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Multifidelity methods for simulation of wax deposition in single-phase and two-phase flow

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Abstract

The description of wax deposition in the presence of (often turbulent) flow is challenging since it requires the understanding of the fluid dynamics, heat and mass transfer, the thermodynamic effects, and the deposit formation and removal. The length and timescales involved vary over many orders of magnitude making a complete simulation of the full phenomena prohibitively expensive for any industrial situations. Different simplifications may be used, depending on the desired compromise between generality, robustness, speed, and accuracy.

In this work, a set of different modelling techniques for wax deposition based on fundamental methods or data-driven approaches is proposed, implemented, and validated. These included more complete, local descriptions of the flow, namely interface-capturing, graph networks, and thin film models, as well as global models using mechanistic considerations and/or regressions based on data.

An interface-capturing model from the literature is implemented and tested, and, due to its high computational cost, a graph network based data-driven approach is tested for acceleration of the computations. Following that, a simplification based on a thin film assumption is also examined, which can result in significant savings in computational cost. Focusing on a more industrial application, a mechanistic model for pipe flows is proposed and extensively validated with data from single and multiphase flows. Finally, a framework for generation of surrogate models based on an active-learning technique, for complex models, is analyzed.

The models presented here have been validated whenever possible, and as far as possible, against experimental data from the literature and could be used in the design and/or operation of equipment subject to wax deposition (and, more generally, any deposit resulting from a phase change-type transformation), or used in the development of other novel techniques.

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Dedication

To my parents, for all the love and support that made this work possible.

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Nomenclature

$\dot{m}$	Mass transfer rate
$\mathbf{b}$	Boundary encoding vector
$\mathbf{e}$	Edge features
$\mathbf{v}$	Node features
$\mathbf{y}$	Node targets
A	Area
c	Concentration
c_p	Heat capacity
D	Diameter
e	Specific internal energy
f	Friction factor
g	Gravity acceleration
H	Holdup
h	Specific enthalpy
K	Equilibrium constant
k	Thermal conductivity
L	Length

L_x	Mole fraction of liquid
M	Molecular weight
p	Pressure
q	Heat transfer rate
R	Universal gas constant
S	Perimeter
T	Temperature
t	Time
U	Velocity
U_S	Superficial velocity
Y	Mass fraction

Greek letters

α	Volumetric fraction
χ	Interfacial area density
δ	Thickness
ϵ	Roughness
Γ_m	Molecular diffusivity
μ	Dynamic viscosity
ϕ	Inclination
ρ	Density
σ	Interfacial tension
τ	Shear stress
θ	Wetted angle

κ Interface curvature

Nondimensional numbers

Co Courant number

Gz Graetz number

Le Lewis number

Nu Nusselt number

Pr Prandtl number

Re Reynolds number

Sc Schmidt number

Subscripts

D Deposit

f Film

G Gas

i Interface

L Liquid

s Slug

w Wall

Chapter 1

Introduction

Wax deposition in the flow of crude oils is a complex phenomenon with high industrial importance - improvements in predictions can lead to huge savings in energy expenditure and cost of design and operation of pipelines. Although it has been an object of study for several decades, fundamental mechanisms of solid deposition and removal remain under discussion in the literature. Many one-dimensional models have been proposed for prediction of wax characteristics in industrial settings, but the number of studies that looked into the fundamental phenomena through direct simulations of the flow is relatively limited.

The deposition in two-phase flow of gas and oil has been subject of relatively few studies, both experimental and numerical. In this case, the presence of a third phase has an effect on both the hydrodynamics as well as the thermodynamic properties. Although the effects can usually be described qualitatively, discrepancies between predictions and observed results can be significant (Liu et al., 2020). The lack of theoretical knowledge is reflected in industrial simulators, with studies showing the high dependence of deposit properties on the choice of the specific closure relations (Zhang, Pedrosa, et al., 2019). Ultimately, conservative predictions have to be used in the design and operation of pipelines and equipment, leading to inefficient installation and operation.

Numerous methodologies exist for description of such complex flows, with trade-offs between computational cost, accuracy and robustness. The approaches range from complex physical

models that aim to resolve all local scales of the flow, to models based solely on global observations of key variables, or hybrid methods in between. Although the data driven approaches can often present high predictive performance, they have limited applicability outside the range of their training data, while physics based models can often provide at least qualitatively correct insights in a large range of situations (Pan et al., 2022).

This work aims to provide an overview of the state of the art physical and data-driven methods that can be used for description of complex flows in pipelines and equipment, particularly under the presence of gas and liquid phases and solid deposits at the wall. The structure of the thesis is presented in schematic form in Fig. 1.1.

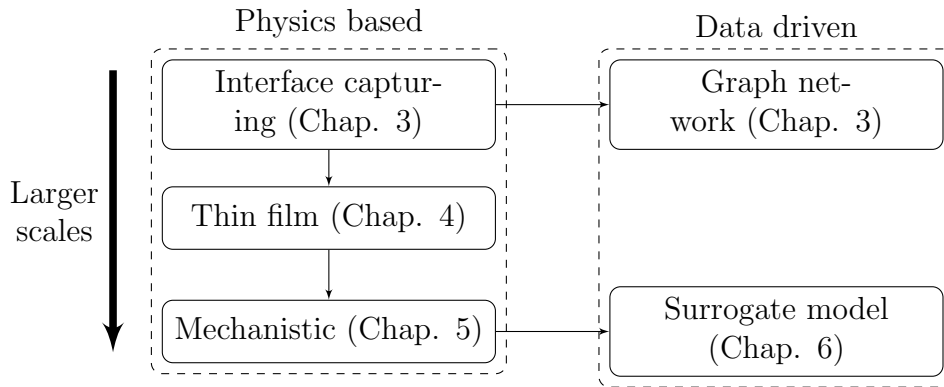


Figure 1.1: Structure of the thesis.

Firstly, on Chap. 3, a state of the art model for detailed modelling of solid deposition with an interface capturing approach will be implemented on an open source platform. Although very useful to analyze small scale effects of parameters on flow and deposition, this approach is very high computationally intensive, and the real time and length scales observed in applications are hard to reproduce. Magnini and Matar (2019) addressed this problem by increasing the rate of deposition artificially, but it is questionable whether that preserves the relevant dynamics. With that taken into account, alternative approaches for accelerating the calculations will be analyzed, starting with a graph based data-driven technique trained on time-dependent flow fields.

On Chap. 4, a model simplification with an assumption of a thin deposit will be proposed. The simplified model will be compared to the fully resolved simulation framework presented before. Finally, the method will be applied to several cases of engineering interest, namely single-phase

and stratified gas-liquid flow, as well as flows on bends. Validation will be presented, based on experimental observations from the literature.

Chap. 5 will present an alternative mechanistic modelling approach for pipe flows. The one-dimensional model has a low enough computational cost that full pipelines can be simulated, or large parametric studies can be executed. It relies, however, on numerous closure relations, which require external information and may have limited range of application.

In Chap. 6 a comparison of techniques for constructing surrogate models for key outputs of costly simulations will be performed. This will be applied to some simple CFD test cases, as well as to deposition calculations of a physics-based model.

Finally, Chap. 7 will present the general conclusions and suggestions of future work.

1.1 Statement of Originality

The content presented here is original material produced by the author. Citations have been provided to all the references used.

1.2 Publications

- Gabriel F. N. Gonçalves et al. (2020). “Data-driven surrogate modelling and benchmarking for process equipment”. In: *Data-Centric Engineering* 1: e7, pp. 1–19. DOI: 10.1017/dce.2020.8
- Gabriel F. N. Gonçalves and Omar K. Matar (Sept. 2022a). “Mechanistic Modelling of Two-Phase Slug Flows with Deposition”. In: *Chemical Engineering Science* 259, p. 117796. ISSN: 0009-2509. DOI: 10.1016/j.ces.2022.117796
- Gabriel F. N. Gonçalves and Omar K. Matar (2022b). “Simulation of single- and two-phase flows with wall deposition in arbitrary geometries using a thin film model”. In: *Chemical Engineering Science* (submitted)

Chapter 2

Literature review

2.1 Wax deposition

2.1.1 Wax deposition in single-phase flow

Single-phase flow with wax deposition has been studied for decades through experimental and theoretical approaches and although some key points are still the subject of discussion, some consensus has been reached regarding the fundamental mechanisms. In their seminal work, Burger et al. (1981) studied the mechanisms of wax deposition using, as basis, data from the Trans Alaska Pipeline System (TAPS). The authors argue that precipitated and dissolved crystals move towards the wall through a combination of diffusion, shear dispersion and Brownian motion effects. A mechanistic model was proposed to estimate deposition rates, and comparison to field data was relatively successful, with predicted values being within a factor of 1.6 of the measurements. Svendsen (1993) also proposed a one-dimensional transient model for the prediction of wax thickness in a pipe. The deposition rate was computed by considering a solid-liquid two-component equilibrium and by assuming that the radial mass flux follows a diffusion law. Two typical cases, on laboratory and industrial scales, were analyzed but no removal or ageing effects were taken into account. Svendsen (1993) presented a qualitative analysis of the deposition dynamics over time, but no experimental validation was performed.

The model of Singh, Venkatesan, et al. (2000) assumed that dissolved wax molecules migrate from the bulk fluid to the deposit interface through molecular diffusion, and must penetrate the solid also through a diffusion process. The growth of the layer and increase in wax concentration, or ageing, comes from a balance between these two mechanisms. The authors assume that after an incipient gel layer is formed, diffusion of high molecular weight components into the gel (as well as the counter-diffusion of light components in the opposite direction) causes the increase of solid wax content in the deposit over time, which would represent the ageing effects. This change of composition naturally alters thermophysical properties such as the thermal conductivity. Zhang, Queimada, et al. (2014) proposed a model for wax deposition considering effects of the multi-component mixture thermodynamics, shearing and ageing effects. Validation was performed using data from flow-loop experiments and two full scale sub-sea pipelines. According to the simulations performed, removal of material due to shearing has an important effect in controlling the growth of the deposit and neglecting it may lead to an overly conservative and inefficient operation. The ageing effects, on the other hand, were observed to have no effect on the thickness itself although they heavily influence the mechanical properties of the deposit.

Coutinho, Edmonds, et al. (2006) proposed a practical thermodynamic model for the prediction of properties of waxy oils which was widely adopted in the literature. Validation was performed for a set of databases of crude-oils with and without dissolved gases. The model proved capable of accurately predicting the wax appearance temperature and the amount of wax precipitated based on the distribution of components, with no experimental fitting required. Singh, Lee, et al. (2011) compared the predictions of a wax deposition simulator to field data obtained in a 23 km long sub-sea pipeline. They evaluated the impact of the choice of models for oil properties, deposition, ageing and shear removal. “Film Mass Transfer” was observed to provide higher deposition rates than the “Equilibrium Model”, and a better match to the data. The tested wax removal models, on the other hand, either had negligible impact on the results or over-predicted the effect of shear.

Aside from the simplified formulations, some authors have also proposed more fundamental models based on the full solution of the momentum, temperature, and concentration transport equations in a two- or three-dimensional domain. Lee (2008) analysed the energy and mass

transport in the boundary layer to propose a more fundamental description of the deposition phenomenon. They showed that the coupling of heat and mass transfer is significant. The influence of the Reynolds number on deposition rates in turbulent flow was investigated using numerical simulations by Albagli et al. (2017). A two-equation turbulence model was used for the liquid along with an enthalpy-porosity model for the deposit. Deposition rates were determined through a thermodynamic equilibrium calculation based on all fluid components. The proposed model is capable of describing the reduction of deposit thickness with shear rate and non-uniform composition of the deposit layer.

