaluate the accuracy of the program, by comparing its predictions with experimental data obtained in laboratory conditions or, if possible, in industrial situations. This comparison will provide us with information regarding the quality of the prediction. As the objective of this work is to predict cement kiln flames, experimental data of full-size furnaces would be useful for validation. Unfortunately, because of the nature of rotary kilns, useful and reliable data are not easily obtainable (see chapter 1). Thus, experimental data obtained in the laboratory will be used for validation in the present study.

In the present study, the validation work was effected in two stages. Firstly, attention was directed towards the modelling of the isothermal flow. For this purpose, a scale model of a cement kiln was constructed. A full description of this experiment is provided in section 6.1. Secondly, the combustion related routines were validated using experimental data obtained in an experimental furnace fired with a parallel flow burner similar to those used in cement kilns (See Bortz 1983). This validation is described in section 6.2.

After obtaining acceptable results in validation studies the code was applied to predictive work, an example of which is given in the last section of this chapter.

6.1 ISOTHERMAL VALIDATION

6.1.1 Preamble

The objectives were to recreate experimentally the running conditions of a full sized kiln while respecting the axial symmetry and the turbulence level requested by the computer model. The resulting flow would be visualised and compared with computed results. Data for the running conditions of a rotary kiln were given by Lafarge Coppée Recherche. The kiln is 90m long by 5m diameter. The burner is shown in fig. 6.1.1 It has three concentric inlets. The internal inlet has a swirl generator. Pulverised coal is transported in the intermediary inlet. The relatively small section of the external inlet provides a high momentum flow in order to control the shape of the flame.

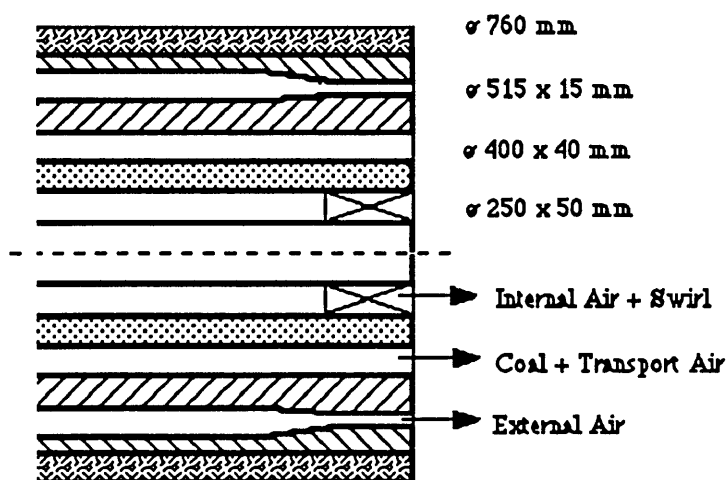


figure 6.1.1 The Cement Kiln Three-way Burner

6.1.2 Description of the Water Model

The arrangement: (see fig. 6.1.2) Mechanical restrictions did not allow the construction of a burner smaller than 1/20th of the original one. The volume flow rate

necessary to reach turbulence in a small geometry is such that it was decided to substitute water for air as the working fluid.

The body of the 'furnace' was a 2m long by 25 cm diameter and 2.5 cm thick acrylic cylinder. It was located in a rectangular box of acrylic filled with water in order to avoid the visual effects associated with its cylindricity.(see photograph at the end of this section , fig 6.1.4 and 6.1.5) Two stainless steel cones were fitted at both ends thus allowing the secondary water flow to be supplied and extracted. These fittings were connected to the rest of the system using flexible hoses to avoid the vibrations of the pumps being transmitted to the body of the 'furnace'. The rest of the piping system was constructed from 2" and 4" PVC pipes. The three way burner was composed of concentric stainless steel pipes separately fed by flexible hoses. It was located in the axis of one of the cones. Two pumps were used to inject the water into the rig. The first one for the secondary flow was a centrifugal pump providing up to 15 l/s at 40 m head. The flow excess was recirculated through a by-pass. The second pump, a Grundfos CR4-120, providing 1.75 l/s at 70 m head, was used to supply the three primary flows. The separate flow rates were regulated using angle seat valves for the primary and a ball valve for the secondary. The flow rates were measured using three rotameters for the primary flows and a rotameter with an orifice plate for the secondary. The whole rig was fitted with a series of gas cocks for purging any air bubble. The water at the outlet of the rig was sent back to the feed tanks to be recirculated.

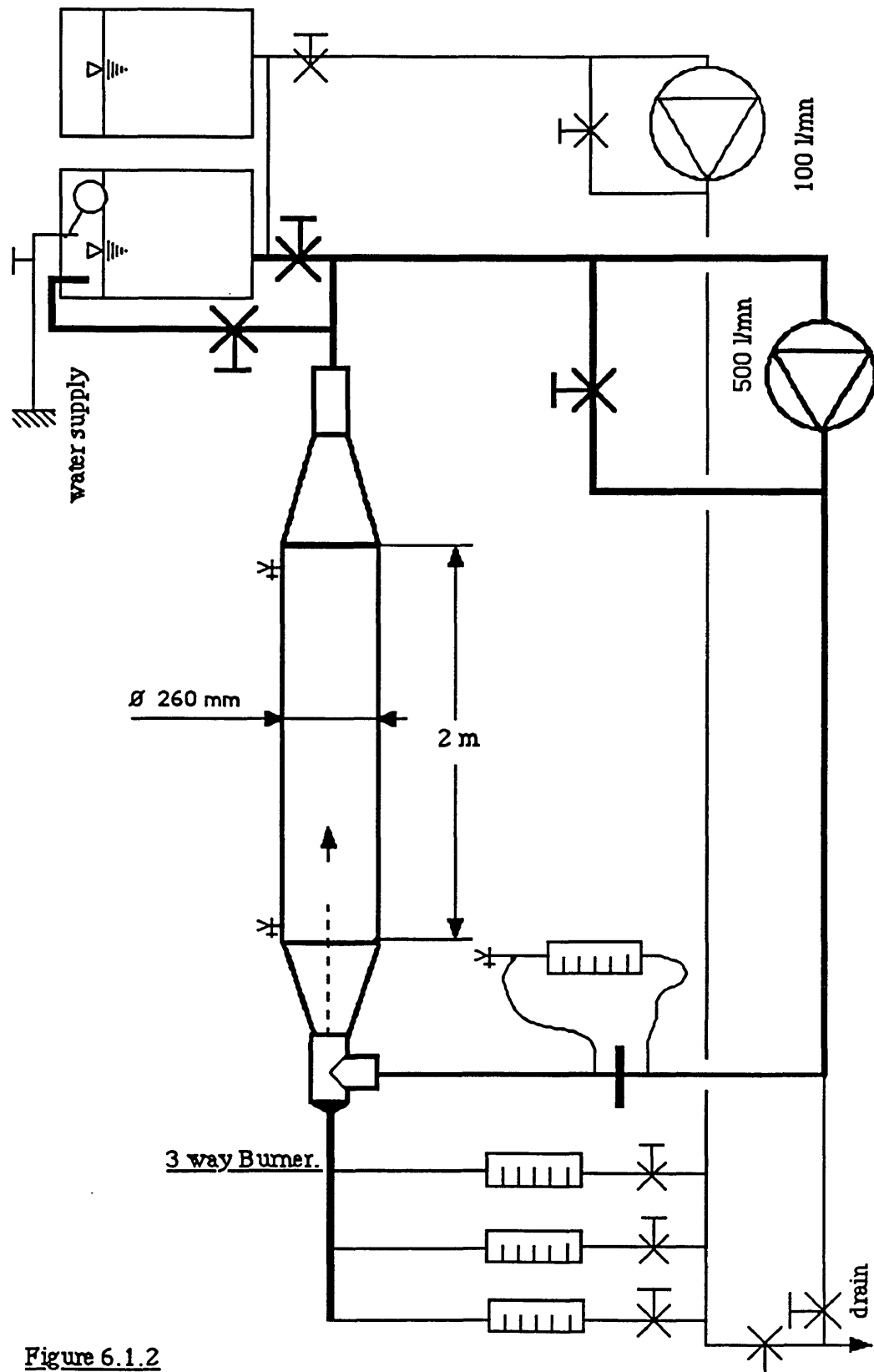


Figure 6.1.2

GENERAL ARRANGEMENT OF THE MODEL FURNACE

The measurements: (fig. 6.1.3) The flow visualisation was performed using the laser sheet technique. A 1mW argon laser beam was sent through a cylindrical lens spreading it into a sheet. (see fig. 6.1.6) This sheet of coherent light illuminated the flow in an axial plane. Polystyrene beads of approximately 200 μm were introduced in the water as seeds. They were illuminated by the laser when in the plane of the sheet. The resulting image was photographed. (see next section)

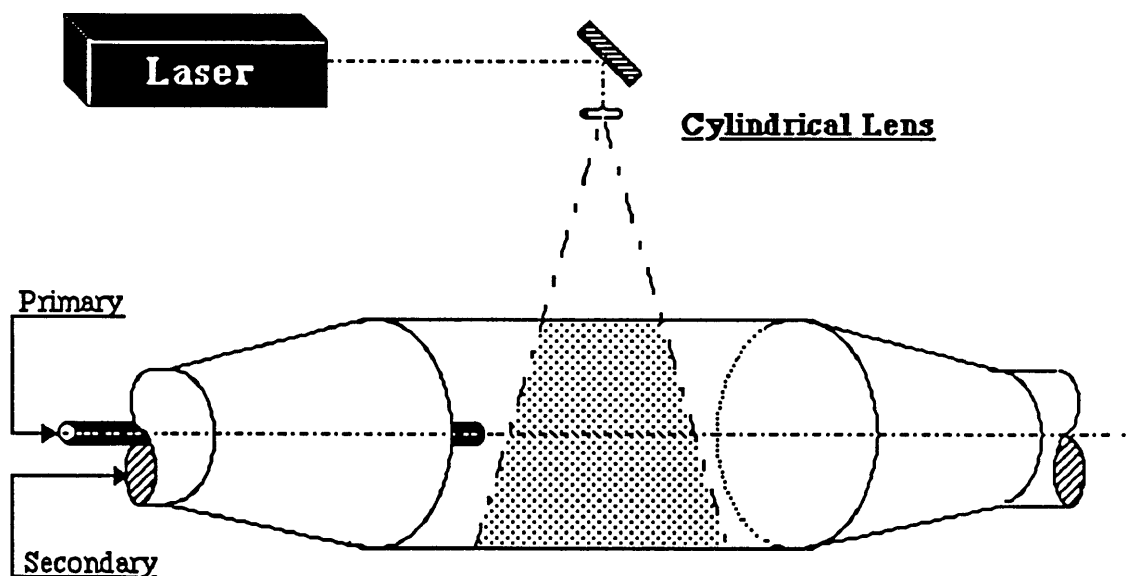


figure 6.1.3

Flow Visualisation by the Laser Sheet Technique

6.1.3 Discussion of the Results

Three different running conditions were set-up. Unfortunately the cross section of the external burner inlet was easily blocked and it was not possible to have a significant flow through it. The flow settings are shown in table 6.1.1

Flow rates in l/s

Setting	Primary			Secondary
	Internal	Transport	External	
1	0.350	0.350	--	8.300
2	0.830	0.830	--	8.300
3	0.830	0.830	--	5.000

Table 6.1.1 Running Conditions for the Water Model

The photographs showing the visualisations for the three settings are presented at the end of this section (fig. 6.1.7, 6.1.9 and 6.1.11) together with the predicted axial velocity, u (fig. 6.1.8, 6.1.10 and 6.1.12)

It can be seen that both prediction and visualisation in no case show any external recirculation.

Setting 1: This setting is characterised by a small primary momentum compared with that of the secondary flow. The photograph (fig. 6.1.7) shows a parallel flow with almost no turbulence in the secondary stream. The primary jet does not mix well with the secondary stream. The prediction shows a small velocity gradient.(fig. 6.1.8)

Settings 2 and 3: Increasing the primary flow (setting 2.) and then decreasing the secondary flow (setting 3.) tends to create vortices on the boundary between the secondary and the primary jets. These vortices are clearly seen on the photographs (fig. 6.1.9 and 6.1.11). They are the result of higher stress levels due to higher velocity gradients. These gradients are well predicted as can be seen on figures 6.1.10 and 6.1.12. Decreasing the secondary air flow does create a small central recirculation zone very close to the burner (fig 6.1.12). This is representative of a high degree of turbulence.