Magnini and Matar (2019) performed high-fidelity simulations of wax deposition and removal in pipes using an interface-capturing model based on the Volume-Of-Fluid method. The phase-change model of Svendsen (1993) was adapted to a local formulation and used to describe the deposit formation and growth. Due to the necessity of fully-resolving the timescales of both phases, the simulations were limited to small durations, and the deposition was enhanced for qualitative analysis of the effect of the different parameters. The authors hypothesized that a streamwise flow of the wax layer driven by the interfacial shear stress was the mechanism behind the removal of material. The viscosity of the deposit was considered to be a free parameter, determined by comparison of the deposit growth rate to the measured experimental values. Validation was performed through comparison to estimates of instantaneous deposition rate in a long duration flow loop experiment. Extensive parametric analysis was then performed with enhanced deposition rates in order to keep computational times achievable. Finally, a simple model for steady-state deposit thickness was also proposed, assuming that the movement within it is well described as a Couette flow.

2.1.2 Wax deposition in oil-gas flow

In contrast to the single-phase flow case, the deposition in two-phase flow of gas and oil has been the subject of relatively fewer studies, both experimental and numerical. In this case, the presence of a third phase has an effect on both the hydrodynamics as well as the thermodynamic properties. Although the effects can usually be described qualitatively, discrepancies between

predictions and observed results can be significant (Liu et al., 2020). The lack of theoretical knowledge is reflected in industrial simulators, with studies showing the high dependence of deposit properties on the choice of the specific closure relations (Zhang, Pedrosa, et al., 2019). Ultimately, conservative predictions are used in the design and operation of pipelines and equipment, leading to inefficient installation and operation. In important work, Matzain (1999), Matzain et al. (2002) and Apte et al. (2004) performed experiments and proposed a semi-empirical model for intermittent, annular and bubbly flow. The observations of the deposition profile in horizontal flow can be summarized by Fig. 2.1. In annular flow, the deposit is uniform along the circumference. In stratified flow, the deposit occurs only on the liquid-wetted surface, being thicker in the bottom region than on the sides. When wavy, however, regions of thicker and rougher deposit are observed near the interface. Finally, for intermittent flows, the deposit is present along the full circumference, but is thicker on the top than on the bottom of the pipe.

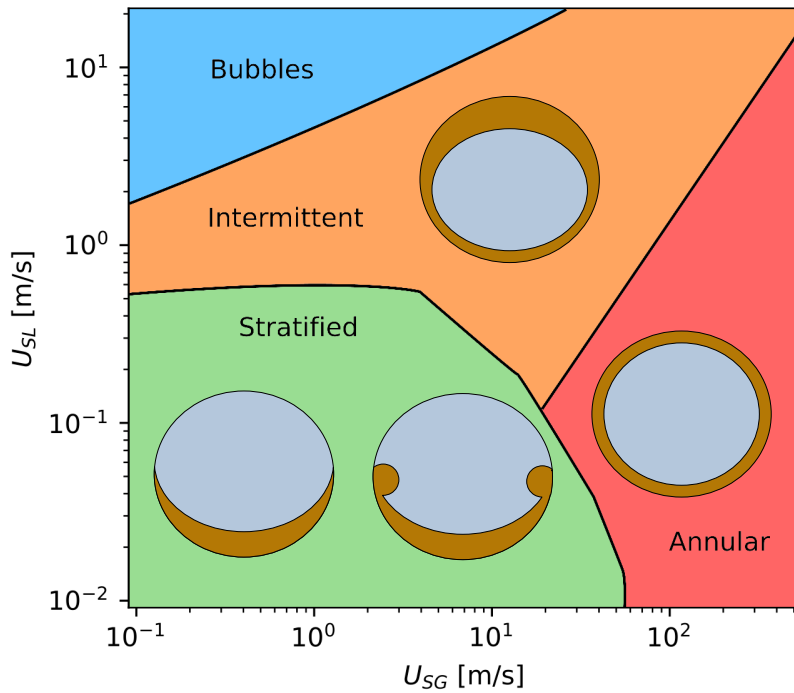


Figure 2.1: Schematic representations of the expected deposition profiles in the various regimes in horizontal gas-liquid flow according to the observations of Matzain et al. (2002).

In the model proposed by Matzain (1999), the growth of the deposit layer is given by:

$$\frac{d\delta_d}{dt} = \frac{\Pi_1}{1 + \Pi_2} \Gamma_{wo} \left[\frac{dC_w}{dT} \frac{dT}{dr} \right] \quad (2.1)$$

where δ_d is the deposit thickness, Γ_{wo} is a diffusion coefficient, C_w is the mass concentration of wax in solution, T is the fluid temperature, r and t denote the radial coordinate and time, respectively, and Π_1 represents the effects of ageing:

$$\Pi_1 = \frac{C_1}{1 - C_L/100} \quad (2.2)$$

where C_1 is a constant, and C_L is defined as

$$C_L = 100 \left(1 - \frac{Re_o^{0.15}}{8} \right) \quad (2.3)$$

in which the Reynolds number Re_o given by

$$Re_o = \frac{\rho_o U_o 2R_{\text{eff}}}{\mu_o} \quad (2.4)$$

Here, ρ_o and μ_o denote the density and viscosity of the fluid phase, U_o is a characteristic fluid velocity, and R_{eff} corresponds to the effective pipe radius accounting for the presence of the deposit. The other correction factor, Π_2 , takes into account the effects of the wall shear, and depends on the gas-liquid flow pattern:

$$\Pi_2 = 1 + C_2 Re_{GL}^{C_3} \quad (2.5)$$

in which the definition of the Reynolds number Re_{GL} depends on the flow regime and is given by

$$Re_{GL} = \begin{cases} \frac{\rho_o U_o \delta_d}{\mu_o}, & \text{for single-phase or stratified flow} \\ \frac{\rho_m U_o \delta_d}{\mu_o}, & \text{for bubble or slug flow} \\ \frac{\sqrt{\rho_o \rho_m} U_o \delta_d}{\mu_o}, & \text{if annular flow} \end{cases} \quad (2.6)$$

where ρ_m is the average density of the oil and gas mixture, and C_2 and C_3 are constants.

Recently, some authors have carried out important analyses of deposition under specific gas-liquid flow patterns, looking for insights into the fundamental differences in behaviour due to the phase distribution. Rittirong (2014) performed a set of detailed measurements of deposit

thickness and wax fraction in conditions of slug flow. They showed that the deposit layer was thicker at the top of the pipe due to a very thin film wetting the wall during the passage of the long bubbles. The model of Panacharoensawad (2012) was adapted for the geometry of a slug unit cell, with the introduction of a new parameter related to the deposition due to the thin film in the bubble region.

For stratified flows, Duan, Liu, Guan, et al. (2016) proposed a wax deposition model for gas/oil stratified flow. The velocity, concentration and temperature profiles were obtained for each cross-section in a bipolar grid system and mixing length theory was used to model the turbulence in the gas and oil phases; this study was followed up with subsequent studies by Duan, Liu, Jiang, et al. (2017) and Duan, Deng, et al. (2018), where the effects of interface shape and oil and gas superficial velocities were analyzed in detail. Chi (2019) performed experiments and modelling of wax deposition in stratified gas-liquid flow and thickness measurements were carried out at the sides and the bottom of the pipe. Interested in industrial operating conditions, Zhang, Pedrosa, et al. (2019) evaluated the impact of the choice of multiphase flow and wax deposition rate models for the prediction of actual field wax deposition cases, within a one-dimensional formulation. Discrepancies between the predictions provided by the multiphase flow models OLGAS[®] and Beggs-Brill were observed for some inclinations, with an important impact on deposition rates. Particularly in a case with vertical flows, the pressure profile provided by the latter differed significantly from the measured data. The authors also observed that in some field conditions, the neglect of shear removal effects led to an order of magnitude overestimation of deposited volume.

2.1.3 Deposition mechanisms

The first matter that needs to be discussed when addressing wax deposition is the mechanism that makes it so that the wax particles migrate from the fluid towards the walls. Burger et al. (1981) identified the possible wax deposition mechanisms as molecular diffusion, Brownian diffusion, shear dispersion and gravity settling.

Recently, Sousa et al. (2019) analyzed the order of magnitude of the different deposition mech-

anisms, and developed criteria to determine the the predominant effects for a given flow based on the magnitude of the relevant nondimensional numbers.

Molecular diffusion

It is generally assumed that for wax deposition to occur, the temperature at the wall must be larger than the temperature in the bulk flow (Yang et al., 2020). Since the solubility of wax increases with temperature, a radial gradient in the concentration of dissolved wax is also created, which leads to a flux of molecules towards the wall.

This effect is modelled with Fick's law:

$$\begin{aligned}\dot{m}_d &= \Gamma_m A \nabla C_w \\ &= \Gamma_m A \frac{dC_w}{dT} \nabla T\end{aligned}\tag{2.7}$$

where $\dot{m}$ is the rate of mass deposition at the wall.

The general consensus in the literature is that molecular diffusion is the dominant effect (Singh, Venkatesan, et al., 2000; Liu et al., 2020).

Brownian diffusion

Brownian diffusion is the phenomenon in which particles in suspension (e.g. wax crystals) move due to random movement of the continuous phase's molecules, generated by the thermal effects.

The diffusion law in this case has the following form:

$$\dot{m}_b = \Gamma_b A \nabla C_p\tag{2.8}$$

The diffusion coefficient Γ_b for small spherical particles is given by the Stokes–Einstein equation:

$$\Gamma_b = \frac{k_B T}{3\pi\mu_L D_p} \quad (2.9)$$

where k_b is Boltzmann’s constant and D_p is the diameter of the articles.

Most authors argue that the concentration of precipitates must be higher at the wall than in the bulk, since it decreases with higher temperatures. That would mean that the diffusion would take place in the opposite direction as the one observed in practice, with the particles being remove from the near-wall region.

Some authors, however, have argued that the impact of Brownian diffusion cannot be neglected in some operating conditions. According to Azevedo and Teixeira (2003), the solid particles in the wall region may be trapped by the deposit, leading to a concentration of effectively zero and making the migration of particles towards the wall relevant.

Shear dispersion

The shear dispersion refers to the movement of particles from the region of high velocity to the region of low velocity.

The flow rate due to shear dispersion is:

$$\dot{m}_{sd} = \Gamma_{sd} \rho A \nabla C_{vp} \quad (2.10)$$

where C_{vp} is the volumetric fraction of particles.

For low volumetric fractions, the shear dispersion coefficient Γ_{sd} of spherical particles has been shown experimentally to be approximately: Burger et al. (1981) and Eckstein et al. (1977)

$$\Gamma_{sd} = \frac{D_p^2 \dot{\gamma} C_{vp}}{40} \quad (2.11)$$

where $\dot{\gamma}$ is the shear rate.

There is not a clear consensus in the literature about whether this effect is relevant in practical conditions. Azevedo and Teixeira (2003) have argued that in conditions of no heat flux, any shear dispersion effects would dominate. Since it is well accepted that deposition does not usually occur in these situations, the shear effect must be negligible.

Gravity settling

Since the wax crystals are denser than the oil, in the absence of flow they would eventually deposit at the bottom of the pipe. In practice, however, gravity settling of crystals on the wall has been observed to be insignificant in general; there is no evidence of the deposit thickness being larger in the lower part of horizontal pipelines. It is possible that the shear dispersion counteracts this effect in pipe flows (Burger et al., 1981).

2.1.4 Thermodynamic equilibrium of waxy oils

The deposition rate depends on the solid-liquid equilibrium state of the mixture. The mixture is characterized by the mass fraction of component i , Y_i , for N different components. For waxy oils, the most used model is the one proposed by Coutinho (Coutinho and Stenby, 1996; Coutinho, Edmonds, et al., 2006).

The molar fraction of each component in the the mixture, z_i , is:

$$z_i = \left(\sum_{j=1}^N \frac{Y_j}{M_j} \right)^{-1} \frac{Y_i}{M_i} \quad (2.12)$$

where M_i is the molar mass of component i .

The equilibrium constant K_i represents the ratio:

$$K_i = \frac{x_i^S}{x_i^L} \quad (2.13)$$

where x_i^k is the molar fraction of each component i in a given phase K (L , liquid, or S , solid).

According to Coutinho and Stenby (1996), it is equal to:

$$K_i = \frac{\gamma_i^L}{\gamma_i^S} \exp \left(\frac{\Delta H_i^f}{RT_i^f} \left(\frac{T_i^f}{T} - 1 \right) + \frac{\Delta H_i^{tr}}{RT_i^{tr}} \left(\frac{T_i^{tr}}{T} - 1 \right) - \frac{\Delta C_{p_i}}{R} \left(\frac{T_i^f}{T} - \ln \left(\frac{T_i^f}{T} \right) - 1 \right) \right) \quad (2.14)$$

where γ_i^L and γ_i^S are activity coefficients, which may in turn depend on the molar fractions themselves.

The number of moles in the liquid phase, L_x , is given by:

$$\sum_{i=1}^N \left(z_i \frac{K_i - 1}{1 + L_x (K_i - 1)} \right) = 0 \quad (2.15)$$

The molar fraction of the components in the liquid and solid phases is obtained from:

$$x_i^L = \frac{z_i}{1 + L_x (K_i - 1)} \quad (2.16)$$

$$x_i^S = \frac{z_i K_i}{1 + L_x (K_i - 1)} \quad (2.17)$$

The system composed of Eqs. (2.14) to (2.17) must be solved for L_x and all x_i^L , x_i^S and K_i , which generally requires a numerical solution.

Svendsen (1993) assumed that γ_i^L and γ_i^S are independent of the composition and $N = 2$, in order to obtain the following algebraic solution to Eq. (2.15):

$$L_x = \frac{K_1 K_2 - z_1 K_2 - z_2 K_1}{1 + K_1 K_2 - K_1 - K_2} \quad (2.18)$$

2.1.5 Methods for simulation of wax deposition

Most of the studies in the literature have been focused on one-dimensional formulations. Since the process of deposition is very slow, very long simulations are required for industrial applications, and as such simplified approaches are required. Despite that, some studies have found it necessary to include more sophisticated models in order to fully understand the dynamics of

the flow, including effects of boundary layers and interfaces.

Table 2.1 summarizes some of the main modelling work presented in this chapter.

Table 2.1: Methods for simulation of wax deposition.

Reference	Technique	Flow pattern
Svendsen (1993)	Mechanistic model	Single-phase
Singh, Venkatesan, et al. (2000)	Mechanistic model	Single-phase
Matzain (1999)	Mechanistic model	Several gas-liquid patterns
Lee (2008)	Mass and heat transport equations for the boundary layer (2D)	Single-phase
Veiga et al. (2012)	Two fluid model, mass, momentum, energy and wax concentration of the mixture (2D)	Single-phase
Rittirong (2014)	Mechanistic model	Slug flow
Duan, Liu, Guan, et al. (2016)	CFD simulation of the pipe cross section	Stratified flow
Xie and Xing (2017)	RBF network	
Magnini and Matar (2019)	VoF model, mechanistic model for equilibrium thickness	Single-phase
Shahdi (2019)	Mass and heat transport equations for the boundary layer	Single-phase
Chi (2019)	Mechanistic model, CFD	Stratified flow
Municchi et al. (2020)	Mixture model	Single-phase

2.2 Simulation of multiphase flow

2.2.1 Computational fluid dynamics

There are several possible techniques for the simulation of multiphase flow with computational fluid dynamics, with trade-offs between fidelity and simulation speed. Each model also requires different sets of closure relations.

Among simulation techniques for multiphase flow, Eulerian-Eulerian, Lagrangian and interface tracking methods are the highlights (van Wachem and Almstedt, 2003). For the first, both phases are treated as interpenetrating continua, with individual mass and momentum equations for all phases, everywhere in the domain. In the case of Lagrangian models, individual particles or droplets of a dispersed phase are tracked, while the continuous phase is modeled as a continuum. Finally, in the one-fluid framework, a single set of mass and momentum conservation equations is solved for the full domain. Extra terms are included in the equations to account for interfacial forces; which act on singular regions of the solution, and properties are assigned according to which phase is present is a given position (Prosperetti and Tryggvason, 2007).

If one defines an indicator function $\chi_k(\mathbf{x}, t)$, such that its value is unity in a position where phase k is present and zero otherwise, the volume fraction α_k is defined by (Yeoh and Tu, 2010):

$$\alpha_k = \lim_{V \rightarrow \infty} \frac{1}{V} \int_V \chi_k(\mathbf{x}, t) d\mathbf{x} \quad (2.19)$$

Since the balance equations are written in an integral form, the interface singularity can not be obtained directly from the discrete volume fraction field, and its effects must be taken into account in the numerical treatment of the solution. The existing VoF schemes can be generally divided in two classes: geometric and algebraic (Roenby et al., 2016). In the former, the interface is reconstructed explicitly and advected, while in the latter these steps are replaced by simplified assumptions, which makes the implementation much more convenient. Figure 2.2 shows an example of the interface positions reconstructed from a volume fraction field with the

geometric technique of Scheufler and Roenby (2019).

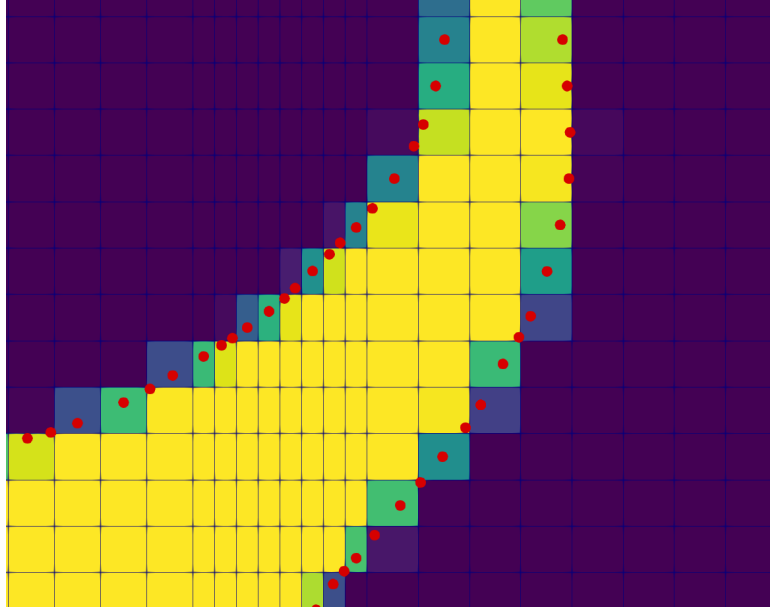


Figure 2.2: Volume fraction and cell centers (red dots) reconstructed with a geometric technique.

2.2.2 Gas-liquid mechanistic models

Despite the usefulness of detailed CFD simulations for the understanding of fundamental phenomena and specific design considerations, in many engineering applications, the computational cost of these analyses is prohibitive, and the main tools are based on simplified models. The main multiphase pipe flow simulation industrial codes are based on mechanistic models (Zhang, Wang, et al., 2003; Bendiksen and Maines, 1991). Since often the pipe lengths can be on the order of kilometers, and the phenomena of interest can occur over days or months, the utilization of coarse grids and large-timesteps is desirable. The direct resolution of individual slugs and waves can be prohibitively expensive; instead, an averaged formulation can be utilized as a "subgrid" term, such that large-scale transients can still be captured (Nydal, 2012).

De Henau (1996) presented such a formulation for a transient, isothermal, two-fluid model based on the unit cell approach for description of the interphase momentum interactions. The focus of the model was terrain-induced slugging, which can't be described by simple zero-dimensional formulations, for example. In De Henau and Raithby (1995), the model was validated with

experimental and numerical data of pressure and liquid fraction in steady-state and transient slug flow. Such unit cell models also have the advantage of being readily adaptable to steady state flow and being able to take insights from steady state models, since the closure relations are essentially the same.

Alternatively, the small scales of slugs and long bubbles may be resolved in detail, with the techniques of front capturing or front tracking, or hybrid approaches (Nydal, 2012). In front capturing, a very fine fixed grid is utilised, and the shape of each wave or bubble is resolved fully. With the tracking method, a Lagrangian grid is defined, with grid points coinciding with at start and end of the long bubbles.

2.2.3 Thin film models

Thin film flows are common in a large range of applications in engineering, geophysics and biophysics (Craster and Matar, 2009). The OpenFOAM CFD framework contains a thin film model tool based on Meredith, Vries, et al. (2011). Due to the small thickness of the film, the diffusion effects are only relevant in the wall-normal direction and advection effects, in the tangential directions. This allows for an integration of the governing equations in the normal direction, transforming a three-dimensional problem into a two-dimensional one; film thickness and other quantities are obtained over the relevant surfaces. In Meredith, Xin, et al. (2011) and Meredith and de Vries (2013), an energy transport equation was added to the model and validated.

2.3 Data-driven methodologies for CFD simulations

2.3.1 Graph-based methods

Graphs are very general structures for representing relationships between data, and can be seen as generalizations of many common representations such as images, linked lists and vectors. In

scientific and engineering applications, they have been particularly studied due to the possibility of representing complex geometries, present in all sorts of applications: from structures of molecules, for discovery of pharmaceuticals, to the analysis of interactions in social networks (see Fig. 2.3). Recently, a lot of attention has been focused on graph neural networks. In these models, outputs of interest can be calculated based on arbitrary entities (nodes) and pairwise relationships (edges), with directed or undirected links. Due to the local structure of the connections, the same model can naturally be used for different topologies.

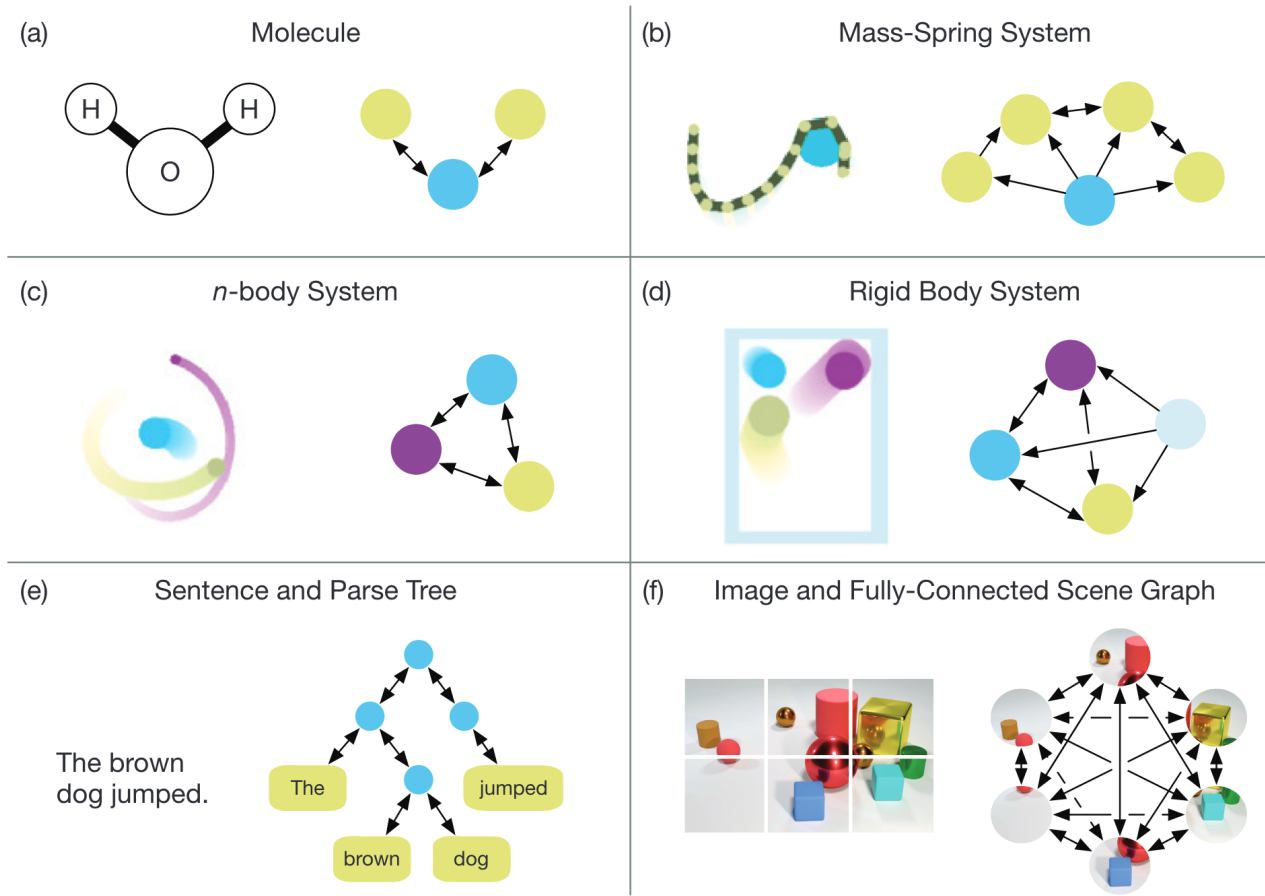


Figure 2.3: Examples of the representation of various types of data as graphs (from Battaglia et al. (2018)).