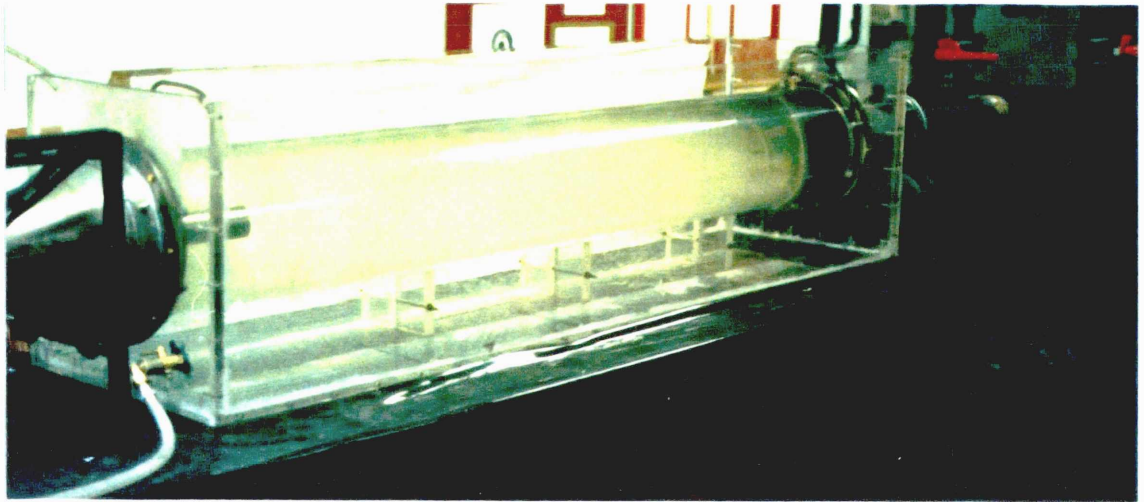


Figure 6.1.4 A General View of the Water Model

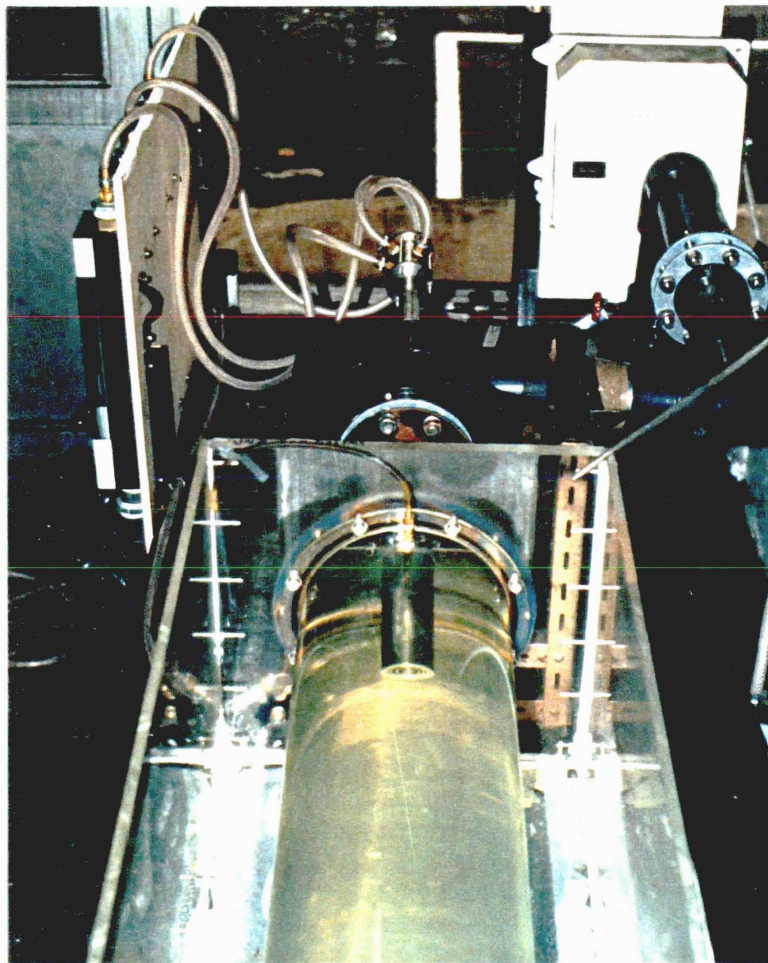


Figure 6.1.5 Detail of the Water Model

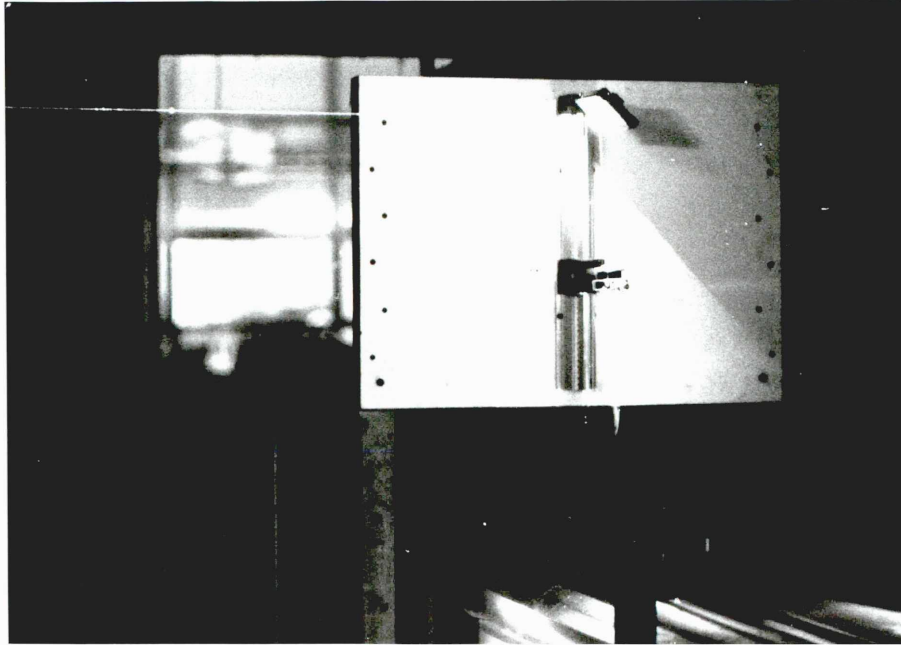


Figure 6.1.6 View of the Laser Beam and the Mirrors

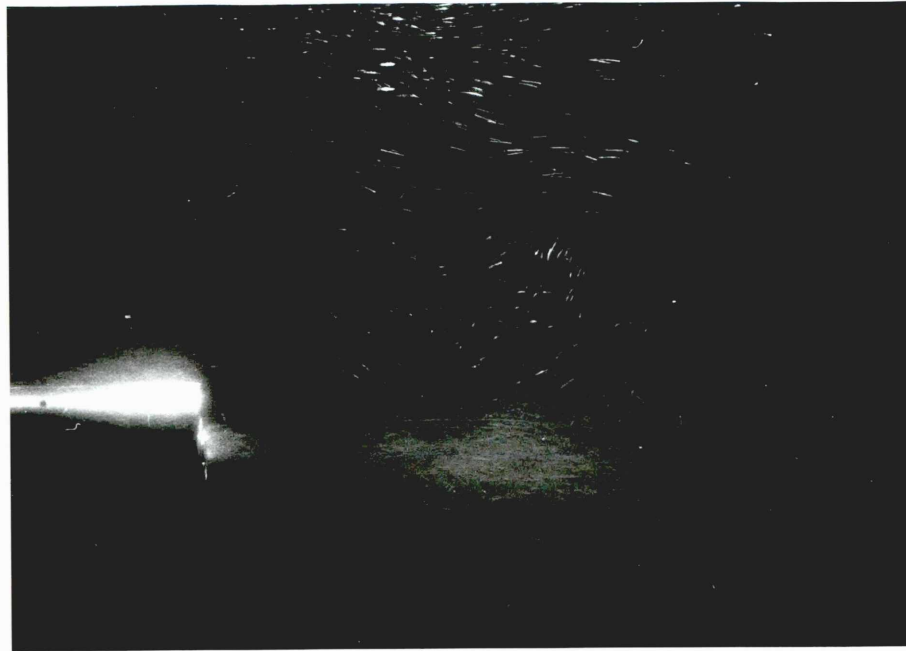


Figure 6.1.7 Flow Visualisation - Setting 1

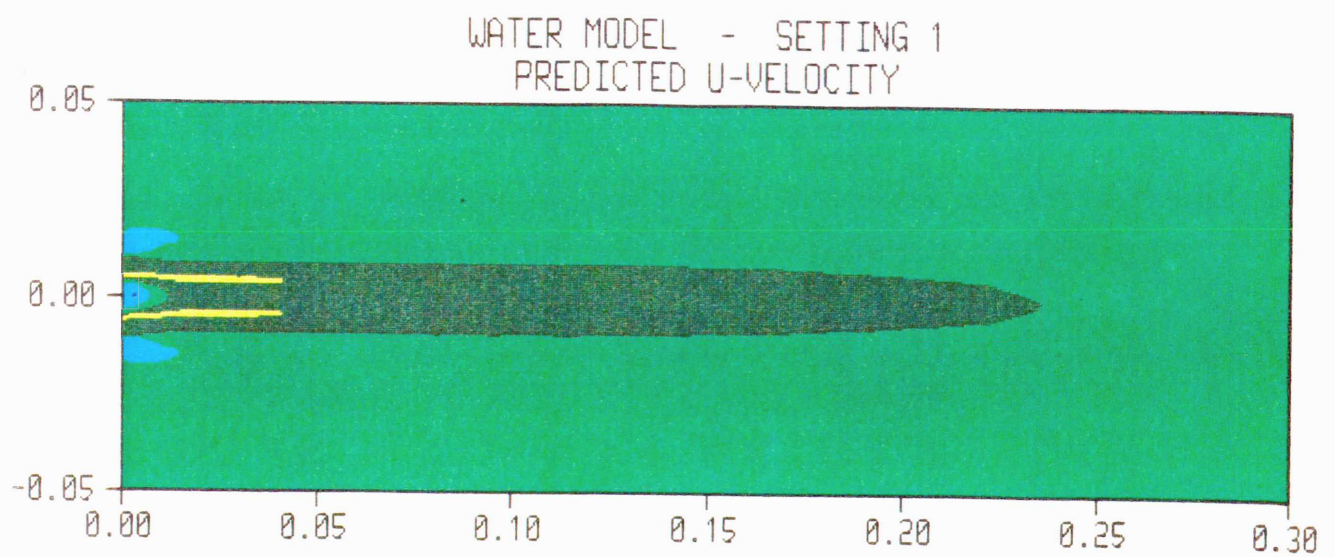
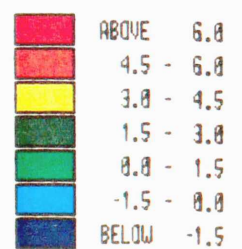


Figure 6.1.8 Predictions of Axial Velocity - Setting 1



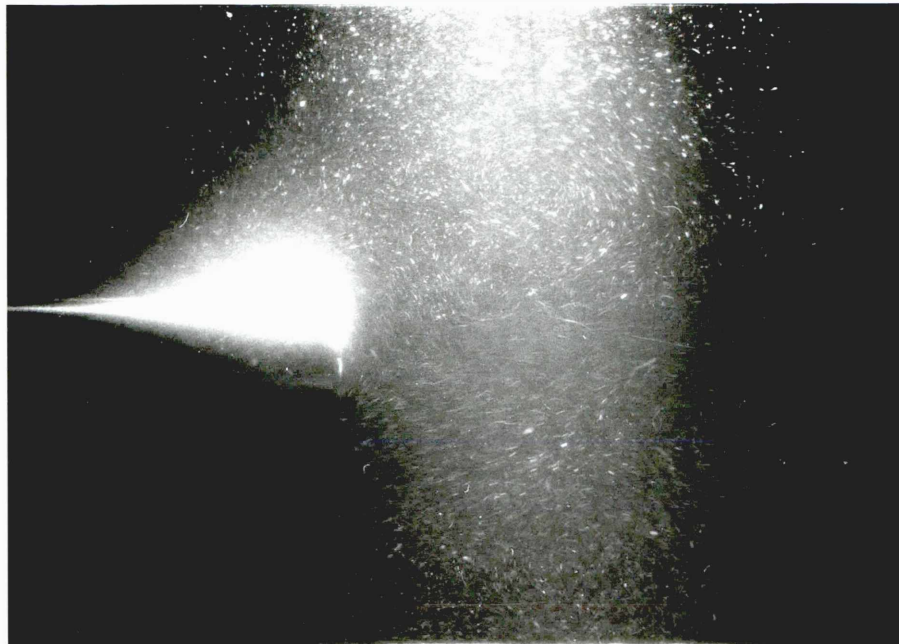


Figure 6.1.9 Flow Visualisation - Setting 2

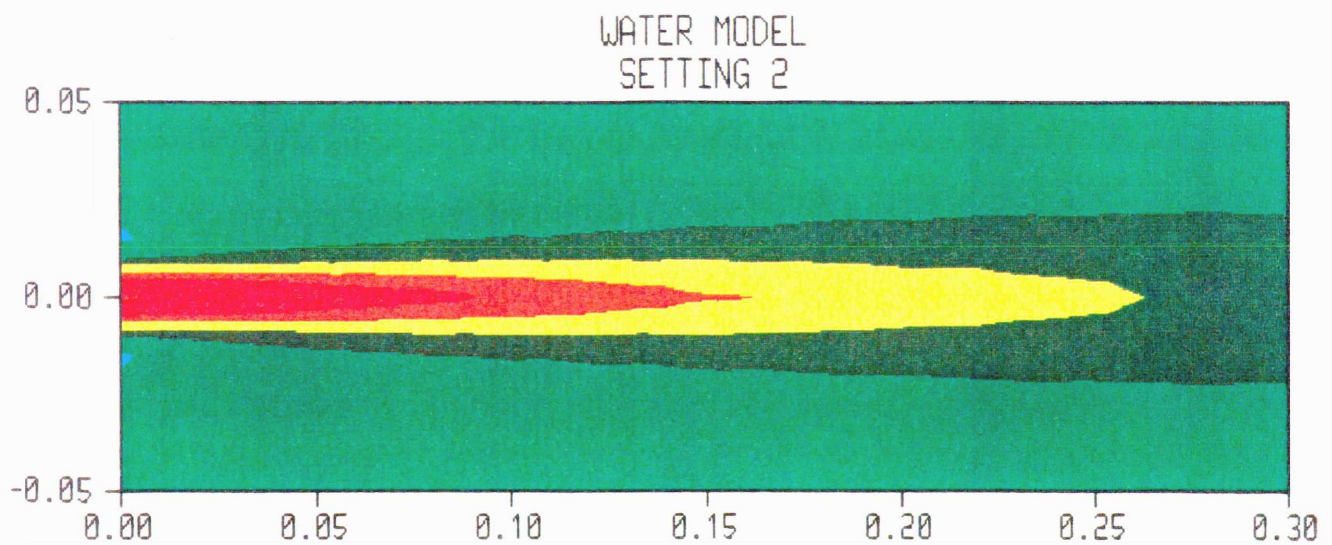
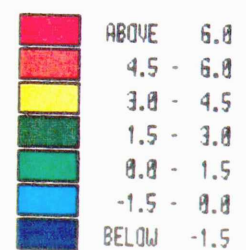


Figure 6.1.10 Predictions of Axial Velocity - Setting 2



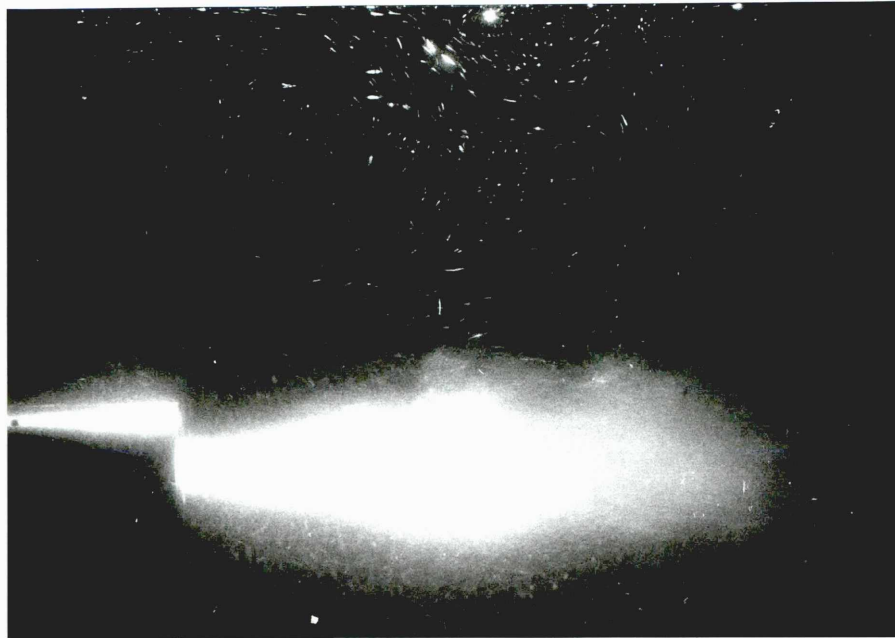


Figure 6.1.11 Flow Visualisation - Setting 3

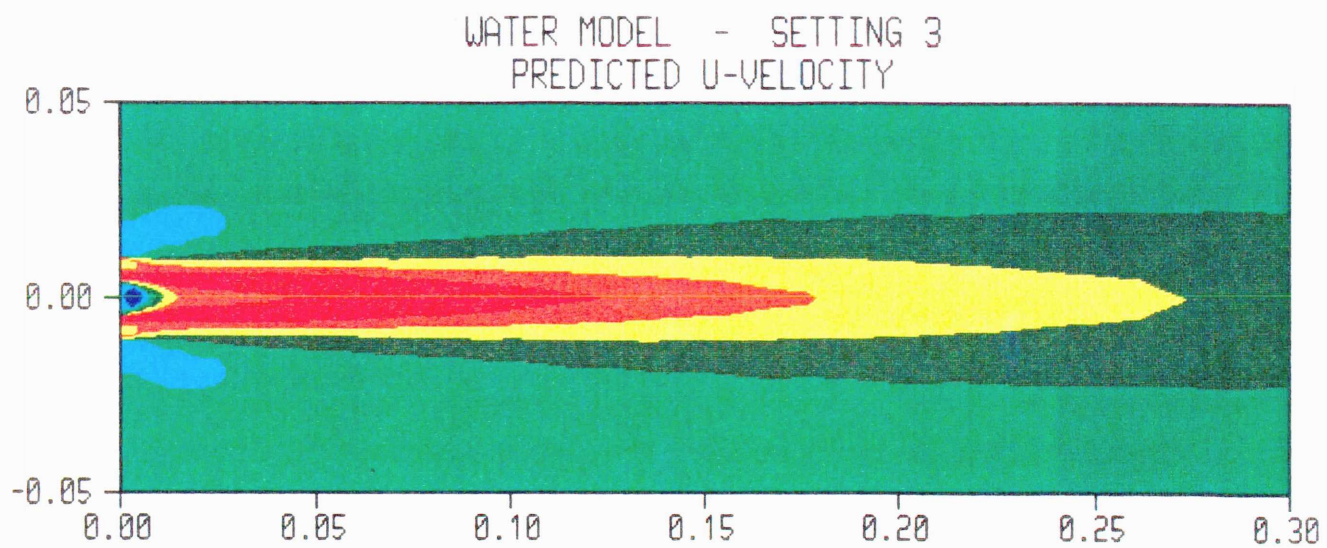
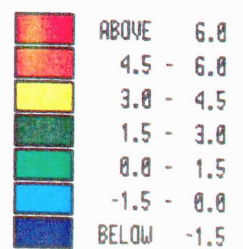


Figure 6.1.12 Predictions of Axial Velocity - Setting 3



6.2 VALIDATION OF COMBUSTION

The combustion validation involves all the routines of the program. The quality of the predictions will be judged as a whole, in the absence of the direct possibility of determining which modelling element is more or less accurate than the others.

6.2.1 Description of the Experimental Data

The data used in the combustion validation was taken from a report involving trials carried out at the International Flame Research Foundation (IFRF) (see Bortz (1983)). In this investigation, an experimental parallel flow burner was used for the combined firing of coal and gas in the IFRF n° 1 furnace. This furnace is horizontally fired and has the approximate dimensions 2.0 x 2.0 x 6.0 m (see fig. 6.2.2). The furnace chamber is refractory lined and in order to simulate the temperature field within a cement kiln, no cooling facilities were installed in the first 2.5 meter of the furnace. However, in order to reduce and control the flue gas temperature six cooling loops were placed in the exhaust end of the furnace. Experimental details can be found in Bortz (1983).

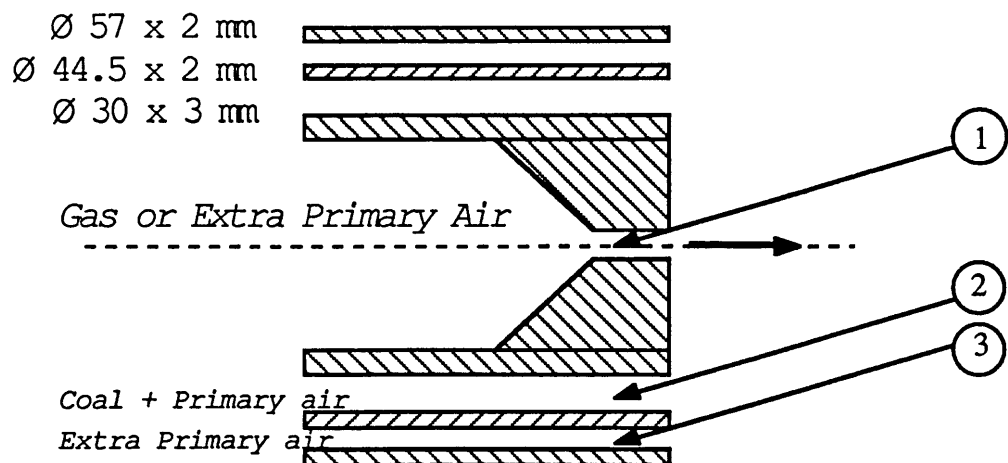


Fig. 6.2.1
The IFRF Burner

The burner had three different inlets (fig. 6.2.1). The central one ① was used for air or for gas, the external one ③ for air, and the middle one ② for coal transport. The burner was fitted along the axis of the furnace. (fig. 6.2.2).