Relatively few studies have focused on the prediction of fluid flows. They are, however, a natural tool for existing engineering workflows, which often deal with complex geometries represented by two or three dimensional meshes.

Belbute-Peres et al. (2020) proposed a methodology for prediction of flow fields in fine meshes based on coarser mesh results, applied to flows around airfoils. A graph convolutional network

was used, with geometrical information and global simulation parameters being used as input features. The upscaled results obtained with the coarse mesh simulation are appended to the latent vector at an intermediate processing layer.

Sanchez-Gonzalez et al. (2020) proposed an architecture for Graph Networks based on a encode-process-decode for particle-based simulations. Pfaff et al. (2021) used a similar model to predict flow fields in static or dynamic non-structured meshes. The approach of Meyer et al. (2021) is based on direct time prediction, where timesteps are predicted directly from the initial conditions, without an iterative time advancement. They highlight the difficulty of dealing with the Poisson equation, since it relies on long-distance effects. They address that with several mesh levels for pressure equation.

2.3.2 Surrogate models with active learning

Process models are used in the design and operation stages of a process plant for a wide array of tasks including design optimisation, sensitivity analysis and uncertainty quantification among others. Most common process models use regression, where a variable of interest (e.g. a drag, or heat transfer coefficient) can be mapped as some function of operating conditions, fluid properties and/or geometric parameters. Usually, experimental tests are performed in down-scaled versions of the system of interest, and the measurements are used to develop regression functions on an *ad hoc* basis. Computational fluid dynamics (CFD) simulations are an attractive tool to complement such a methodology as once a model has been set up and validated, parametric analysis can be easily performed manually or automatically. Additionally, numerical computations allow for the exploration of parameters that could not be easily replicated in laboratory conditions due to infrastructure or measurement limitations.

Despite the aforementioned advantages, realistic CFD simulations suffer from major limitations in terms of computational cost. Simulating moderately-sized industrial systems may take hours to days on high-performance computing clusters, which means that in practice the total number of simulations in a given study will rarely be greater than a few dozen. The regression algorithm should therefore have the highest possible sample efficiency, i.e. be able to provide

good estimates of interpolated values with the lowest number of simulations possible. Traditional techniques used in the design of computational experiments include Latin hypercubes, Hammersley sequence sampling, orthogonal arrays and uniform designs (Simpson et al., 2001). These methods aim to distribute the input features such that the space of parameters is filled as “evenly” as possible. In the context of machine learning, different strategies have been used for dealing with small sample regression problems where obtaining samples is costly. They include transfer learning, semi-supervised learning, and active learning (Wu et al., 2019) among others. This study will focus on the last strategy, since it requires minimal interference on the surrogate development algorithm and is also agnostic of the underlying CFD model. Note, however, that these techniques are not necessarily exclusive, and combinations of methods could also be explored for further improvements.

Active learning consists of a mathematical criterion, a sampling strategy, to select the most “informational” parameters from a pool of possibilities. In the present case, this consists of selecting the next expensive simulation to be performed and is decided algorithmically, possibly making use of the underlying structure of the solution estimated with previous results. This avoids an extremely expensive grid search of all parametric permutations, a procedure that is infeasible in moderately complex systems. Such grid search techniques suffer from the “curse of dimensionality” where the number of possible combinations of simulations increases exponentially with respect to the increase in dimensionality, making such techniques computationally intractable. Active learning techniques for regression problems have been the subject of relatively few studies, when compared to classification tasks. RayChaudhuri and Hamey (2002) utilized the “query-by-committee” scheme for active learning with a neural network. Several copies of the model were trained on random subsets of the data and the discrepancy of the predictions was used as a criterion for selecting samples.

Cai et al. (2013) proposed an active learning algorithm which selects the examples expected to affect the predictions the most. The expected change is estimated based on the comparison between models, which were trained in subsets of the data. O’Neil (2015) compared active learning techniques in the context of linear regression models. From all the schemes investigated, only the diversity-based approach was found to significantly outperform the baseline results.

Wu et al. (2019) analyzed the performance of six sample selection algorithms for regression, of which two were proposed by the author, on datasets from various domains. The five active learning techniques were found to outperform random selection consistently. The strategy based on greedy sampling of both inputs and output was verified to be particularly effective.

However, there does not seem to be a generic active learning strategy which can outperform all others for every class of problems. On the other hand, empirical and systematic comparison of algorithms in different domains of knowledge may be useful for a practitioner interested in applying such techniques to a specific class of problems. The present idea is to build a set of industrially relevant problems which are generic enough to cover similar types of CFD problems and benchmark different active learning algorithms to assess their efficacy and provide directions for best practices to users in similar domains. Following that, the selected strategy will be used for developing surrogates for the wax deposition model proposed, which could be used in analysis or optimization of industrial systems.

Chapter 3

Deposition using interface-capturing and graph-based models

3.1 Introduction

The most complete approach for modelling a complex multiphase flow is the full solution of the fundamental conservation equations, in an arbitrary grid, with a detailed description of the volume fraction fields and interfacial phenomena. These phenomena could correspond to the formation of interacting three-dimensional large-amplitude waves, and changes in interfacial topology resulting from breakup of the interface; the latter may arise from the interaction between the interface and the prevailing hydrodynamics that could overcome stabilising viscous and capillary forces. In order to analyze that methodology, the model developed by Magnini and Matar (2019) that was based on the use of a volume-of-fluid (VoF) method implemented within a commercial code, ANSYS Fluent, was re-implemented in the open-source platform OpenFOAM; allows for a more thorough investigation of the numerics and algorithmic details on the emergent solutions. The major disadvantage of this high-fidelity approach that incorporates all the relevant physics is its high computational cost, which often renders it prohibitively expensive; this is often exacerbated by the presence of turbulence, extreme physical property contrasts in two- and multiphase flows, and complex geometries typical of industrially relevant

settings. In order to alleviate these issues, a graph-based data-driven model is also evaluated for extrapolation of CFD results with an open-source library being developed for manipulation of the OpenFOAM simulations data. We also present preliminary results from a hybrid multi-fidelity approach that combines data-driven extrapolations with physics-based corrections in a framework designed to provide efficient and reliable solutions. The details of these approaches are provided herein but we begin by providing a concise description of the VoF method.

3.2 VoF Modelling

3.2.1 Main equations

The interface-capturing VoF model is based on a one-fluid formulation, where the conservation equations are written for the mixture of deposit and liquid phases, and an equation for the volume fraction of phase i , α_i , is solved to determine the mixture properties and interface location. A schematic of the model is shown in Fig. 3.1. The deposit is a gel that is formed as the thermodynamic equilibrium drives the multicomponent mixture towards a higher fraction of solid phase, due to the low temperature of the wall. At the same time, the precipitation changes the local fraction of waxy components in the oil, generating a gradient of concentration and consequently a diffusive mass flux. Here, the deposit is treated as a fluid rather than a solid phase albeit with potentially spatio-temporally evolving rheological properties which may cause it to ‘age’ and ‘harden’. The continuity equation for the mixture is given by:

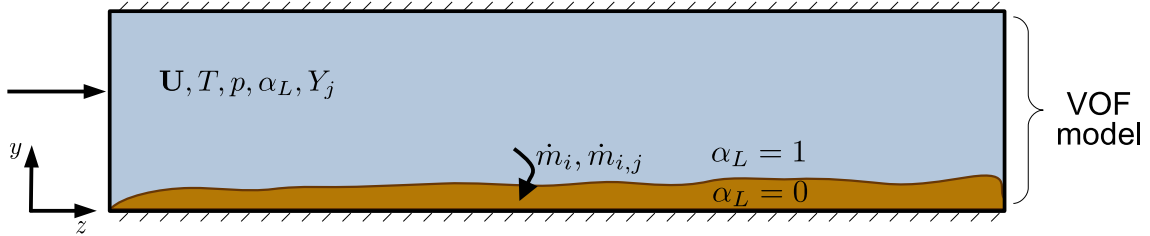


Figure 3.1: Schematic of the interfacial capturing model.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0 \quad (3.1)$$

where ρ is the mixture density, $\mathbf{U}$ is the mixture velocity, and t is time. The momentum equation is given by:

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot (\rho \mathbf{U} \mathbf{U}) = -\nabla p_d - \rho \mathbf{g} + \nabla \cdot (\mu_{\text{eff}} \nabla \mathbf{U}) + \sigma \kappa \nabla \alpha \quad (3.2)$$

where μ_{eff} is the mixture viscosity, σ is the interfacial tension, κ is the interface curvature, α is the volume fraction, and $\mathbf{g}$ is the gravitational acceleration. The conservation of internal energy leads to:

$$\frac{\partial \rho c_p T}{\partial t} + \nabla \cdot (\rho c_p \mathbf{U} T) = \nabla \cdot (k_{\text{eff}} \nabla T) + \dot{q} \quad (3.3)$$

where c_p is the heat capacity of the mixture, T is the temperature, k_{eff} is the mixture thermal conductivity, and $\dot{q}$ represents energy source terms.

For each phase i , mass conservation yields:

$$\frac{\partial \rho_i \alpha_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{U} \alpha_i) = \dot{m}_i \quad (3.4)$$

where in the case of just two phases:

$$\dot{m}_2 = -\dot{m}_1 \quad (3.5)$$

Similarly, an equation for the mass fraction of each component j in phase i , $Y_{i,j}$, may be obtained:

$$\frac{\partial \rho_i \alpha_i Y_{i,j}}{\partial t} + \nabla \cdot (\rho_i \mathbf{U} \alpha_i Y_{i,j}) = \dot{m}_{i,j} \quad (3.6)$$

where, again, in the case of two phases:

$$\dot{m}_{2,j} = -\dot{m}_{1,j} \quad (3.7)$$

For the two-phase flow case under consideration in the present work, the relationship between ρ , μ , $\alpha_1 \equiv \alpha$, and $\alpha_2 = 1 - \alpha_1 = 1 - \alpha$ is expressed by

$$\rho = \alpha \rho_1 + (1 - \alpha) \rho_2 \quad (3.8)$$

$$\mu = \alpha \mu_1 + (1 - \alpha) \mu_2 \quad (3.9)$$

The expression recommended by Svendsen (1993) for the dependence of density on temperature is given by:

$$\rho = \rho_0(1 - \beta_\rho(T - T_0)) \quad (3.10)$$

where T_0 and ρ_0 denote a reference temperature and density, respectively. For the dependence of the viscosity on temperature, we use the Guzman-Andrade equation which corresponds to an Arrhenius-type relation (Svendsen, 1993):

$$\mu = \mu_0 \exp\left(\frac{\beta_\mu}{T}\right) \quad (3.11)$$

where μ_0 and β_μ are constants. This was implemented in the library presented here, although not used in the preliminary tests, and no deposit ageing is considered.