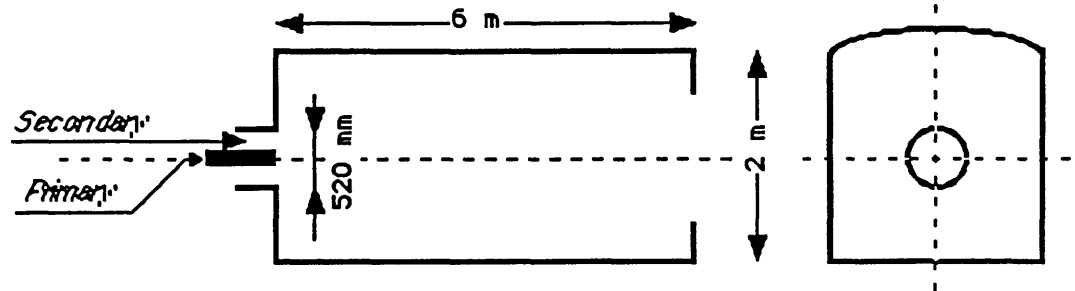


fig 6.2.2 **The IFRF N° 1 Furnace**

The IFRF experimental work was carried out using different settings four of which were selected for the validation work. These settings are shown in fig. 6.2.3

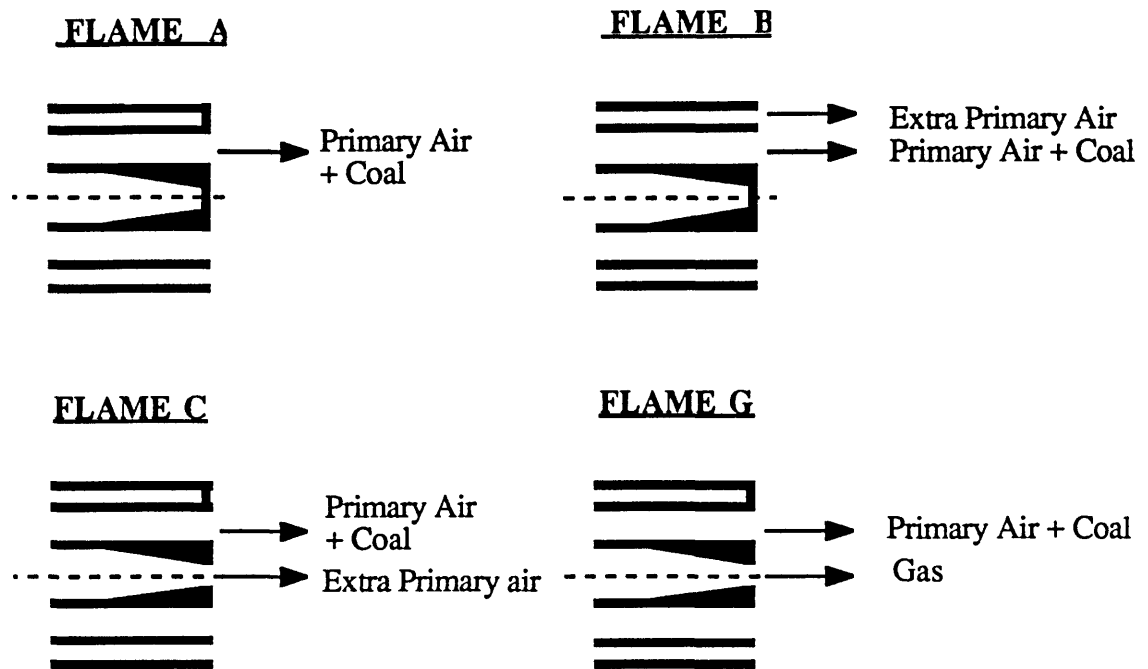


Fig. 6.2.3
Running Conditions

In **flame A**, the central and external inlets were unused. In **flame B**, extra primary air was added in the external flow inlet. In **flame C**, the extra primary air was added in the central flow inlet. In **flame G**, the central air of flame C was replaced by gas. The flow rates of the extra primary air in flame C and gas in flame G were such that they had similar momenta.

The inlet conditions are summarised in table 6.2.1 and 6.2.2 together with the properties of coal and gas.

Table 6.2.1: IFRF Run Conditions (flow rates in kg/hr)

Flame	A	B	C	G
Coal rate	240	240	240	120
Gas rate	--	--	--	80
Secondary air	2611	2390	2564	2665
Primary air	80	80	80	80
Extra Primary Air & Position	--	240 External	106 central	--

Table 6.2.2 Coal Properties as fired (dry basis)

Coal:	Peak Downs	Particle Sizes	
C	78.4 %	> 150 μ	5.8 %
H	4.18 %	> 100 μ	18.0 %
O	3.71 %	> 75 μ	23.8 %
N	1.85 %	> 50 μ	33.0 %
S	0.72 %	> 20 μ	55.4 %
Ash	10.8 %	Natural gas Properties	
Volatiles	18.0 %	CH ₄	85.3 %
LCV (MJ/kg)	31.52	LCV (MJ/kg)	43.85

6.2.2 Prediction Parameters

The predictions of the IFRF experiments were made using a 55 x 45 point grid. The parameters of table 6.2.3 based on the data from Anthony et al. (1975) and Badzioch and Hawkesley (1970) were used and convergence criteria described in chapter 5 were observed.

Q factor:	2.4	ACOMB:	4
	Activation energy	Pre-exponential factor	
Devolatilisation	$74 \cdot 10^6$	$0.382 \cdot 10^6$	
Coal Combustion	$71 \cdot 10^6$	1.7	

Table 6.2.3 Parameters for the IFRF predictions

Although the IFRF furnace has a rectangular cross section, it was considered, for prediction purposes, to be a 2 m cylinder. Finally, the influence of the cooling loops was simulated using the measured wall temperatures as boundary conditions for enthalpy and radiation calculations.

6.2.3 Discussion of the Results

6.2.3.1 Preamble

The results for flames A, C and G are shown in figures 6.2.4.1 to 6.2.6.12 presented at the end of this chapter. In these figures both experimental and predicted data are depicted. Three different kinds of graphs are provided.

Contour plottings. Figures 6.2.4.1 to 6.2.4.6 show contour lines of field temperature and oxygen for the predicted results. These graphs show an image of how the flame might appear in the furnace, and give a good basis for qualitative comparisons.

Axial profiles. Figures 6.2.5.1 and 6.2.5.2 depict the changes of temperature and oxygen along the axis. The predicted results (continuous lines) correspond to the values calculated by FAFNIR in the axial cells which cover an area going up to 4 mm from the axis. The measured data (dots) are shown on the same graphs.

Four different quantities are plotted in figure 6.2.5.3. The first one (bold continuous line) shows the mass sources integrated along the furnace. It represents both the devolatilisation and the char combustion of the particles as calculated by FAFNIR. It is the sum over the radius of all the mass sources S_m from the particulate phase to the gas phase (see chapter 2), divided by the input mass flow rate of carbon (on a dry free ash basis). It is in fact equivalent to the particle burnout along the furnace. The volatile source curve (thin continuous line) uses the same formula with the exception that only the volatile contents of the coal are included. Both curves are almost the same near the burner where char combustion has not yet commenced for all the particles, then when the devolatilisation process has finished (where the volatile source curve has reached its maximum) the mass source curve shows only the char burnout process.

The experimental data is plotted in white and black squares. They were obtained by collecting solid samples and analysing them separately in the laboratory. The plotted data is the result of the following formulae for T_x (white squares) and Z_x (black squares) as calculated by Bortz (1983):

$$T_x = \frac{1 - \frac{A_0}{A_1}}{1 - A_0} = \text{Total combustible burnout} \quad (6.2.1)$$

$$Z_x = 1 - \frac{V_1}{V_p} \cdot \frac{A_0}{A_1} = \text{Volatile burnout} \quad (6.2.2)$$

where A_0 is the input ash concentration at the inlet and A_1 the ash concentration of the sample collected at the local in-flame measuring point. V_p is the volatile matter yield from the proximate analysis and V_1 the volatile matter yield at the local in-flame measuring point.

Radial Profiles. Figures 6.2.6.1 to 6.2.6.12 show the temperature and oxygen radial profiles plotted at the stations (locations along the furnace) where experimental data

was available. That is at 10, 25 and/or 75 cm, and also at 1.0, 1.5, 1.8, 2.8, 3.5 and 5 m from the burner tip. The continuous lines show the predictions and the dots the measured data. Two flames are shown together in order to allow a better comparison. The diagram at the bottom of the figures is a scaled image of the burner tip. It shows the exact position of the different primary inlets, and the different flame settings.

6.2.3.2 The Flames

The flames will now be analysed on the basis of both experimental and predicted data.

Flame A. Contour plottings for this case (fig. 6.2.4.1 and 2) show a flame with a low burning rate. It is slightly lifted and stays relatively cold. The lack of extra primary air probably slows down the global fuel-air mixing. The ignition point is located at around 75 cm from the burner which is where devolatilisation initiates (fig. 6.2.5.1) and where the axial temperature gradient is higher (fig. 6.2.5.2). The predicted maximum temperature on the axis is 1600 °C and is not reached before a downstream distance of 3.45 m. (fig. 6.2.5.2) (the measured maximum temperature is 1575 °C at 3.50 m). The radial oxygen profiles (fig. 6.2.6.3 and 4) show that the consumption of oxygen is concentrated on the centre line and confirms the fact that the particles do not mix well with the secondary air stream.

Flame C. This flame has extra primary high momentum air injected through the central inlet. The main effect of this jet is to increase the shear stress which enhances the mixing between secondary and primary air streams. This mixing rate increases the volatiles combustion in the near burner field as can be seen in figure 6.2.5.3 where the oxygen level decreases much faster than in the previous case. The consequences of this high volatiles combustion rate are seen in figures 6.2.5.2 and 6.2.5.3: the temperature rises sharply and the devolatilisation occurs very rapidly. The ignition point is located at

20 cm from the burner (instead of 75 cm in flame A) and the global level of temperature in the first 2 m is higher than in flame A, with a maximum value on the axis of 1685 °C about 30 cm from the burner, and an even hotter location of 1965 °C situated off-axis at a distance of 5 cm (fig. 6.2.6.5). The temperature then decreases at a slightly greater rate than in flame A. In conclusion flame C is hotter and shorter than flame A.

Flame G. The comparison between flames C and G shows that replacing air for gas in the central burner inlet has little effect on the flame. The overall combustion rate is similar (fig. 6.2.5.3) and so is the general level of temperature. This is due to the fact that the low volatile bituminous coal used for this case contains sufficient volatile matter to ignite the char, as long as there is good mixing between primary and secondary air. The injection of gas would be much more useful for an anthracite coal containing small amounts of volatiles (2- 3 %) (see Bortz 1983)

Flame B. The measurements for this flame show (fig. 6.2.4.3, 6.3.4.4 and fig. 6.2.6.1 to 6.2.6.4) that the coal is entrained by the high momentum annular air of the extra primary stream and that the major combustion zone is no longer on the furnace axis. This entrainment is not very well predicted a fact that will be explained in the next section.

6.2.3.3 Prediction Performance

The quality of the prediction will now be analysed for all the flames. For this purpose figures showing both experimental and predicted data over the furnace will be examined (fig. 6.2.6.1 to 6.2.6.12).

The overall prediction performance is qualitatively good (apart from flame B). The variations of one flame relative to another are well calculated. Quantitatively, predictions are acceptable: flame ignition points, flame lengths and maximum temperatures are within the precision that can be expected from the measurements, especially considering

that the IFRF furnace is actually rectangular and not cylindrical. The predicted axial profiles show a good agreement with the experimental ones, and prediction in the Near Burner Region (NBR) performs fairly well.

Nevertheless it is observed that the predicted oxygen level on the axis is generally much lower than the measured one. The reason for this could be the particle dispersion model used in the calculation. It has been seen (section 3.2.1) that the sign of the particle diffusion velocity due to turbulence cannot be determined since it is a random process.

In order to overcome the problem, it was attempted to give the velocity a randomly determined sign. A 50 % probability was given to the drift velocities $U_{diff\ p}$ and $V_{diff\ p}$ to be either negative or positive. The sign was re-determined every time step along the particle trajectory, when the particle velocity is calculated. This particle dispersion model was tested on the prediction of flame A. The results are depicted in figures 6.2.7.1 to 6.2.7.4. The predictions on the left hand side were calculated with no turbulence dispersion, the ones on the right hand side were calculated using the particle dispersion model. It can be seen from these graphs that the predictions with and without dispersion are unfortunately identical. At this stage, a suitable model could not be found, and the program was run for the rest of the cases with no particle diffusion.

The particle trajectories were therefore unaffected by turbulence eddies. As a result they tend to stay close to the axis. For this reason the consumption of oxygen in the central region was too strong. This problem may also explain the bad prediction of flame B since it is the turbulence created by the high momentum of the annular stream which should have spread the coal jet in the way the experiment showed.

The relatively poor prediction of flame B may also be caused by symmetry problems during the experiment. As a matter of fact, there is a good agreement between prediction and experiment in the NBR. The divergences arise at about 75 cm from the

burner tip. (see fig. 6.2.6.3) If the flame was not perfectly symmetric, that is exactly what could be expected. This explanation can be strengthened by looking at the measured oxygen profile at the end of the furnace. At this location the profile should be flat... (fig. 6.2.6.4)

6.3 PREDICTION OF CEMENT KILNS

The last task of the present study is to demonstrate that the code is able to predict the behaviour of full size cement kilns in a manner convincing to engineers. An example of such runs is presented below. A flame was predicted for a cement kiln using a three-way burner similar to the one described in section 6.1. Two different settings 'MAXI' and 'MINI' were predicted. The two settings differ in the primary air specific momentum. (see table 6.3.1). The axial specific momentum is defined as

$$G_s = \frac{G_u}{\dot{m}_{\text{coal}} \cdot H_{\text{coal}}} \quad (6.3.1)$$

where $\dot{m}_{\text{coal}}$ is the coal flow rate, H_{coal} its calorific value and G_u is the axial momentum calculated as:

$$G_u = \sum_{i=1}^{\text{inlets}} (u_i \cdot \dot{m}_i) \quad (6.3.2)$$

where u_i and $\dot{m}_i$ are respectively the axial velocity and the air mass flow rate for each inlet of the three way burner.

Table 6.3.1 Full Size Cement Kiln Predictions

	Maxi	Mini
Specific Momentum (N/MW)	5.0	2.2
Coal Mass Flow Rate (kg/s)	2.08	2.17
Total Heat Transfer on Walls (MW)	50	49
Predicted Flame Length (m)	30	44
Maximum Axial Temperature (°C)	2170° at 30 m	2110° at 44 m

The flame length is defined as the distance between the burner tip and the point where the coal burnout becomes greater than 98%. Figure 6.3.1 and table 6.3.1 show that a much shorter flame is obtained with a high specific momentum (flame MAXI). It can be also seen in figures 6.3.2 and 6.3.3 that flame MAXI is hotter than flame MINI. It is possible to derive from these predictions information regarding the quality of the produced clinker, and to increase the performance of the kiln: flame MAXI should produce the same amount of clinker but with a smaller coal consumption. This possibility of reducing the fuel consumption was confirmed when these flame settings were experimented at a Lafarge Coppée plant.

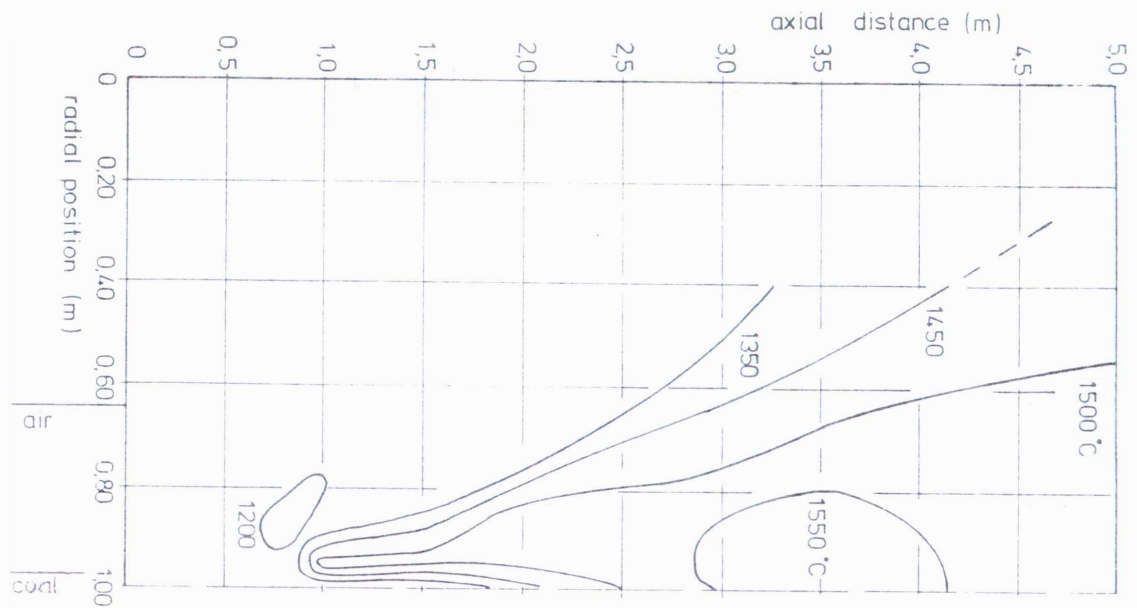


Figure 6.2.4.1 Measured Temperature - IFRF - Flame A



Figure 6.2.4.2 Predicted Temperature - IFRF - Flame A



Figure 6.2.4.3 Measured Temperature - IFRF - Flame B

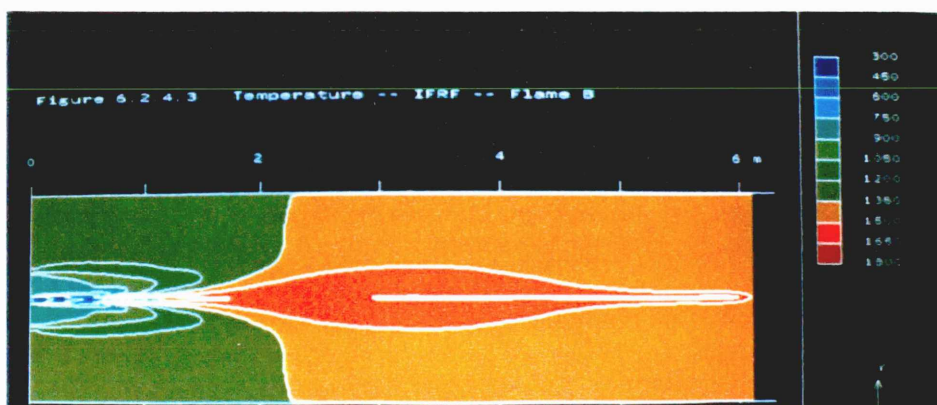


Figure 6.2.4.4 Predicted Temperature - IFRF - Flame B

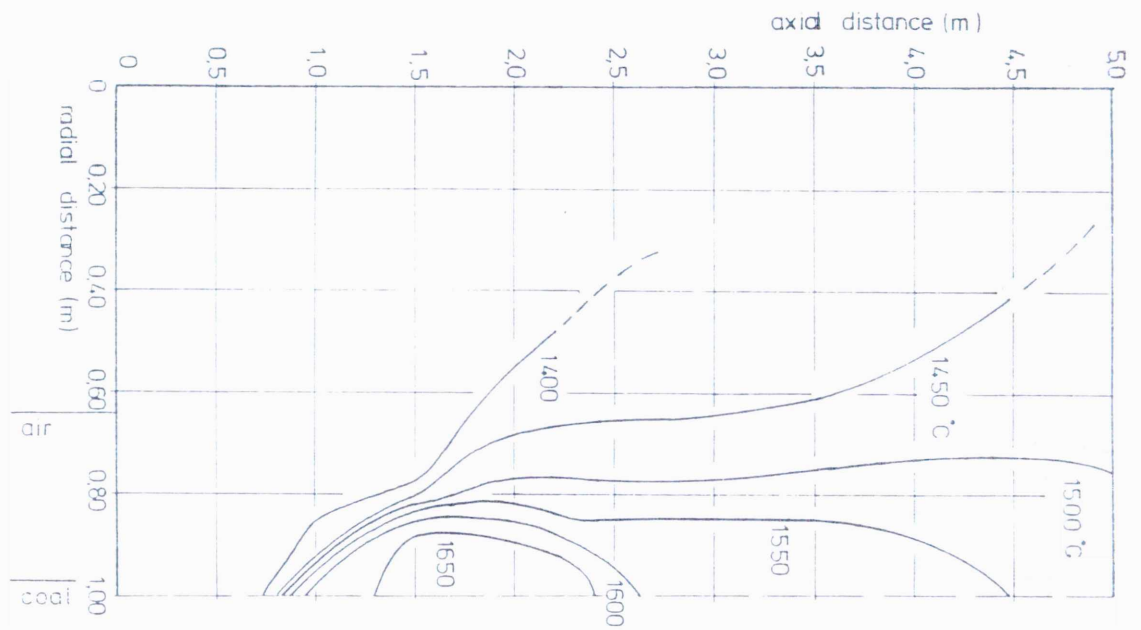


Figure 6.2.4.5 Measured Temperature - IFRF - Flame C

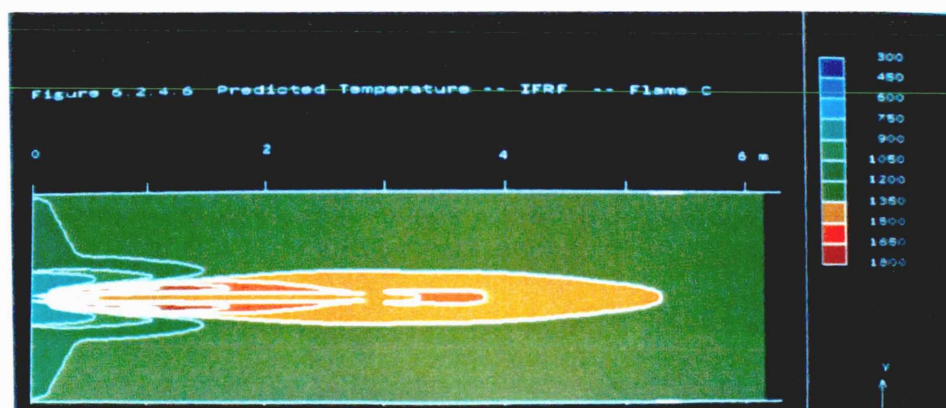


Figure 6.2.4.6 Predicted Temperature - IFRF - Flame C

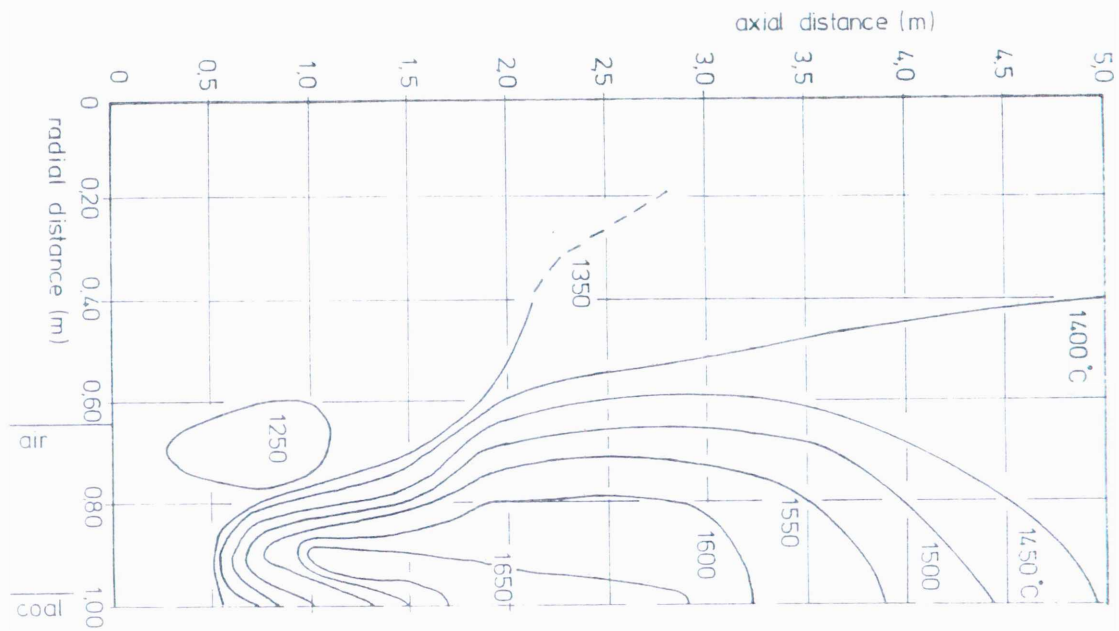


Figure 6.2.4.7 Measured Temperature - IFRF - Flame G



Figure 6.2.4.8 Predicted Temperature - IFRF - Flame G

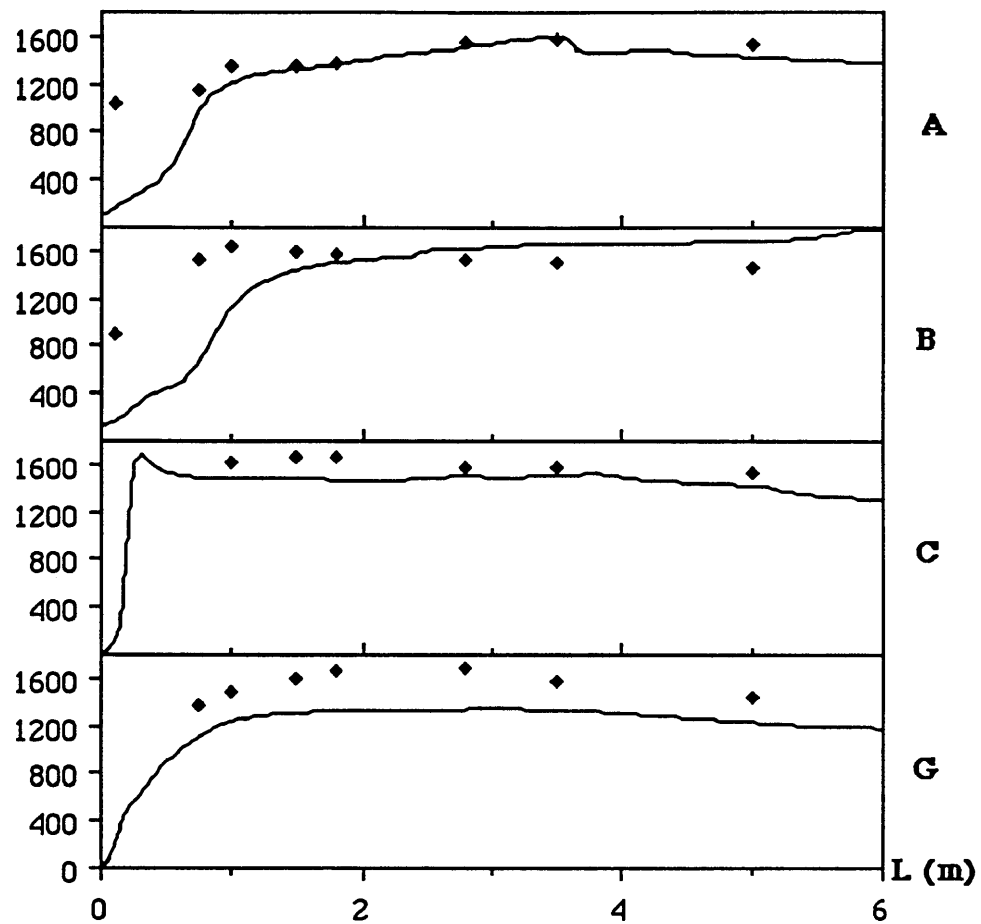
Temp. ($^{\circ}\text{C}$)

Figure 6.2.5.1

Temperature Axial Profiles for flames A, B, C, and G

— Predicted
♦ Measured

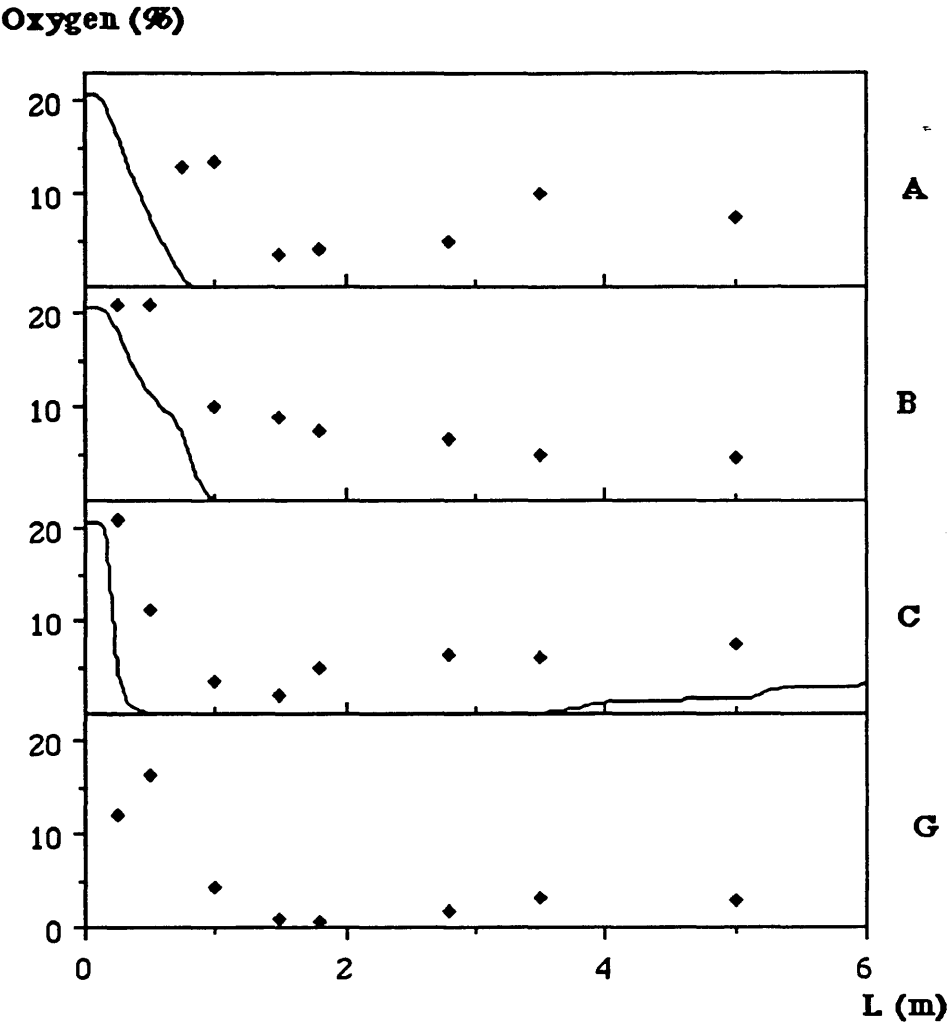


Figure 6.2.5.2
Oxygen Axial Profiles for flames A, B, C, and G

— Predicted
♦ Measured

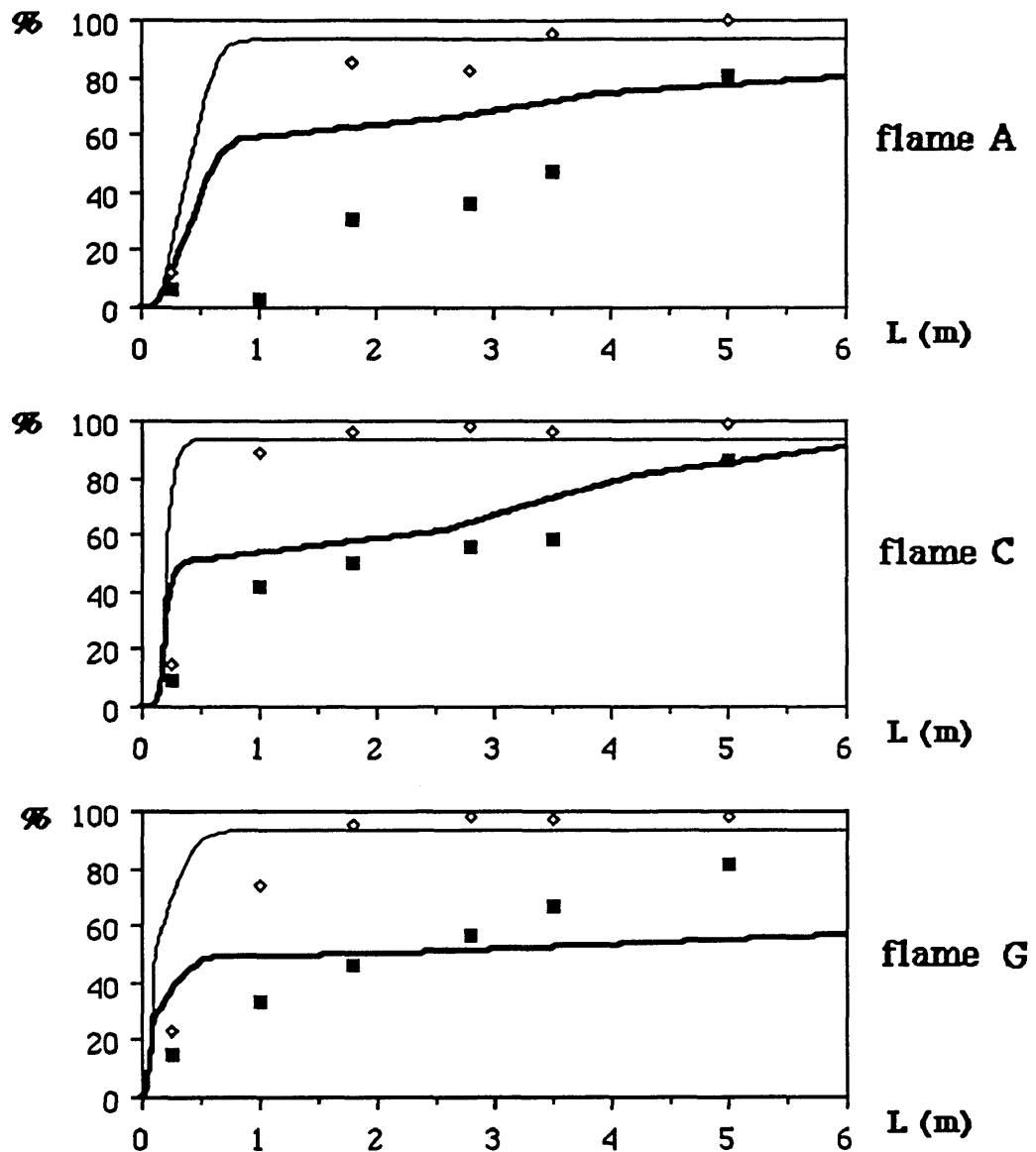


Figure 6.2.5.3
Comparison of Axial Profiles of
Volatiles and Char Burnout for flames A, C, and G