3.2.2 Phase-transfer model

The inter-phase mass transfer rate in the present work is given by the formulation of Svendsen (1993) in which he assumed that the deposition may take place at the wall or at the interface of an already existing deposit layer. The mass transfer rate per volume is given by:

$$\dot{m}_{i,j} = -\Gamma_m \rho \eta_{i,j} \frac{\nabla T \cdot \hat{\mathbf{n}}}{T} \chi \quad (3.12)$$

where Γ_m is a diffusion coefficient, $\hat{\mathbf{n}}$ is the outward-pointing unit normal to the interface, and χ is the interfacial area density. According to Magnini and Matar (2019), the interfacial area density χ and interface normal direction $\hat{\mathbf{n}}$ are given by:

$$\chi = \begin{cases} |\nabla \alpha|, & \text{if a cell contains an interface} \\ A_{\text{wall,cell}}/V_{\text{cell}}, & \text{if a cell touches a wall} \end{cases} \quad (3.13)$$

$$\hat{\mathbf{n}} = \begin{cases} \nabla \alpha / |\nabla \alpha|, & \text{if a cell contains an interface} \\ \hat{\mathbf{n}}_w, & \text{if a cell touches a wall} \end{cases} \quad (3.14)$$

where $A_{\text{wall,cell}}$ is the area of the cell face that belongs to a wall, V_{cell} is the volume of the computational cell and $\hat{\mathbf{n}}_w$ is the wall normal vector. We refer to this methodology for the calculation of the source term as “diffuse”. Here, the methodology proposed by Soh et al. (2016) is used instead where the area and normal obtained by the interface reconstruction technique are used for the calculation of the mass transfer:

$$\chi = \begin{cases} A_{\text{PLIC}}/V_{\text{cell}}, & \text{if a cell contains an interface} \\ A_{\text{wall,cell}}/V_{\text{cell}}, & \text{if a cell touches a wall} \end{cases} \quad (3.15)$$

$$\hat{\mathbf{n}} = \begin{cases} \hat{\mathbf{n}}_{\text{PLIC}}, & \text{if a cell contains an interface} \\ \hat{\mathbf{n}}_w, & \text{if a cell touches a wall} \end{cases} \quad (3.16)$$

where the subscript PLIC denotes quantities obtained with the geometric reconstruction of the interface.

The authors have shown that this method is better at preserving the interface shape; the effect of the chosen methodology on the emergent solutions in terms of the temporal evolution of the deposit mass will be assessed below.

The function $\eta_{i,j}$ in Eq. (3.12) is given by:

$$\eta_{i,j} = Y_{i,j} \left[T(1 + \theta)^2 \frac{\partial L_x}{\partial T} + \theta \frac{M_j \Delta h_{f,j}}{RT} \right] \frac{K_j}{(1 + \theta K_j)^2} \quad (3.17)$$

with θ expressed by

$$\theta = \frac{1 - L_x}{L_x} \quad (3.18)$$

Here, M_j , $\Delta h_{f,j}$ and K_j are the molecular mass, enthalpy of fusion and equilibrium constant of component j , and R is the universal gas constant. The equilibrium constant K_i for component i is given by:

$$K_i = K_{0i} \exp \left(\frac{\Delta h_{f,i}}{RT} \left(1 - \frac{T}{T_{f,i}} \right) \right) \quad (3.19)$$

in which $T_{f,i}$ and K_{0i} correspond to the temperature of component i at fusion and a constant,

respectively. The mole fraction of liquid phase is:

$$L_x = \frac{b}{a} \quad (3.20)$$

where a and b for the case of two components are given by

$$a = 1 + K_1 K_2 - K_1 - K_2 \quad (3.21)$$

$$b = K_1 K_2 - z_1 K_2 - z_2 K_1 \quad (3.22)$$

The mole fraction z of each component is:

$$z_1 = \left(1 + \frac{Y_{i,2} M_1}{Y_{i,1} M_2} \right)^{-1} \quad (3.23)$$

$$z_2 = \left(1 + \frac{Y_{i,1} M_2}{Y_{i,2} M_1} \right)^{-1} \quad (3.24)$$

A two-phase liquid/solid equilibrium calculation may be performed to obtain the following analytical result:

$$\frac{\partial L_x}{\partial T} = \frac{\sum_{i=1}^2 [(b-a)K_i + (az_i - b)] \Delta h_{f,3-i} K_{3-i}}{RT^2 a^2} \quad (3.25)$$

This is then substituted into Eq. (3.17) to furnish an expression for $\eta_{i,j}$ that can, in turn, be inserted into Eq. (3.12) for $\dot{m}_{i,j}$; the latter represents the source terms in Eqs. (3.6).

3.3 Numerical methodology

Equations (3.1)-(3.4) and (3.6) comprise the core of the model. As they are coupled and non-linear, an iterative procedure is used for solving the system with the solution algorithm presented in Fig. 3.2. The numerical model was implemented on the OpenFOAM-v2006 library (OpenCFD, 2020). Second-order schemes were utilized for the discretization of spatial terms, and a first-order implicit Euler scheme for the time. Although the test cases presented here are of laminar flows, the model is compatible with any of the existing OpenFOAM turbulence models.

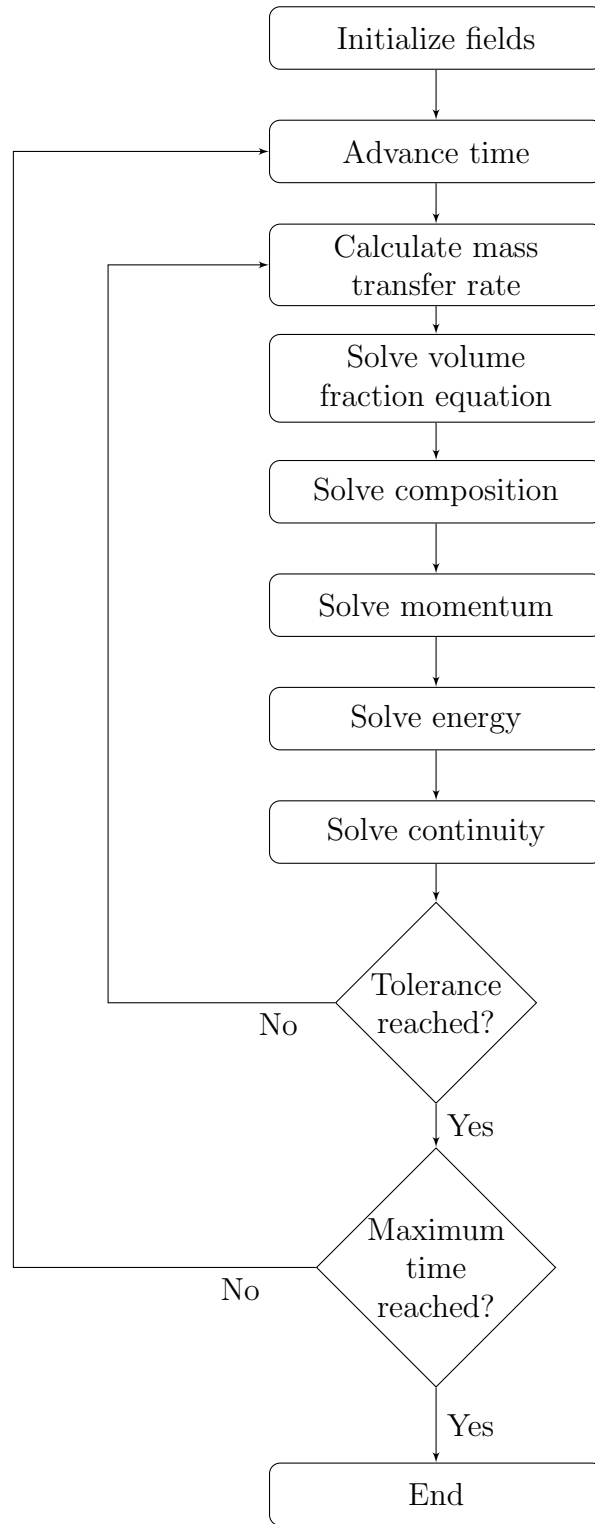


Figure 3.2: Solution algorithm for the wax simulations with interface capturing.

Although the work of Magnini and Matar (2019) carried out using the commercial CFD package ANSYS Fluent included an extensive parametric study of the model, little attention was focused on the effect of the numerical parameters and sub-models on the results. In an open-source implementation, a more in-depth analysis of these effects can be conducted. Here, a base case

is defined based on the two-dimensional channel setup of Magnini and Matar (2019); the case parameters are presented in Tab. 3.1 and a schematic of the boundary and initial conditions in Fig. 3.3. The simulation starts from a clean channel (i.e. volume fraction of deposit is zero everywhere), where the velocity is initialized with the average value and the temperature, with the value for the inlet. The inlet assumes similar values, except for the fact that a parabolic laminar flow profile is used for the velocity. The initial and inlet values for the light and heavy components in the oil are calculated according to the lumping procedure presented in Magnini and Matar (2019). The same values are used for the deposit phase, although it is not present initially, in order to prevent numerical issues.

In the current model, there is no special treatment for the initial nucleation of the solids at the wall. In fact, a non-penetration boundary condition is used, along with the mass transfer expressions introduced before; the appropriate area and normal vectors are considered for wall-adjacent cells. The low temperature of the wall (or, later in the process, in the deposit interface) drives the thermodynamic equilibrium to a higher fraction of solid phase, which naturally generates mass transfer source terms in that region.

Note that, as in the original work of Magnini and Matar (2019), the diffusion constant Γ_m in Eq. (3.12) was increased to a value higher than the one typically measured experimentally in order to obtain significant deposition in a short timescale. This is justifiable since the goal here is not to seek validation against experimental data but to assess the influence of the numerics on the solutions obtained from the numerical procedure.

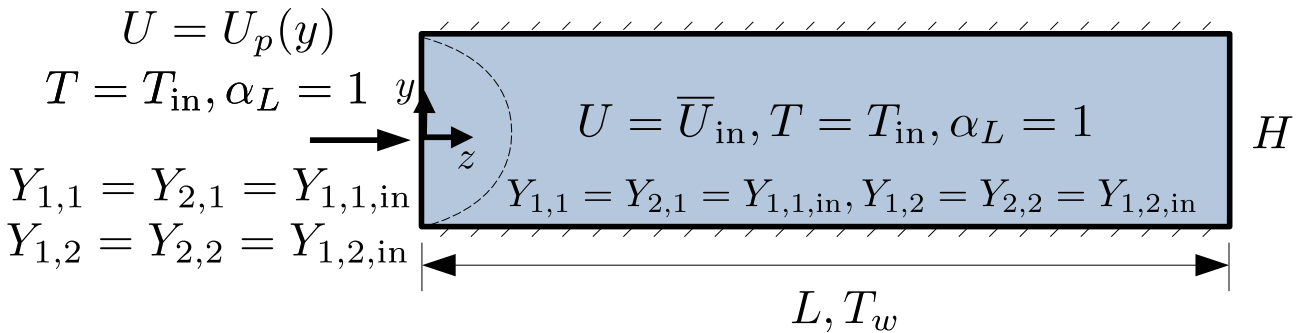


Figure 3.3: Boundary and initial conditions for the VoF simulations.

In Figure 3.4, the total mass of deposit in the computational domain is plotted as a function of time, for three different interface reconstruction techniques. The curves associated with ‘gradAl-

Table 3.1: Parameters utilized for the interface capturing test cases.