- Predicted Volatile Sources
- Predicted Mass Sources
- ◇ Measured Volatile Burnout Z_x
- Measured Total Combustible Burnout T_x

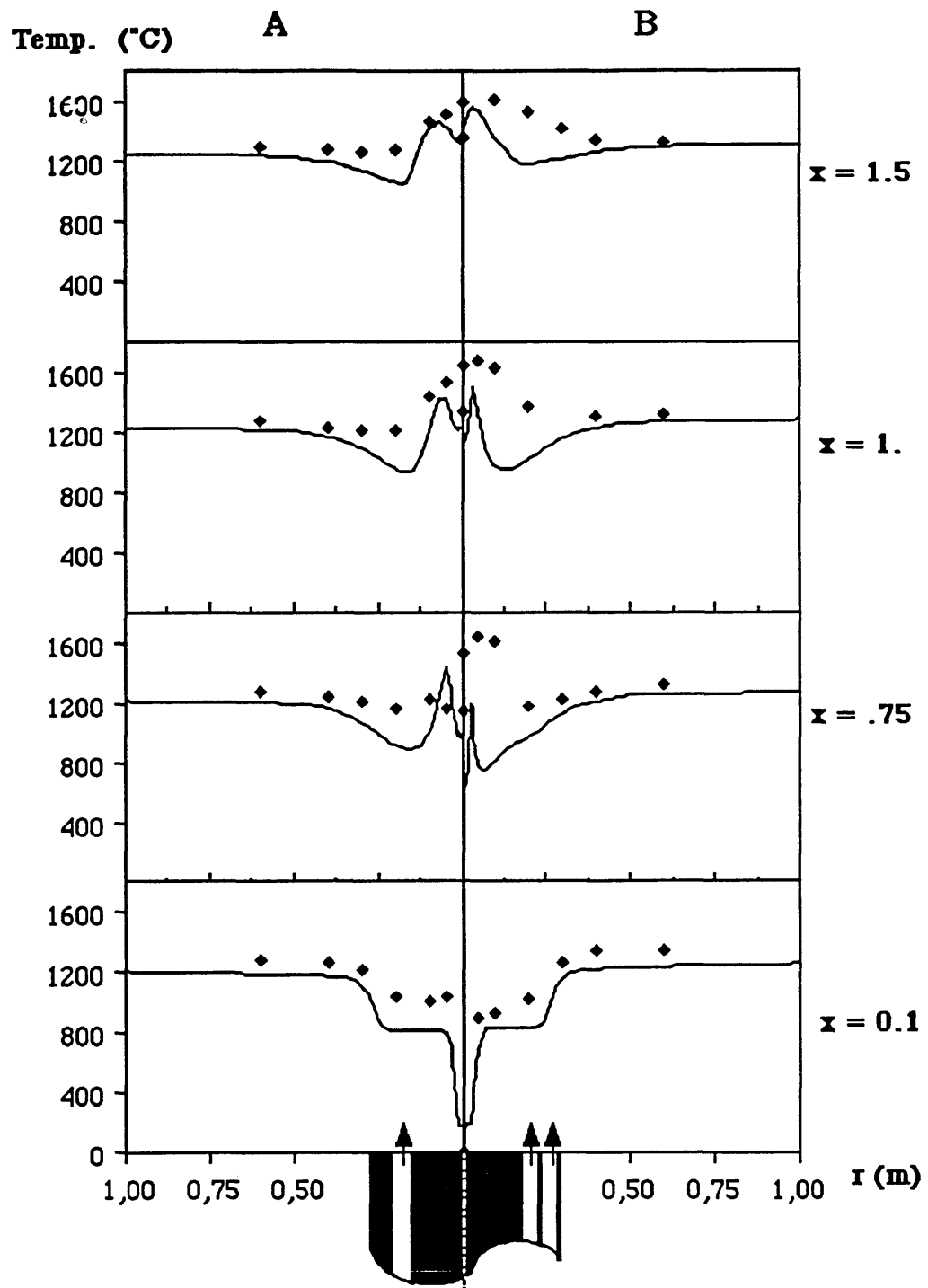


Figure 6.2.6.1

Temperature Profiles of Flames A and B

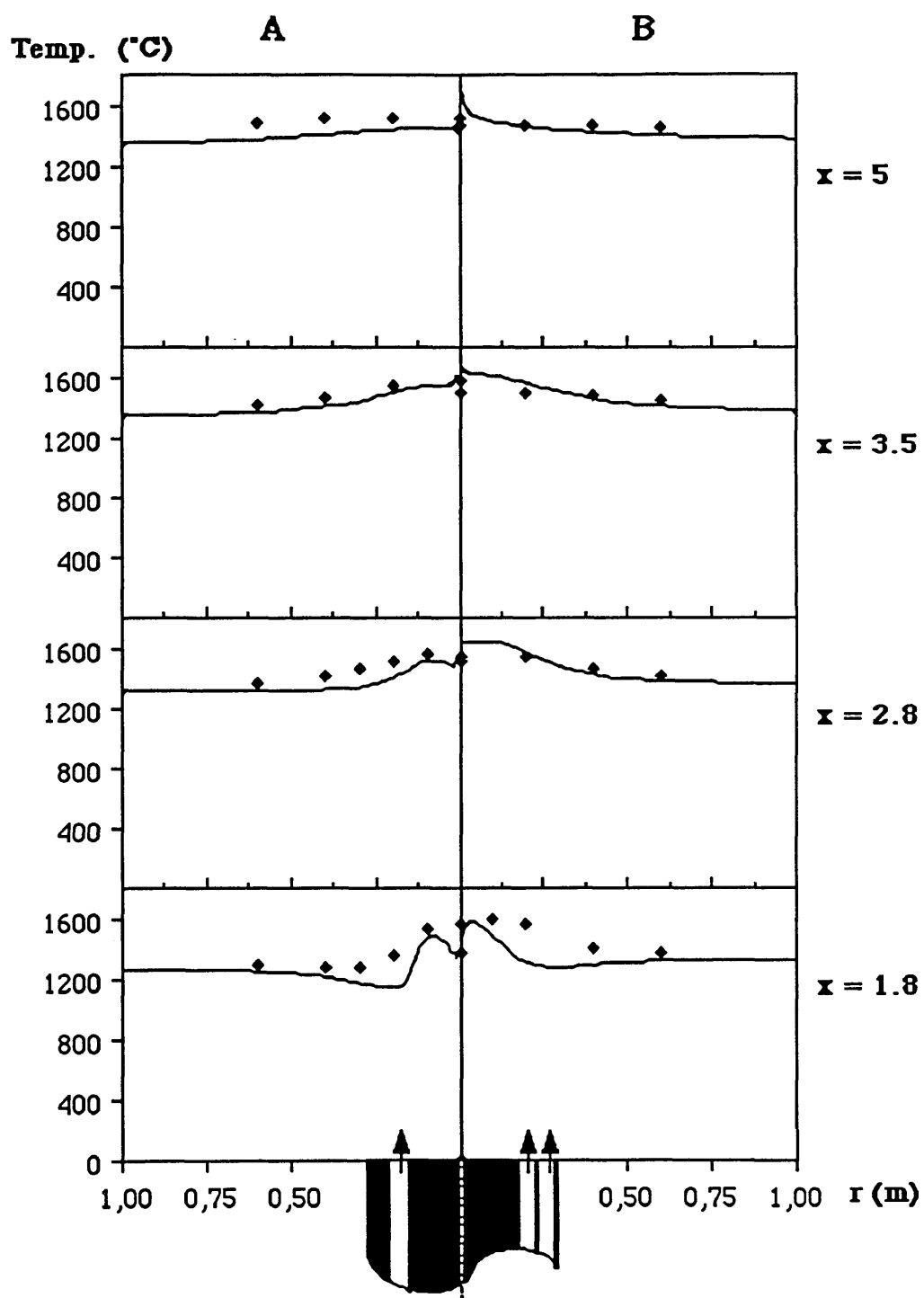


Figure 6.2.6.2

Temperature Profiles of Flames A and B

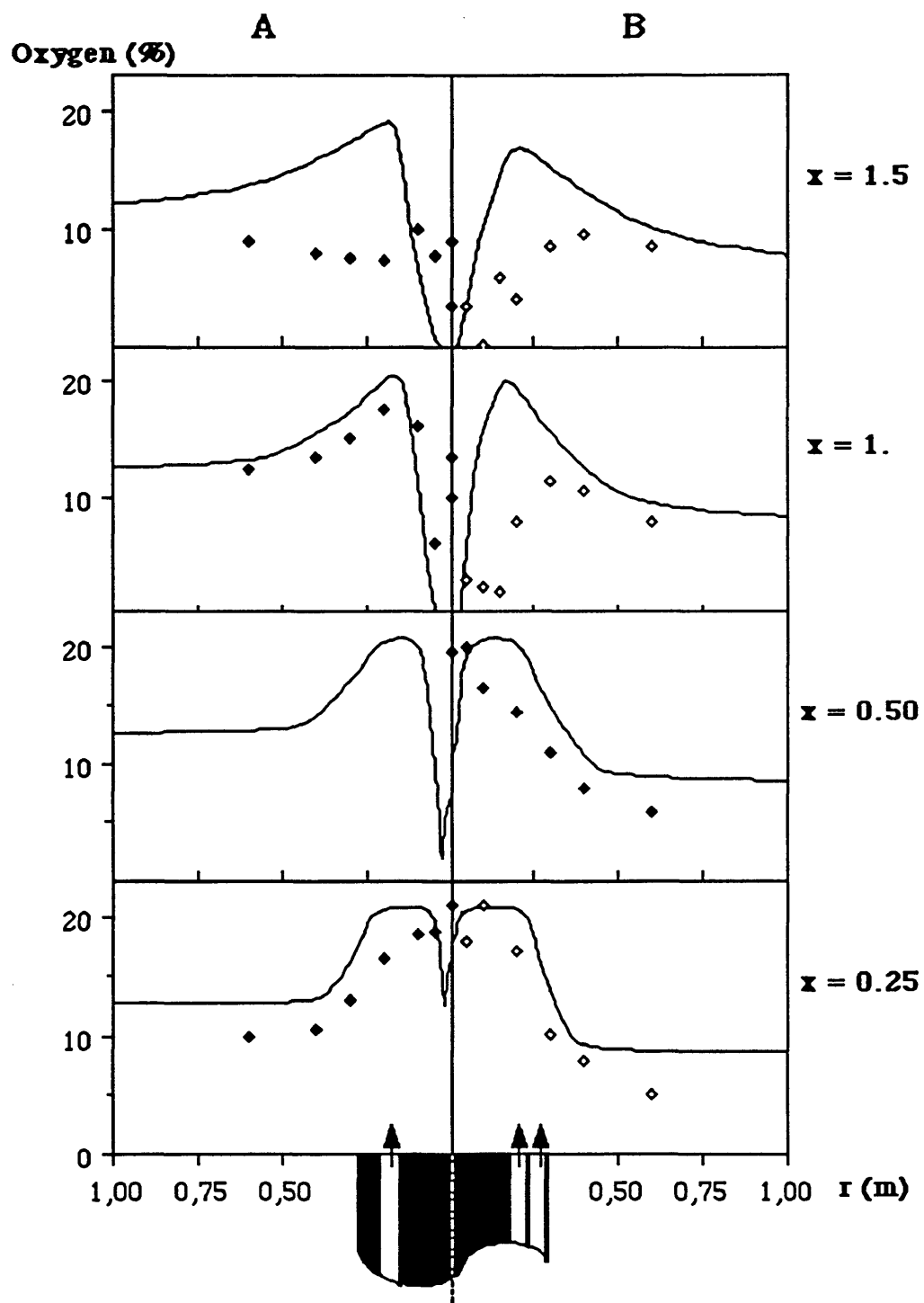


Figure 6.2.6.3

Oxygen Profiles of Flames A and B

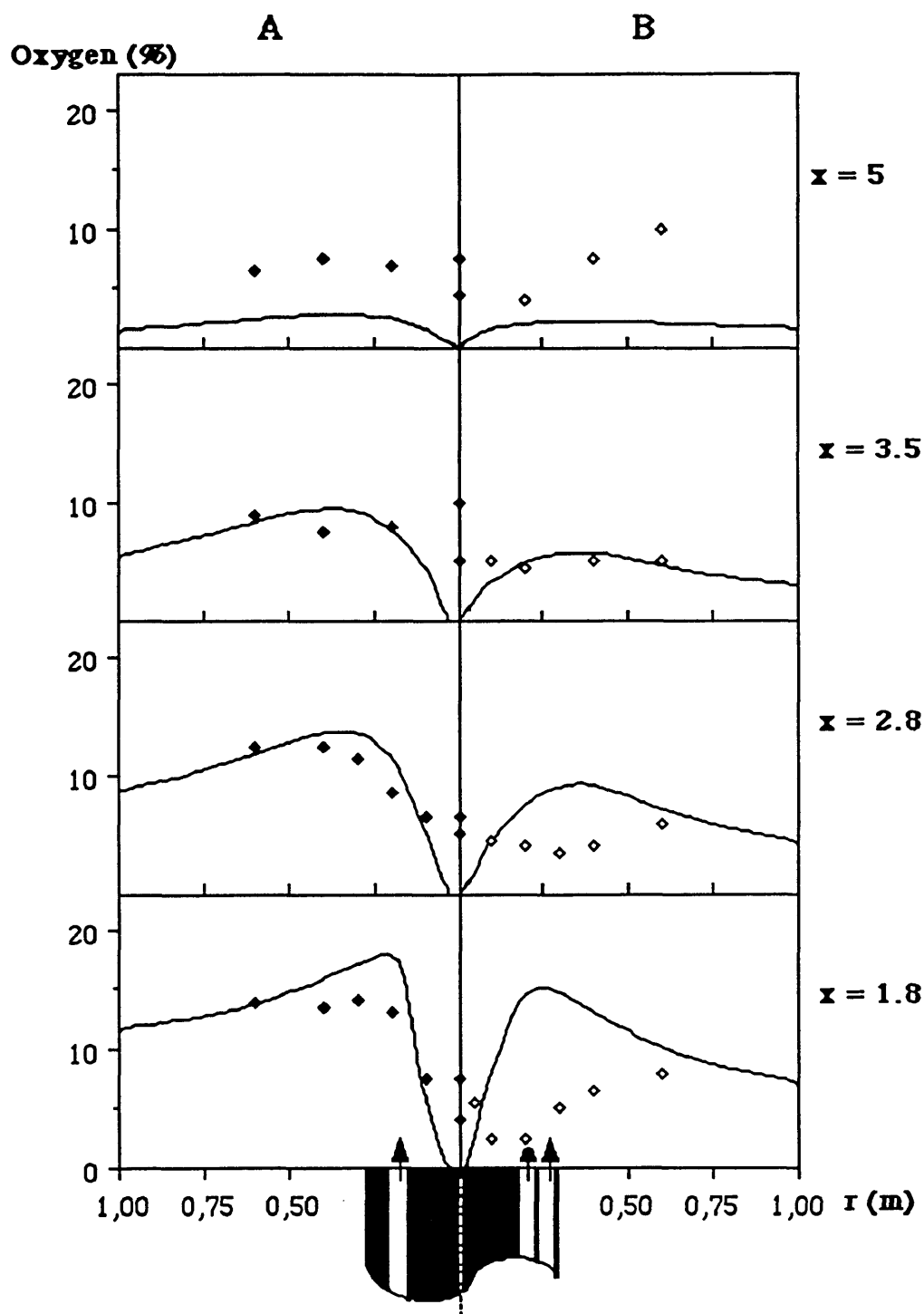


Figure 6.2.6.4

Oxygen Profiles of Flames A and B

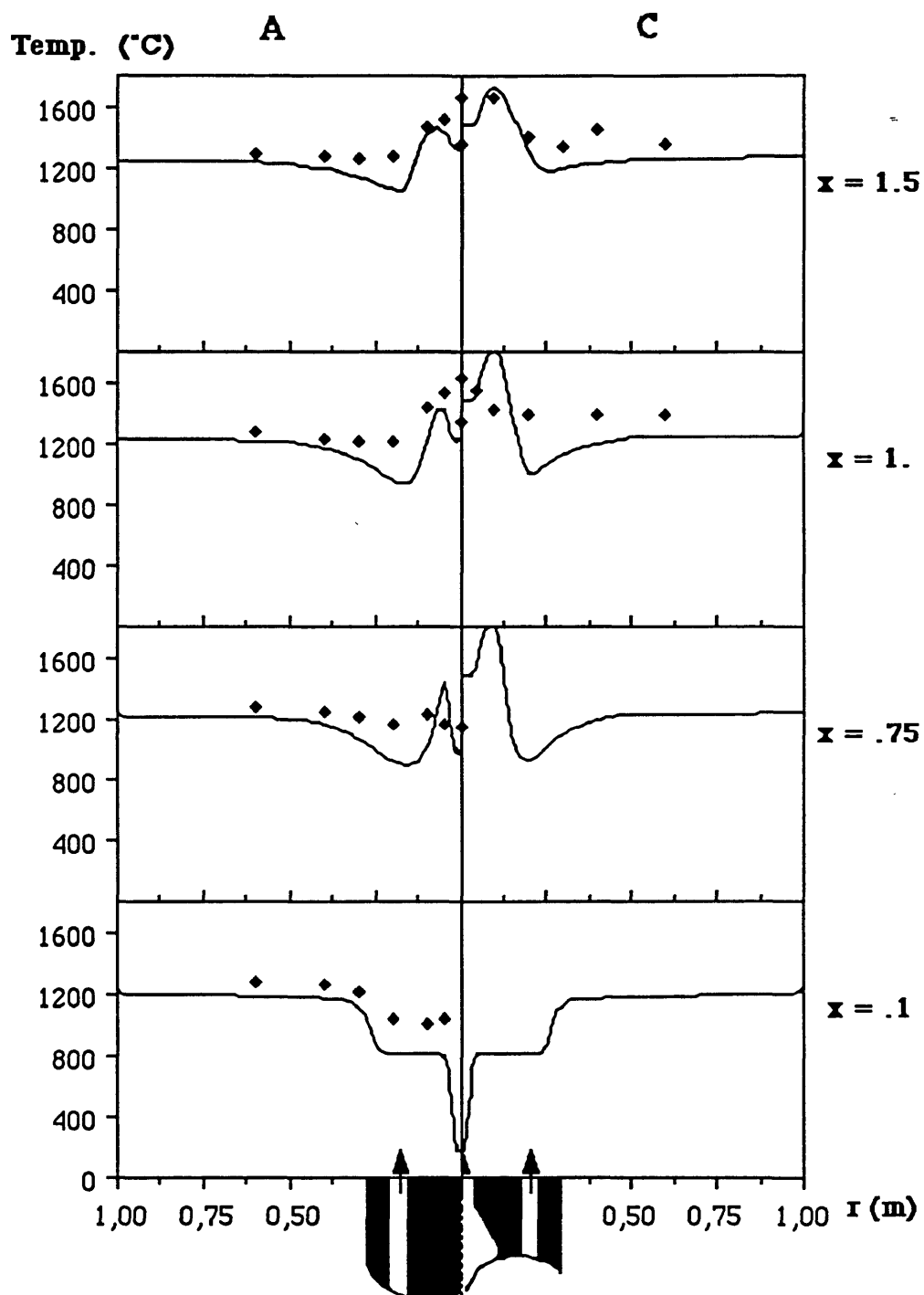


Figure 6.2.6.5

Temperature Profiles of Flames A and C

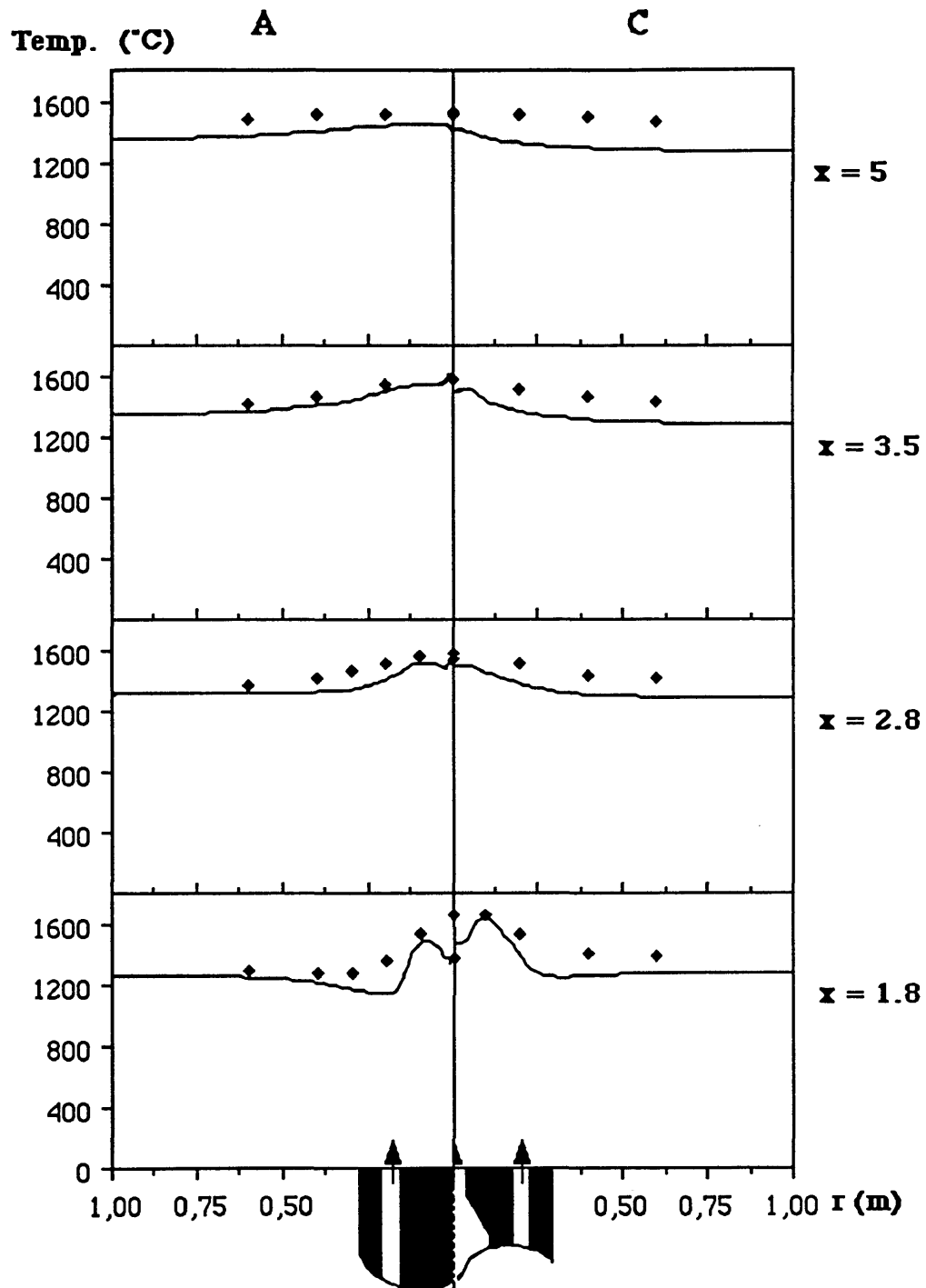


Figure 6.2.6.6

Temperature Profiles of Flames A and C

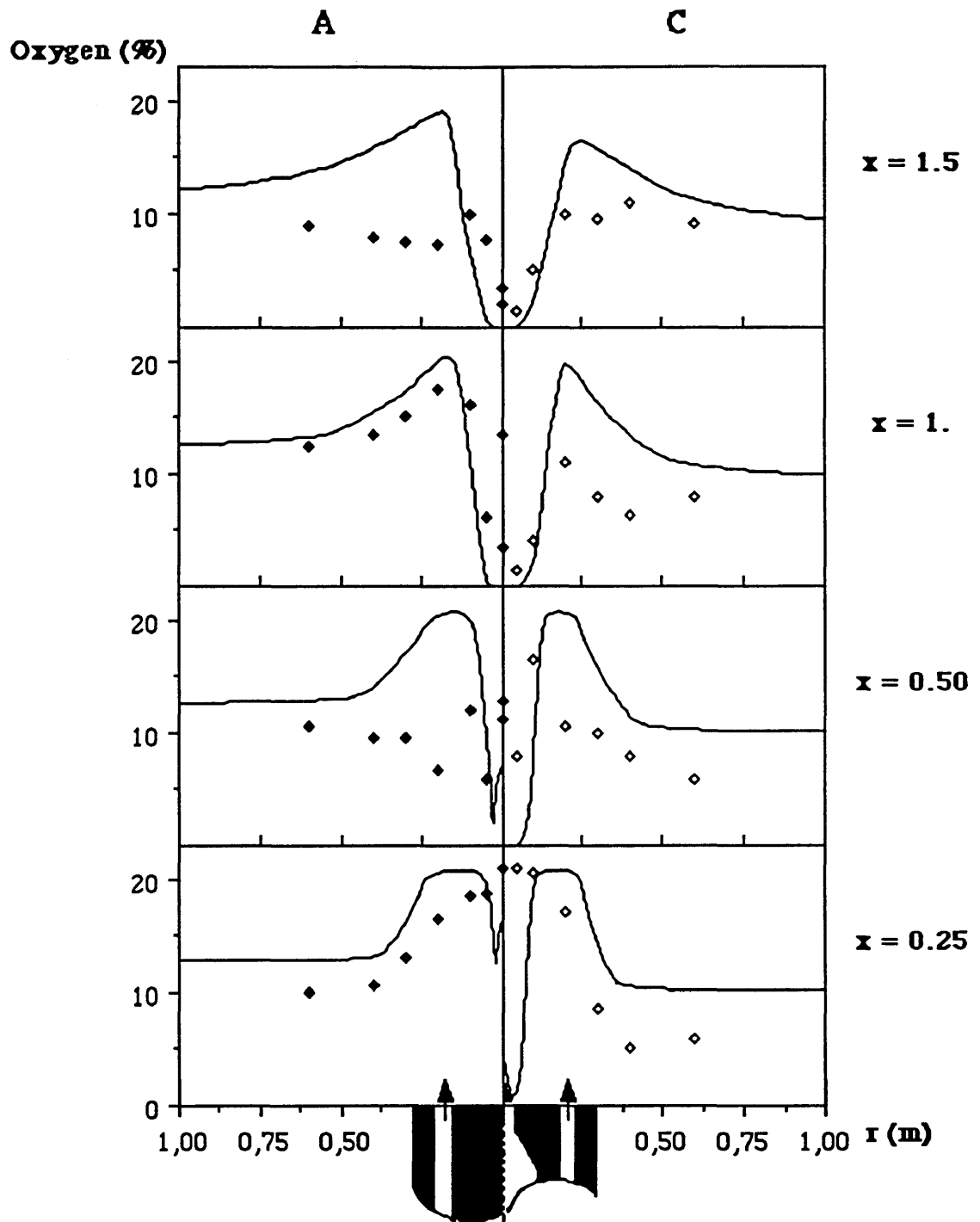


Figure 6.2.6.7
Oxygen Profiles of Flames A and C

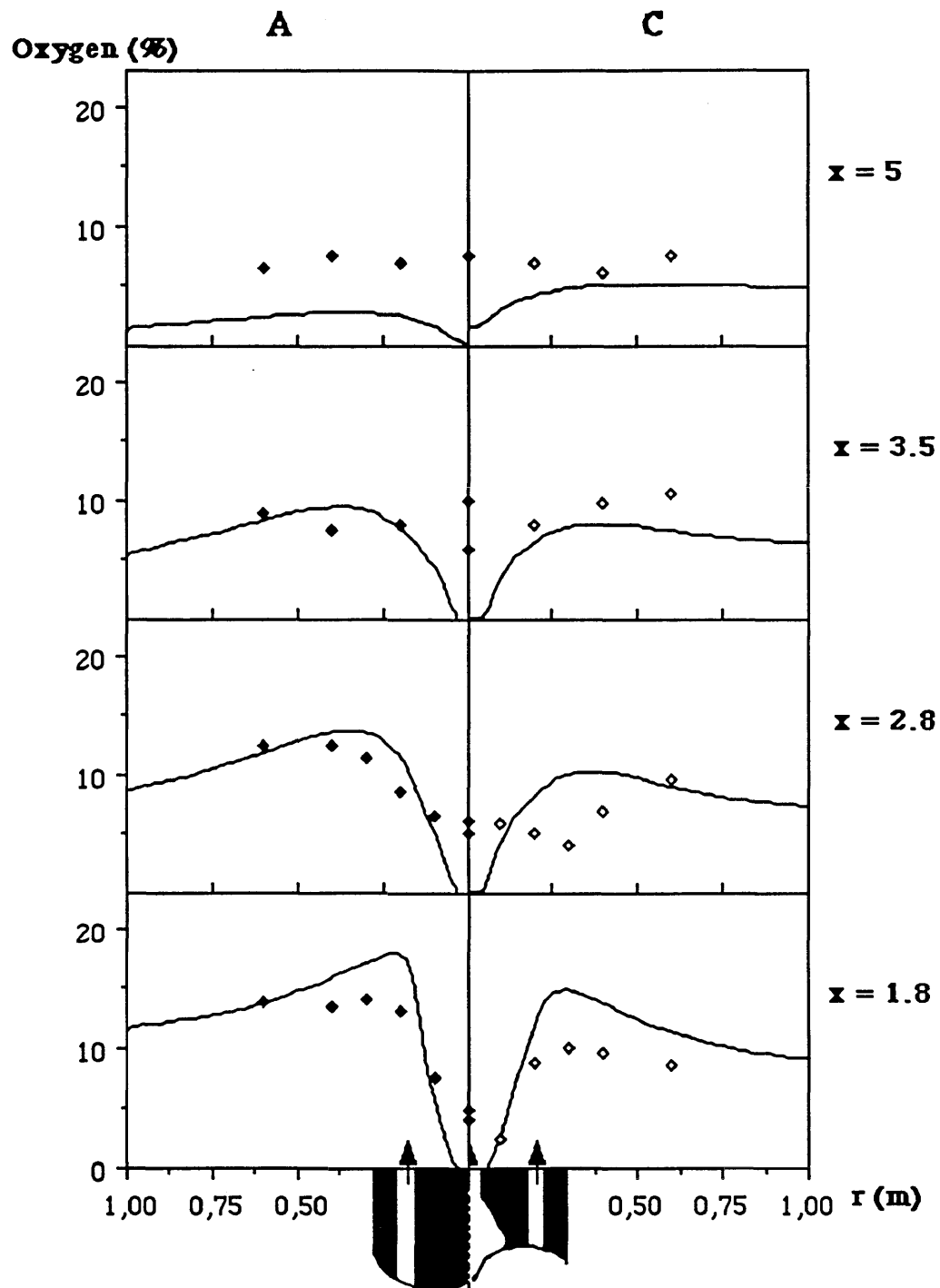


Figure 6.2.6.8

Oxygen Profiles of Flames A and C

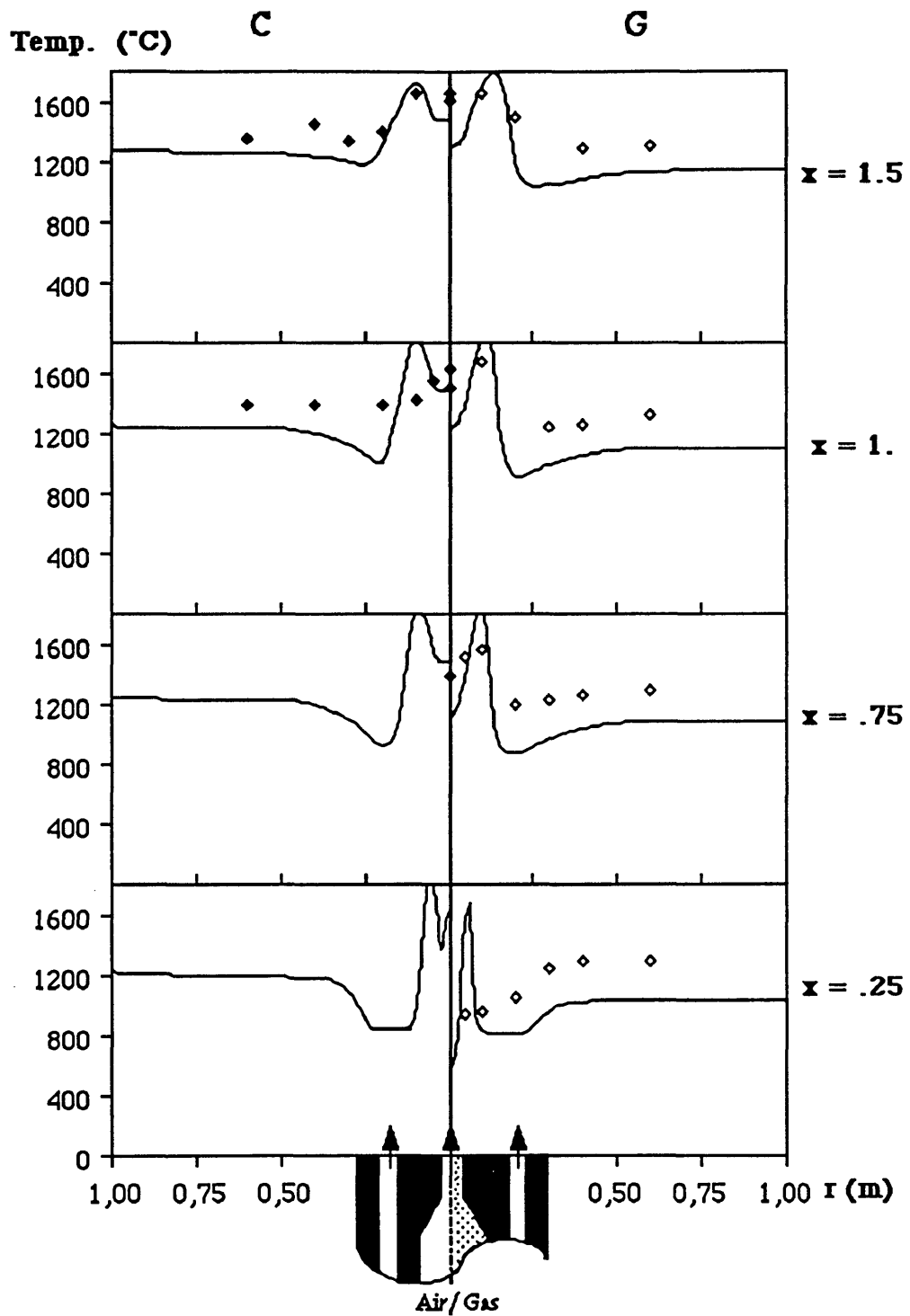


Figure 6.2.6.9

Temperature Profiles of Flames C and G

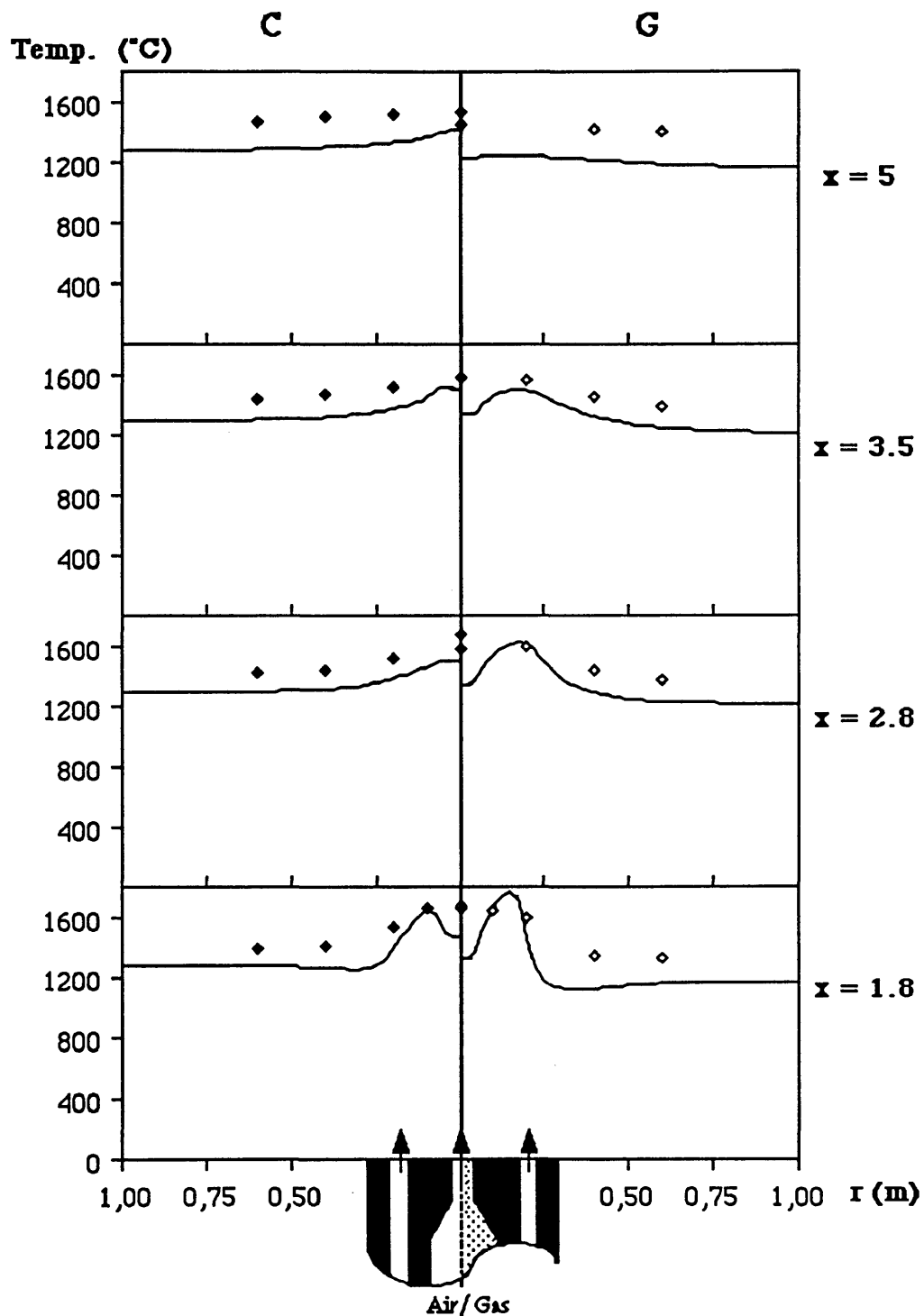


Figure 6.2.6.10

Temperature Profiles of Flames C and G

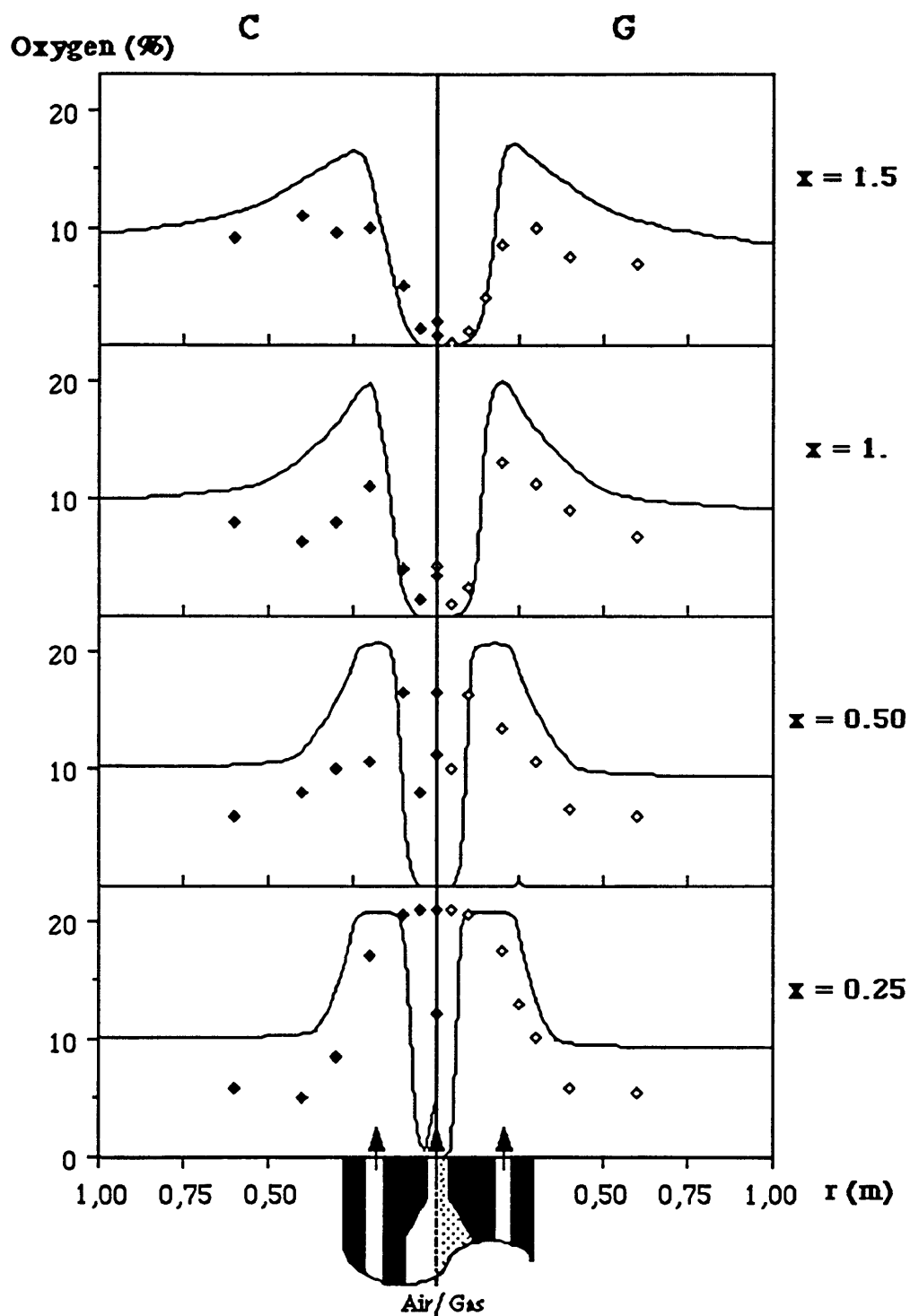


Figure 6.2.6.11

Oxygen Profiles of Flames C and G

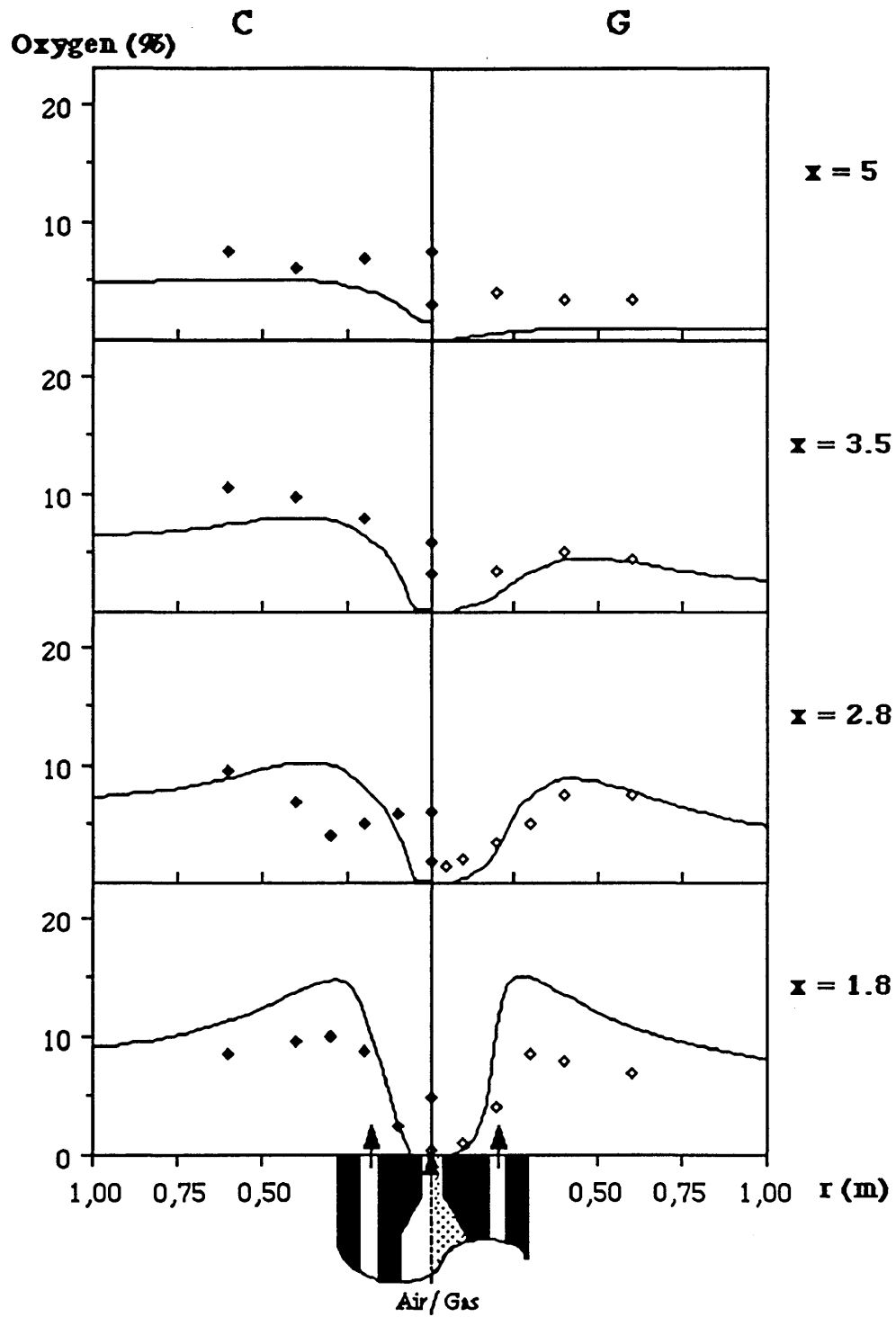


Figure 6.2.6.12
Oxygen Profiles of Flames C and G

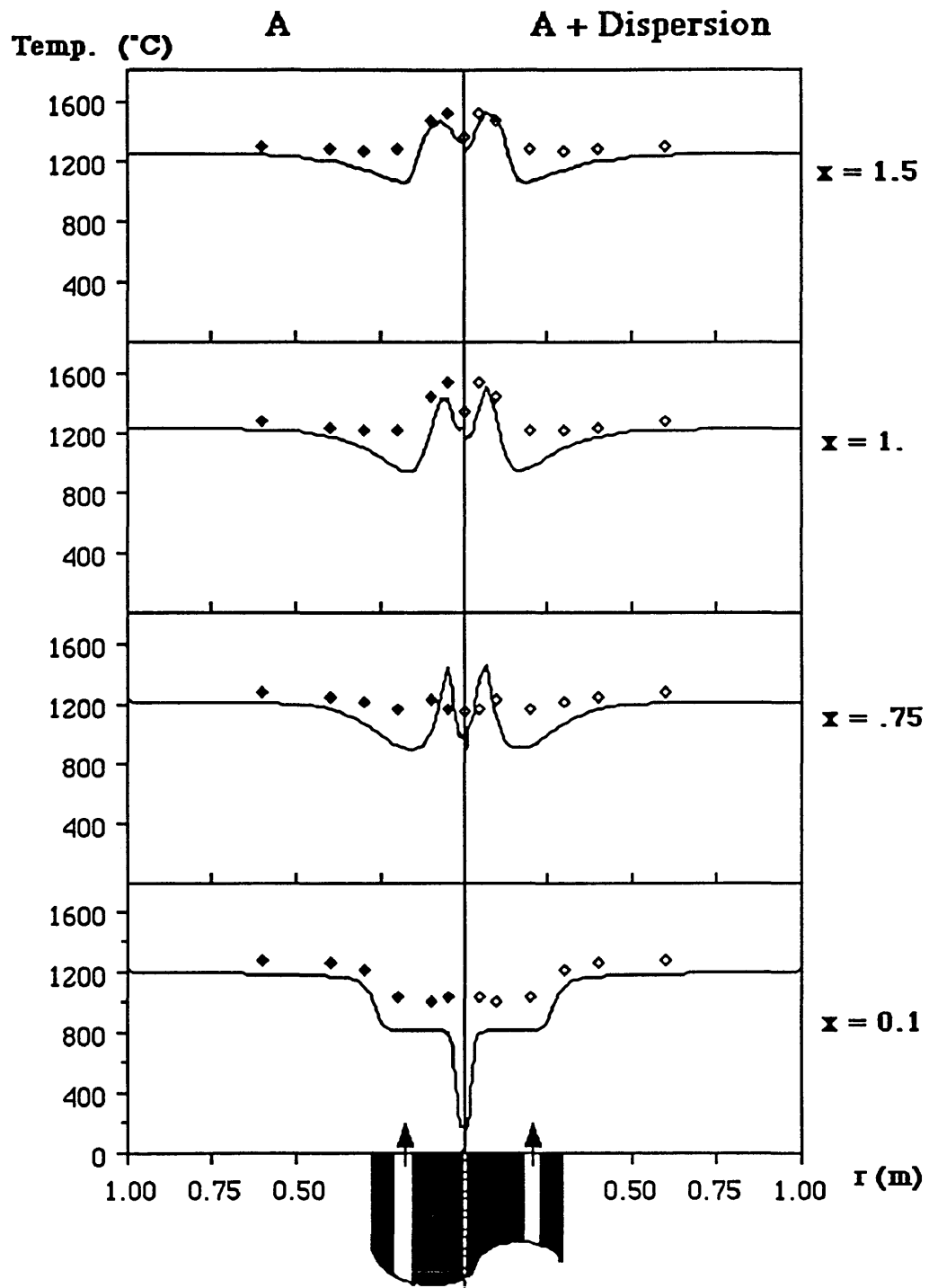


Figure 6.2.7.1

Temperature Profiles of Flame A with and without particle dispersion

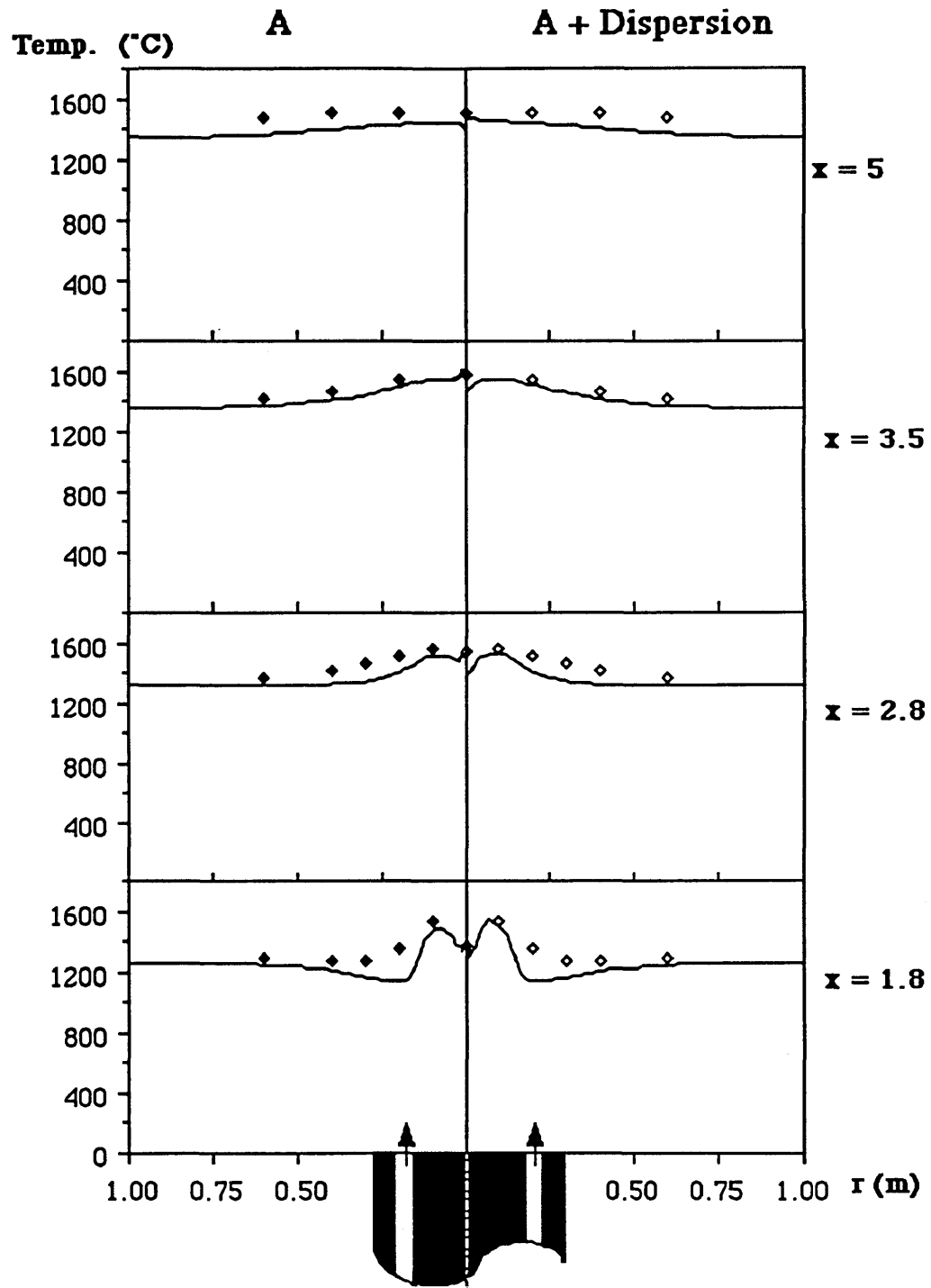


Figure 6.2.7.2

Temperature Profiles of Flame A with and without particle dispersion

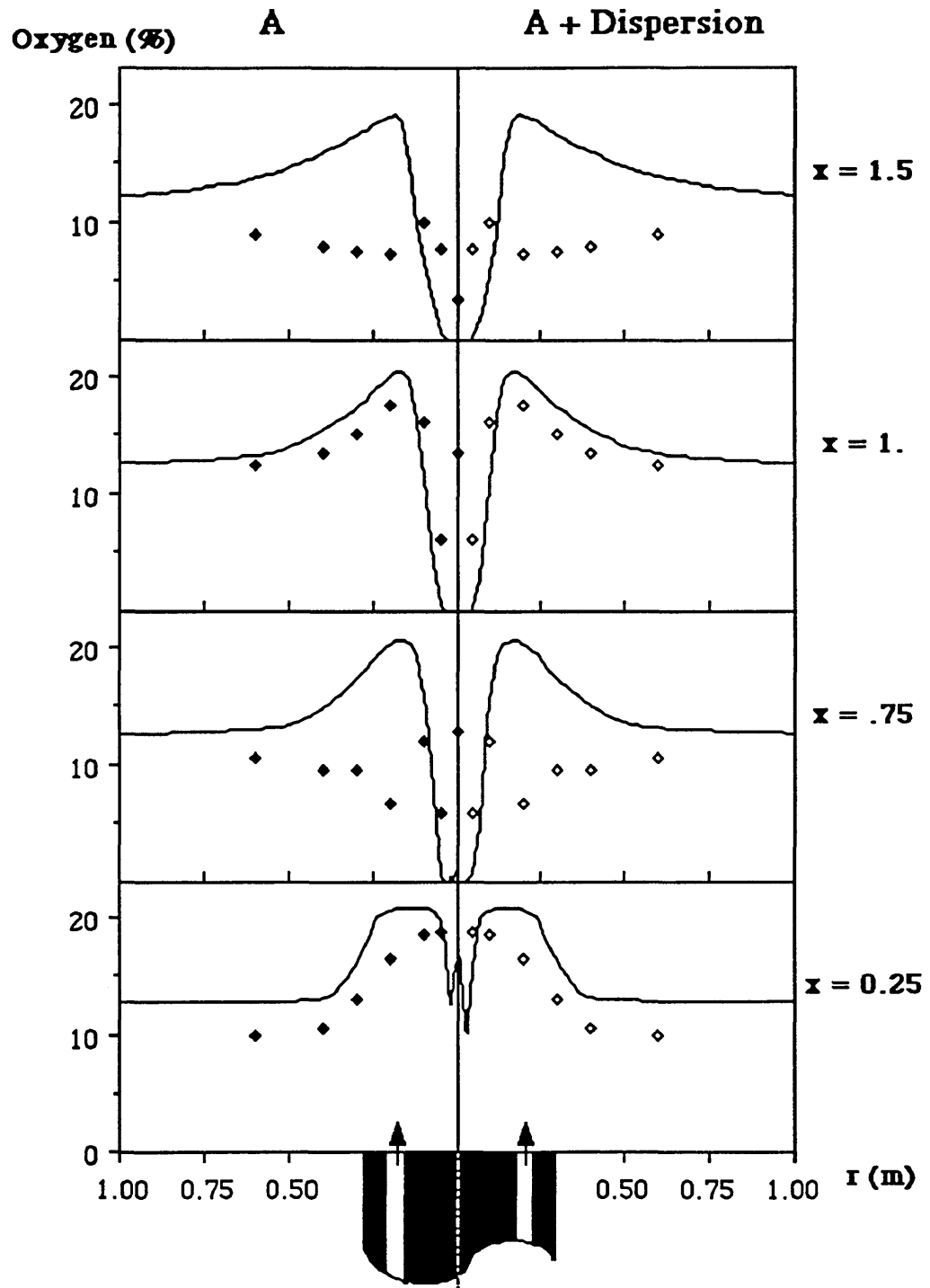


Figure 6.2.7.3

Oxygen Profiles of Flame A with and without particle dispersion

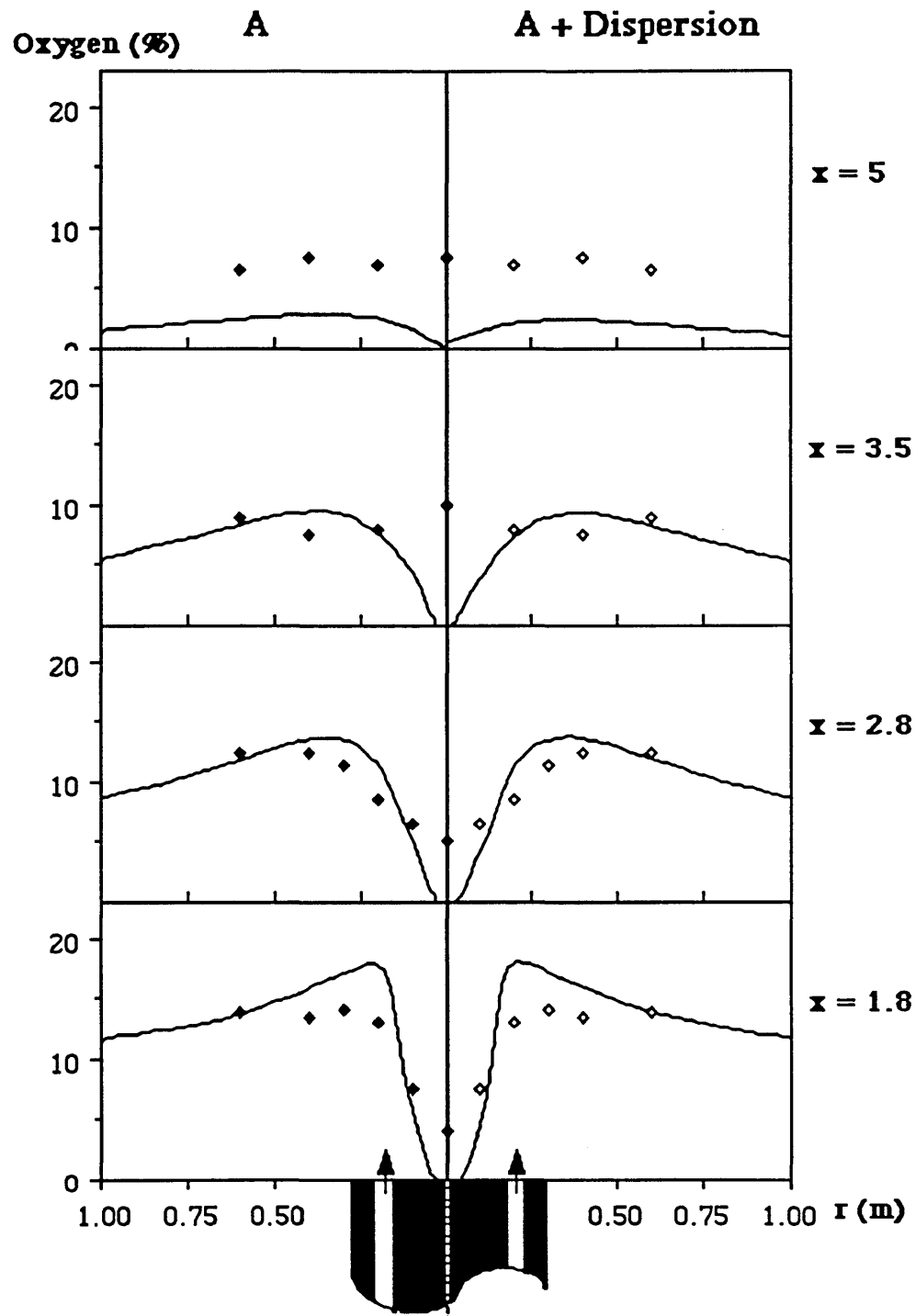


Figure 6.2.7.4

Oxygen Profiles of Flame A with and without particle dispersion

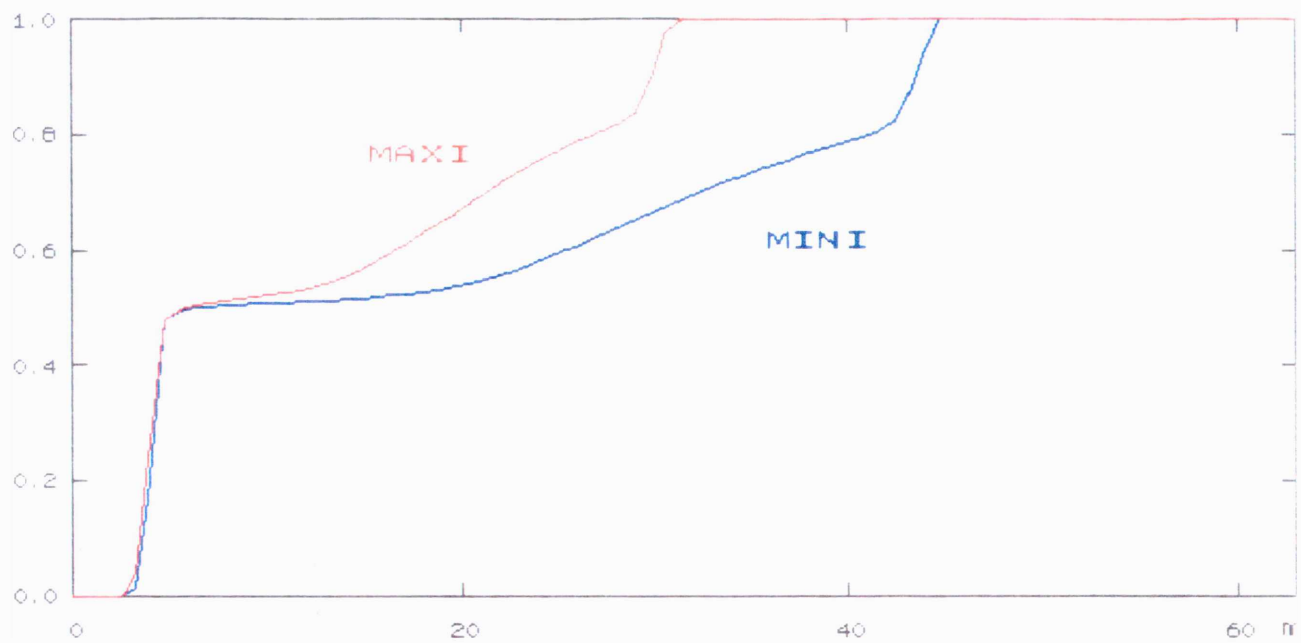