Parameter	Value	Unit
$\bar{U}_{\text{in}}$	0.226	m s^{-1}
H	9.0×10^{-3}	m
L	0.36	m
$Y_{1,1,\text{in}}$	0.85	-
$Y_{1,2,\text{in}}$	0.15	-
T_{in}	303.0	K
T_w	275.0	K
ρ_1	850	kg m^{-3}
ρ_2	850	kg m^{-3}
μ_1	8.7×10^{-3}	Pa s
μ_2	8.7×10^{-3}	Pa s
k_1	0.134	$\text{W m}^{-1} \text{K}^{-1}$
k_2	0.134	$\text{W m}^{-1} \text{K}^{-1}$
$c_{p,1}$	2008	$\text{J kg}^{-1} \text{K}^{-1}$
$c_{p,2}$	2008	$\text{J kg}^{-1} \text{K}^{-1}$
M_1	213	kg kmol^{-1}
M_2	556	kg kmol^{-1}
$T_{f,1}$	272.0	K
$T_{f,2}$	341.0	K
$\Delta h_{f,1}$	34.9×10^3	J mol^{-1}
$\Delta h_{f,2}$	107.8×10^3	J mol^{-1}
K_1	1.0	-
K_2	1.0	-
Γ_m	2.76×10^{-6}	$\text{m}^2 \text{s}^{-1}$

pha’ and ‘plicRDF’ present nearly identical results: rapid deposit growth occurs at early times which is reflected by the sharp rise in the mass; this is then followed by an approximately linear growth culminating in a plateau. Although the use of the isoAlpha interface reconstruction in ANSYS Fluent leads to qualitatively similar results to those obtained via use of ‘gradAlpha’ and ‘plicRDF’, there is a significant offset in the deposition curve during the transient period ($t < 25$ seconds for the parameters used to generate Fig. 3.4). The final dynamic steady-state reached, however, is almost identical for all interface reconstruction methodologies in ANSYS Fluent and OpenFOAM studied herein.

As in Magnini and Matar (2019), the deposit growth in single-phase flow here is governed by a balance between thermodynamic effects promoting deposit formation and the wall shear removal. The first one is mainly governed by the temperatures of the bulk liquid and the

wall, as well as the oil composition. The latter, on the other hand, depends on a complex combination of Reynolds number, flow geometry and deposit rheology. As the deposit gets thicker, the interface moves away from the wall and the velocity and temperature increase, inhibiting further growth.

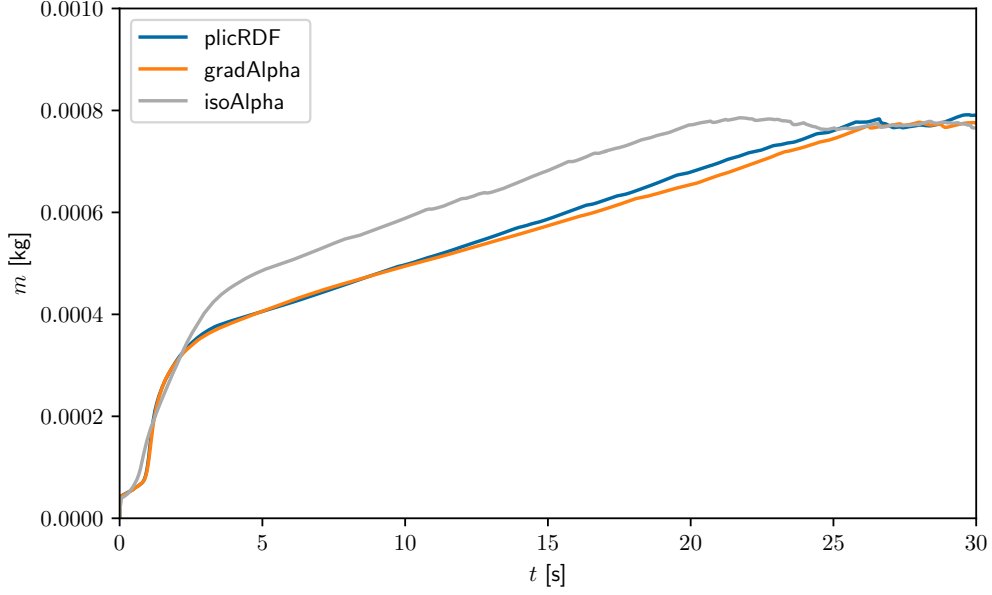


Figure 3.4: Temporal variation of the deposit mass for different interface reconstruction techniques; the parameter values are given in Tab. 3.1.

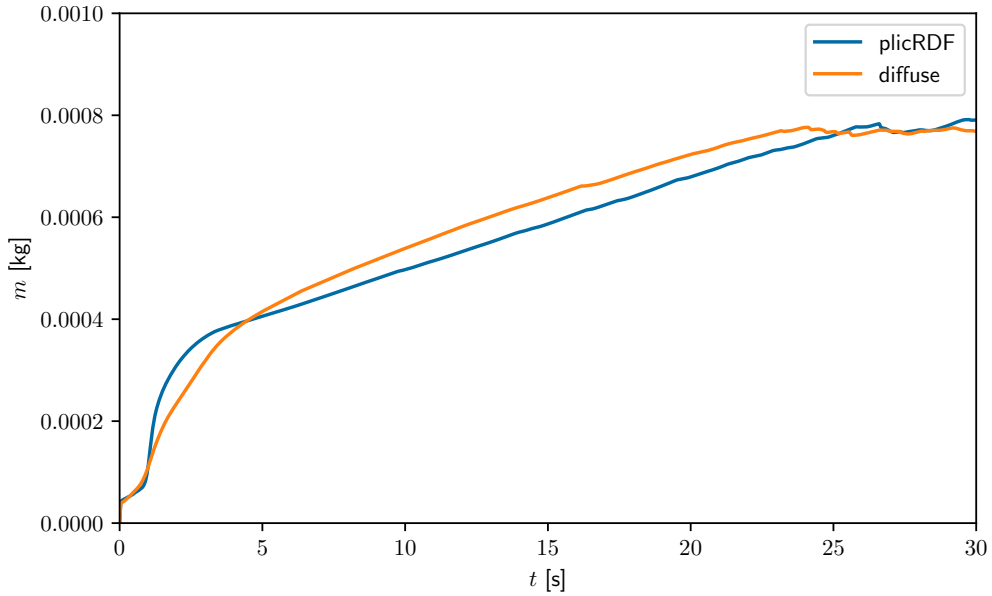


Figure 3.5: Temporal variation of the deposit mass for different methods of obtaining the interface area density χ given by Eqs. (3.13) and (3.15); the parameter values are given in Tab. 3.1.

Figure 3.5 shows the effect of the choice of formulations for the interfacial area density χ , represented by Eqs. (3.13) and (3.15), discussed briefly in Sec. 3.2.2. Close inspection of the results shows that use of the “diffuse” approach, expressed by Eq. (3.13), leads to a more gradual increase in the deposit mass m at early times. In contrast, the PLIC approach (see Eq. (3.15)) leads to a sharper early-time increase in m with the mass remaining below that predicted by the diffuse method during the linear period at intermediate times. Despite these differences, the plateau of deposited mass reached is very similar for both χ formulations.

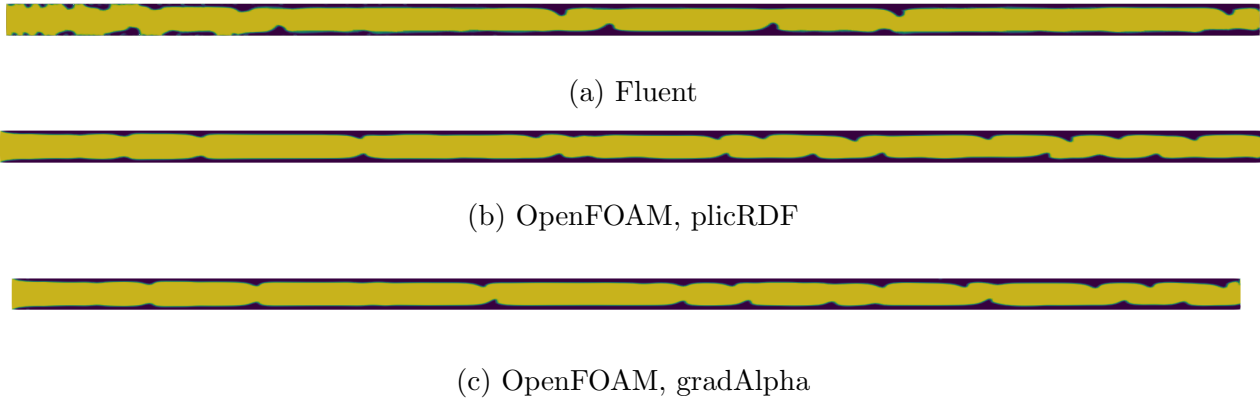


Figure 3.6: Volume fraction of the deposit in the channel at $t = 30$ s for different solvers and interface reconstruction techniques and the same parameters as those listed in Tab. 3.1.

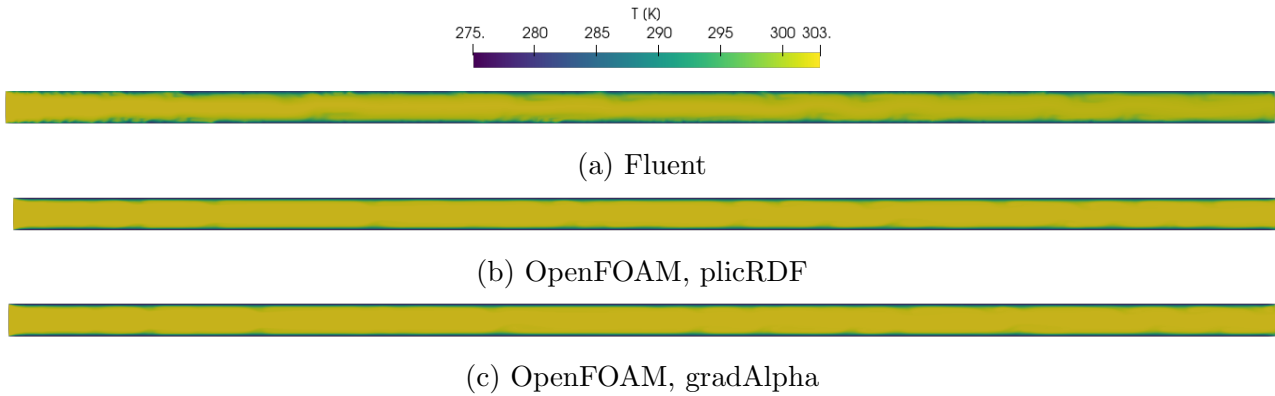


Figure 3.7: Temperature field in the channel at $t = 30$ s for different solvers and interface reconstruction techniques and the same parameters as those listed in Tab. 3.1.

We have also explored the effect of interface reconstruction methods on the interfacial dynamics that accompany the two-phase flow. Figure 3.6 shows sample contours of the volume fraction fields for different solvers and interface reconstruction techniques and the same parameters as those used to generate Fig. 3.4. In each case, the results are qualitatively similar: the two-phase flow is accompanied by the formation of large-amplitude solitary waves in the deposit

that form near the inlet and travel downstream. The temperature results (Fig. 3.7) are also qualitatively similar in all cases, although the field obtained in Fluent is less sharp than the ones obtained with OpenFOAM. Very minor differences are noticeable between the two reconstruction techniques here. The results obtained using VoF implemented within OpenFOAM are quantitatively very similar though not identical, as expected due to the inherent stochastic nature of the flows: wave formation is triggered by tiny perturbations near the inlet which then grow and develop into solitary travelling waves. Furthermore, perturbations can also grow spontaneously from the waveless regions that separate solitary waves leading to additional wave formation. In contrast, the results generated by Magnini and Matar, 2019 in ANSYS Fluent exhibit waves of larger amplitude than those obtained from the OpenFOAM simulations and noticeable deposit-free regions near the inlet (Fig. 3.8b). Since the case setups are identical, these differences can probably be ascribed to different implementation of numerical models such as the interface reconstruction.