Figure 6.3.1 Coal Burnout for Full Size Cement Kiln Prediction



Figure 6.3.2 Temperature for Full Size Cement Kiln Prediction -- Flame MINI

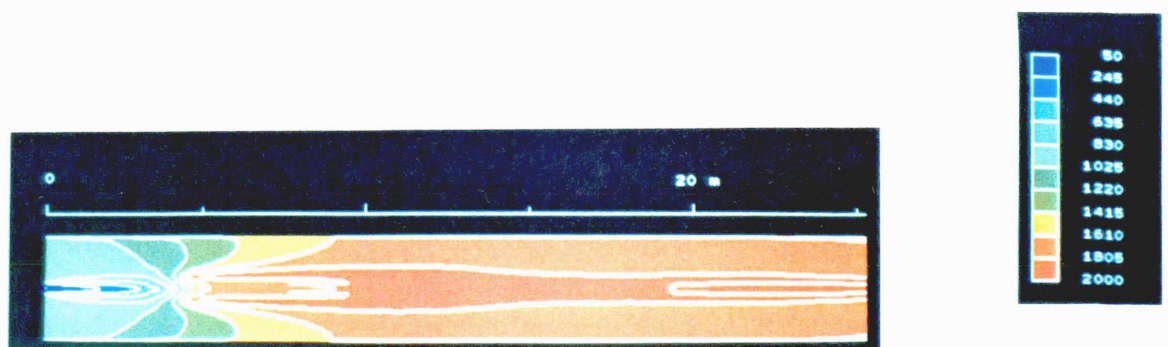


Figure 6.3.3 Temperature for Full Size Cement Kiln Prediction - Flame MAXI

CHAPTER 7

COMPLETION

The objectives of the present study have been stated in section 1.4. In the first section of this chapter the work presented in this thesis is summarised to show the extent to which the stated aims have been attained. In the second section, the suggestions and scope for future work are given.

7.1 RECAPITULATION

7.1.1 FAFNIR the Code

During the first part of this thesis, a new computer code was developed for the prediction of flow and heat transfer in a pulverised fuel fired furnace for axisymmetric, turbulent, recirculating flows with swirl. This program, called FAFNIR, can be run without tampering with the code itself by using an interactive pre-processor, and is open to any further modifications thanks to its structural programming. It has been tested on several computers and operating systems.

The physical and chemical phenomena occurring in a pulverised fuel flame were studied and available mathematical models were chosen according to their performance. Numerical methods for the gas phase (a finite difference method, using an eulerian approach), the particulate phase (a time discretisation method using a lagrangian approach) and the thermal radiation heat (the non-equilibrium diffusion model) were selected and applied. Finally, these models were assembled and programmed into the computer code FAFNIR. A pre-processor and a post-processor were also written to facilitate the running of the code. After some tests, FAFNIR was ready to use. This work is described in the present thesis on chapters 2, 3 and 4 for the mathematical and physical modelling, and chapter 5 for the computing of FAFNIR.