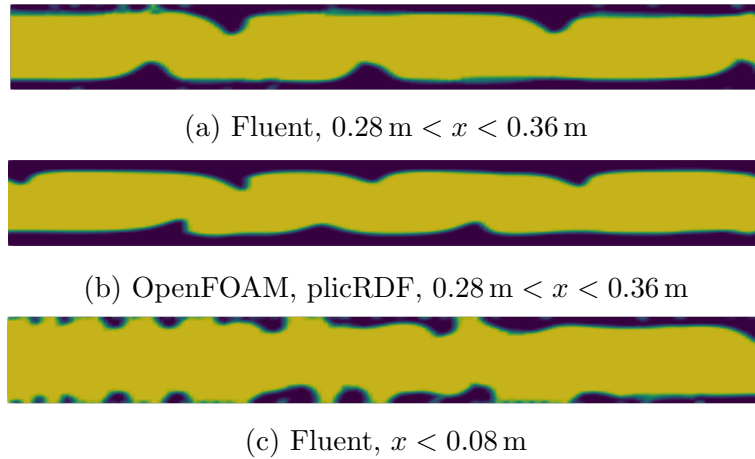


Figure 3.8: Detail of the volume fraction of the deposit in the channel at $t = 30 \text{ s}$ for different solvers and interface reconstruction techniques and the same parameters as in Tab. 3.1.

As the above results have demonstrated, although the interface-capturing model corresponds to the most detailed approach, it is still not completely free of assumptions, and even small implementation choices can result in significant qualitative and quantitative effects. The transient period of deposit growth, in particular, is sensitive to the specific formulation used. The computational cost of this approach is also a concern. The simulation of the base case takes 35 to 45 core hours for each second of simulation, even though the pipe length (0.36 m - see Tab. 3.1) is short, which would make scaling up to hours or days of simulation unfeasible. This

has motivated us to consider alternative, data-driven approaches to circumvent the limitations of the VoF approach; these approaches are presented next.

3.4 Graph-based modelling

As mentioned in the previous section, the interface-capturing technique has very high computational costs, which make data-driven acceleration very attractive. Flow simulation results are naturally represented as graphs, and graph-based machine learning models have shown promising results in many classification and regression tasks (Zhou et al., 2020; Waikhom and Patgiri, 2021). The key information that must to be represented is the following:

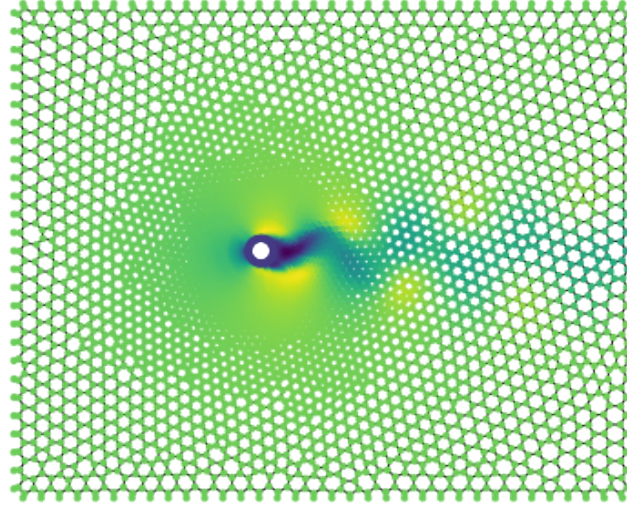
Mesh In most finite volume codes, variables are calculated at the centroid of computational cells. As such, cell centers and faces may be respectively represented as nodes and undirected vertices connecting the respective positions. Boundary faces will typically also include value information so they may be included as additional nodes in the graph.

Volumetric fields Typically, flow fields consist of scalars, vectors, tensors, and symmetric tensors. Figure 3.9 shows an example of the representation of the velocity field for flow past a cylinder generated via a two-dimensional simulation using an unstructured mesh, as a graph. The computational cells are replaced as nodes, which are represented with filled circles placed in the centroid positions (and colored with the quantity of interest), and faces are substituted with black edges between them. The simulation was carried out using OpenFOAM with a Reynolds number $Re = 200$, using the setup of Guerrero (2020) – the full case description is presented in Sec. 3.5.1. As can be seen in this figure, the flow is accompanied by vortex shedding, which is typical of flows past a cylinder beyond a certain, critical threshold.

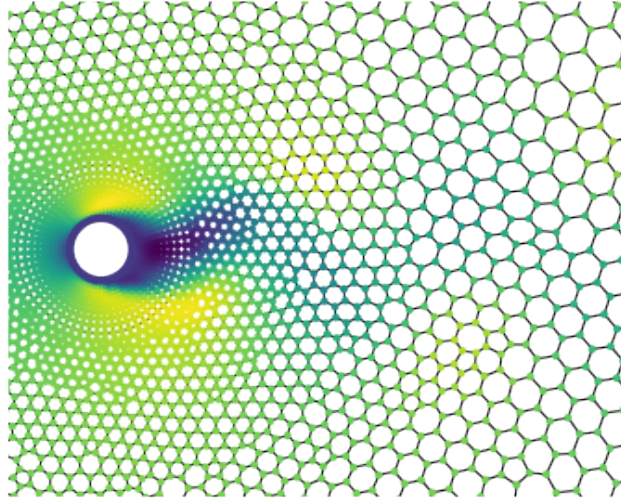
Boundaries All flow calculations require information regarding the type and value of boundary conditions. However, the number of possibilities of boundary conditions is large making the treatment of boundaries quite complex. Here, we adopt the standard encoding strat-

egy for boundaries of assigning a categorical index to each patch, with an extra category for the internal cells. This is demonstrated in Fig. 3.10.

Global fields Global fields are variables that are independent of specific nodes or edges, i.e. independent of position. They can be used to represent field forces, such as gravity acceleration, or constant fluid properties.



(a)



(b)

Figure 3.9: Graph of the velocity field for laminar flow past a cylinder with a Reynolds number of 200, generated via two-dimensional simulations using an unstructured mesh, exhibiting vortex shedding shown in (a); panel (b) provides an enlarged view of the near-cylinder region.

In this work, FOAMGraph was used as a versatile library for importing and manipulating CFD

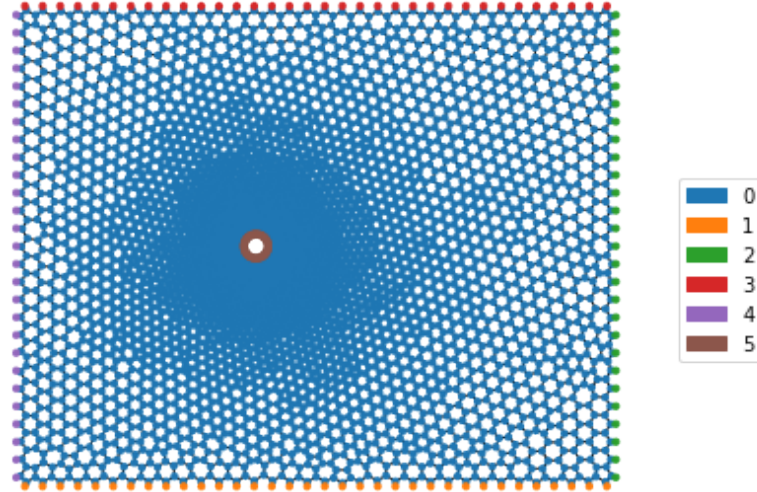


Figure 3.10: An example of a boundary encoding strategy for the simulation of flow past a cylinder shown in Fig. 3.9.

simulation data using graph-based machine learning tools focused on OpenFOAM. FOAM-Graph is implemented as a standalone python package that can be readily used without a complicated setup process, and is available in a public repository¹, with an MIT license. The PyFoam library is used for reading OpenFOAM files. The implementation uses standard data structures defined in the packages PyTorch Geometric (Fey and Lenssen, 2019) and PyTorch Geometric Temporal (Rozemberczki et al., 2021) for representation of spatial and temporal data, which simplifies the integration of novel graph tools and models with CFD data. The data loading functions automatically detect whether the simulation was run with a dynamic mesh or not, and returns the appropriate temporal iterator.

The package is divided into the following submodules:

visualization Contains tools for plotting graphs as two or three dimensional objects.

utils Contains general utilities, including tools for reading and writing OpenFOAM cases to/from graphs.

nn Contains graph neural network models and tools applicable to fluid dynamics problems.

¹https://github.com/gfngoncalves/foam_graph

transforms Contains data transformation functions, for preprocessing of simulations. Includes, for example, a transformation which removes a spatial coordinate, for two-dimensional OpenFOAM results.

Currently, the following boundary conditions are supported, and have been tested:

- Dirichlet boundaries represented with *fixedValue* (and similar ones as *fixedProfile*, *inletOutlet*)
- Neumann boundaries represented with *zeroGradient*
- Empty boundaries, for 1 or 2D cases (*wedge* and *empty*)

Here, we apply the method of Pfaff et al., 2021 for transient flow predictions. Given case-dependent node features $\mathbf{v}_i$ and edge features $\mathbf{e}_{i,j}$, a Graph Network architecture is used to predict node targets $\mathbf{y}_i$. These node targets can be set to be a future state of the system; a schematic of the graph network algorithm is shown in Fig. 3.11.

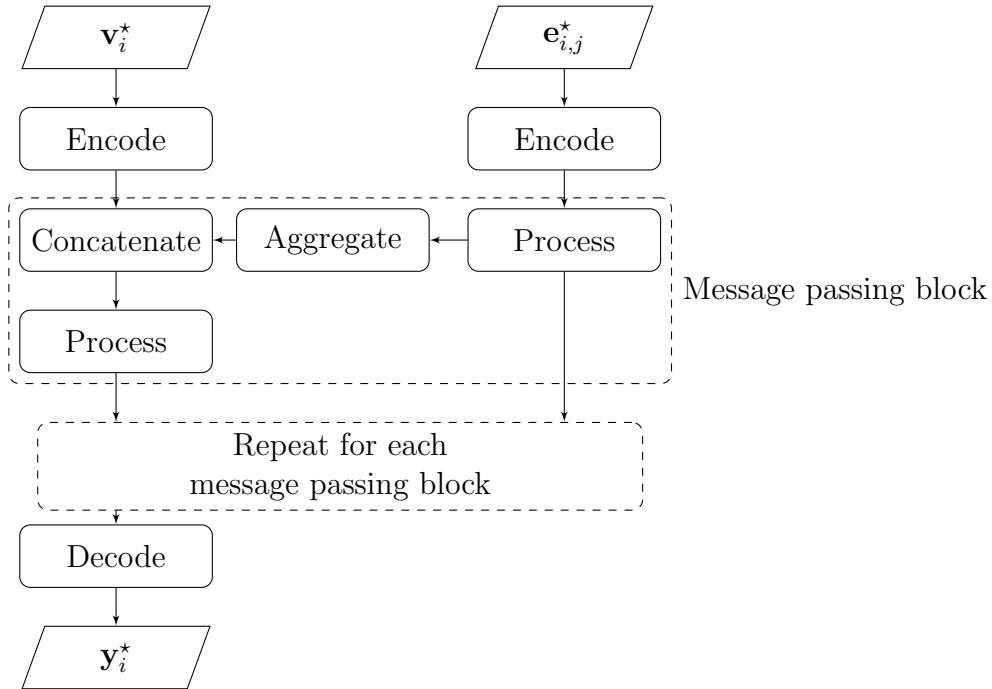


Figure 3.11: Algorithm for the Graph Network method introduced by Pfaff et al. (2021).