7.1.2 Validation

It then became necessary to prove the validity of FAFNIR predictions. For this purpose, the generality of the code became useful, since experimental data on full size cement kiln furnaces is not easily available, and therefore laboratory experiments were used.

Firstly, the validity of the flow calculations were tested. A water scale model of a cement kiln was constructed and a laser sheet technique used to visualise the flow. The comparisons with the predicted flow were found to be satisfactory. (see section 6.1)

Secondly, the global flow and combustion predictive procedure were tested by comparison with experimental data from the International Flame Research Foundation (IFRF) (see section 6.2). Three out of four cases showed a good correlation between experiment and prediction. The fourth case (flame B, in section 6.2.3.3) was not so well predicted, due probably to the particle dispersion model which was not found to be satisfactory, and perhaps due also to symmetry problems that occurred during the experiment.

7.1.3 Cement Kiln Runs

The overall validation results were found to be satisfactory enough to install the program in a cement manufacturer, and test it on a full size kiln. An example of such a run is presented in section 6.3. These runs showed that it was possible to predict a cement kiln flame with reasonable accuracy. It was found that a specific set up could yield an energy gain. This result was confirmed by experimental observation in a cement plant.

Today, the program is commonly used by Lafarge Coppée Recherche for the prediction of cement kilns flames. Firstly on a day to day basis, by helping plant

engineers to solve specific problems. Secondly on a long term basis, by running parametrical studies with paramaters such as input flow rates and velocities, swirl angle, coal granulometry, secondary air temperature etc... The main objective of this thesis, which is to provide the cement industry with a tool capable of predicting the behaviour of pulverised fuel fired cement kiln is therefore attained.

7.2 FUTURE WORK

A computer code would be useless if it could not evolve. This evolution is not only necessary because of more accurate mathematical models will be developped in the future thanks to the research in coal combustion, but also because the necessities of the industry do change as time passes and the conjuncture evolves.

New more accurate mathematical models may be developped both for the devolatilisation and the char combustion process. Today's research uses sophisticated techniques that will probably increase the understanding of these phenomena. The same can be said regarding turbulence modelling and especially regarding particle dispersion models. These may be better predicted in the future thanks to available computer capacities increasing in an exponential way. This evolution in computing capabilites may also allow for complex radiation models to be implemented.

Regarding the evolution of industrial necessities, the programming of liquid fuel combustion modelling in FAFNIR would give the code a wider range of applications. It is also possible to imagine the code being used to predict the behaviour of flames fired with a mixture of different coals or a mixture of coal and liquid fuel. The combustion of certain kinds of industrial wastes might also be predicted (?). Finally, FAFNIR results can be used by another code in order to the predict NO_x or SO_x emissions.

As a conclusion, it is hoped that FAFNIR was effectively written in such a way that the future developments mentioned above can be easily implemented.

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