The models were trained on a single RTX6000 GPU, with Pytorch-Lightning (Falcon and The PyTorch Lightning team, 2019). Parameter adjustment was performed with the Adam

algorithm, with an initial learning rate of 1×10^{-3} . An automatic learning rate reduction by a factor of 10 was used if the validation error did not decrease over 10 epochs, and the training was stopped early if no improvement was observed over 50 epochs. Finally, white noise was added to the training data in order to improve the stability of ‘rollouts’ (extrapolations to system states beyond those used to carry out training), as in the original reference of Pfaff et al., 2021.

In the original work, not much attention was dedicated to the analysis of the effect of the timesteps of the simulation and training data. Typically, the physics of the simulation will provide an upper bound for the simulation timesteps, and training data can be arbitrarily sampled at any frequency. If the timestep of the training data is too low, the amount of available data will be increased, but the effective information may be redundant and the inference might be slow. On the other hand, large steps in time require deeper networks (e.g. more message passing steps) to have the power to describe full physics, leading to costly training and memory limitations. The compromise between these factors depends on the complexity of the analyzed system and the required accuracy, as well as any hardware or cost limitations. Here, the ratio between the sample and the simulation timesteps varied between 20 and 1000, according to the complexity of the problem.

3.5 Application to flow dynamics simulations

3.5.1 Case 1: flow past a cylinder

The capabilities of FOAMGraph are demonstrated on practical CFD cases by applying the method of Pfaff et al. (2021) discussed briefly above. The first test case is a two-dimensional laminar flow around a cylinder, with Reynolds number $Re = 200$; a similar setup was utilized by Pfaff et al. (2021). This is not a particularly challenging test case, due to the periodicity of the flow, but was adopted as an initial verification of the algorithm capabilities. This particular case setup is based on the the one provided in Guerrero (2020), and illustrated in schematic

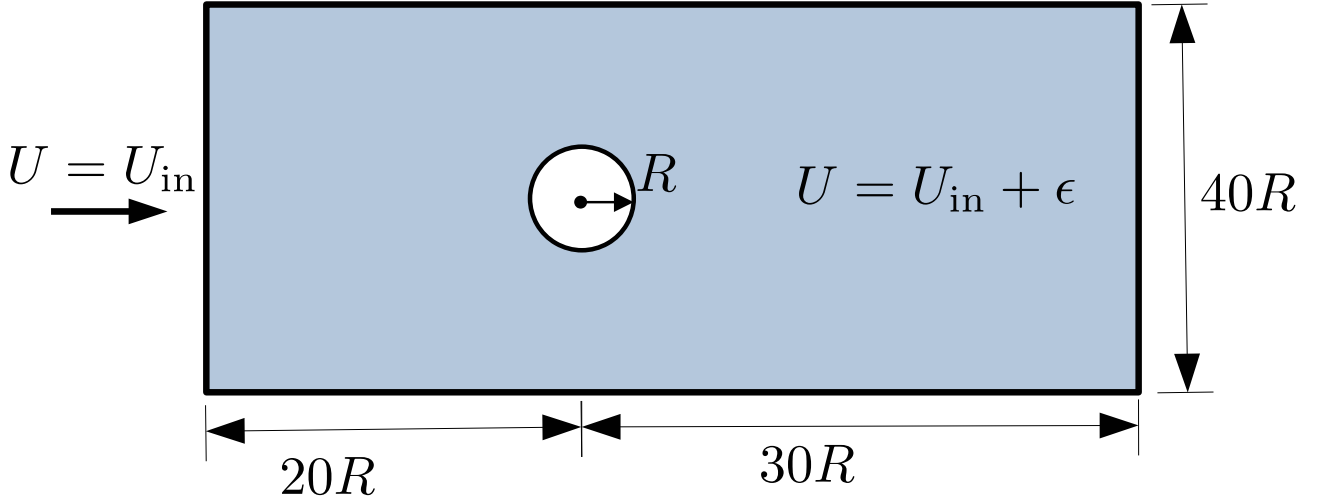


Figure 3.12: Boundary and initial conditions for the simulations of flow past a cylinder.

form in Fig. 3.12. The velocity is initialized with a small perturbation, in order to reach the dynamic steady state faster. The simulation was run within OpenFOAM with a timestep of 0.05s, with snapshots being saved every 1s. A total of 300 snapshots were obtained of which 80% were used for training and the remaining for validation.

With reference to Fig. 3.11, the node, edge features, and node targets, $\mathbf{v}_i$, $\mathbf{e}_{i,j}$, and $\mathbf{y}_i$, respectively, are summarized as follows:

$$\mathbf{v}_i = (\mathbf{U}_i, \mathbf{b}) \quad (3.26)$$

$$\mathbf{e}_{i,j} = (\mathbf{x}_j - \mathbf{x}_i, |\mathbf{x}_j - \mathbf{x}_i|) \quad (3.27)$$

$$\mathbf{y}_i = (\Delta \mathbf{U}_i, p^{t+1}) \quad (3.28)$$

The standard hyperparameters recommended by Pfaff et al. (2021) were used: 128 components on the latent vector, and two hidden layers in all multi-layer perceptrons.

The number of message passing blocks is intrinsically connected to the range of the neighborhood that affects a given node. For advective systems, this depends on the Courant number, Co . Based on that, we propose that the minimum number of blocks is:

$$N_{\text{blocks}} \approx \frac{\Delta t_{\text{samp}}}{\Delta t_{\text{sim}}} Co \quad (3.29)$$

where Δt_{samp} is the sampling timestep and Δt_{sim} is the timestep of the simulation. Following this approach, the number of blocks was set to 15.

After the model was trained with single time-step differences, it was used for rollouts. The results shown in terms of the velocity contours for three periods beyond the training time-step are shown in Fig. 3.13. Inspection of this figure reveals that the periodic nature of the vortex shedding associated with this flow is reproduced very well, with no significant amplification of errors over time. The results shown in Fig. 3.13 therefore demonstrate the promise of graph-based methods in efficient fluid dynamics simulations.

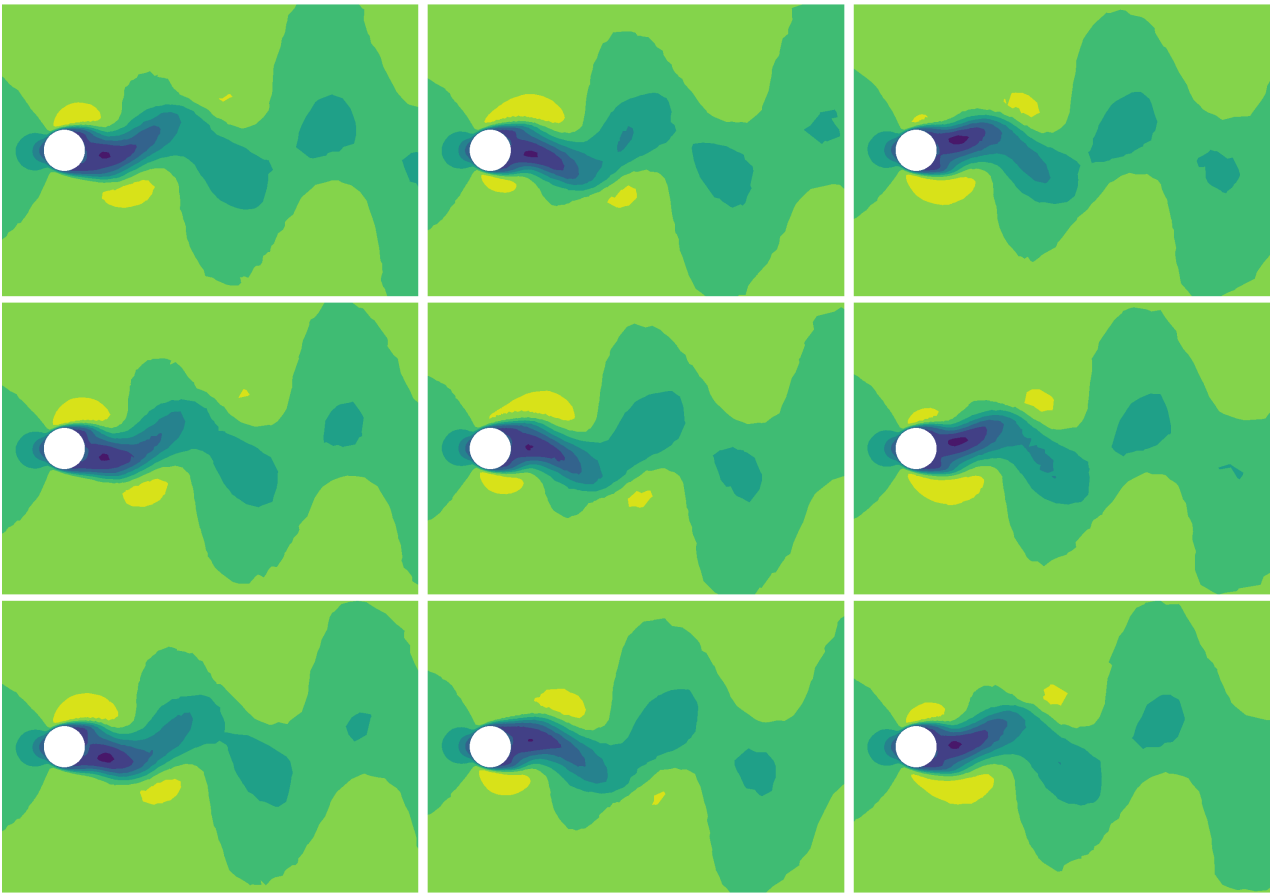


Figure 3.13: Velocity contours for the rollout of test Case 1 of flow past a cylinder with $Re = 200$ for three periods beyond the time-step used to carry out training using the Graph Network method of Pfaff et al., 2021.

Since this case is very simple, the data-driven approach does not provide gains in computational performance: while the full simulation takes 0.47 s per physical second, the neural network inference takes 1.86 s on a CPU. Gains could possibly be observable, however, if a GPU is used

for inference.

3.5.2 Case 2: channel flow with wax deposition

A more challenging test case was also analyzed based on the wax deposition model presented in Magnini and Matar (2019). The channel flow setup used here is the one introduced in Sec. 3.3. The state vector in this situation is a lot more complex, since energy and composition also need to be taken into account. The node and edge features and node targets are summarized as follows:

$$\mathbf{v}_i = (\mathbf{U}_i, \alpha_i, T_i, Y_{w,i}, Y_{o,i}, \mathbf{b}) \quad (3.30)$$

$$\mathbf{e}_{i,j} = (\mathbf{x}_j - \mathbf{x}_i, |\mathbf{x}_j - \mathbf{x}_i|) \quad (3.31)$$

$$\mathbf{y}_i = (\Delta \mathbf{U}_i, \Delta \alpha_i, \Delta T_i, \Delta Y_{w,i}, \Delta Y_{o,i}, p^{t+1}) \quad (3.32)$$

The results of the simulation rollout for the volume fraction and temperature fields are shown in Figs. 3.14 and 3.15, respectively. Inspection of these figures reveals that the extrapolated results for both the volume fraction and temperature remain stable for a very long time, with physically reasonable results being maintained despite the large timestep used for advancing the solution. The interface remains sharp, and the waves propagate and exit the domain as expected. The inference takes 0.17 core hours (using 2 cores) per second of simulation, compared to the original 35 to 45 core hours (using 32 cores) of the full computation. The training process took 10.7 h in the aforementioned GPU. Based on this comparison, it can be inferred that the data-driven approach adopted represents a promising methodology for efficient and reliable simulation of complex, time-dependent two-phase flows.

In order to test the limitations of the graph-based approach, figure 3.16(a) shows a longer rollout solution for the deposit volume fraction generated for the same parameters as in figure 3.14 where each snapshot corresponds to 10 steps (1 s of simulation). The extrapolation begins to break down after around 20-30 steps, with some drying up of the zone near the inlet. After 60-70 steps, the wave behaviour becomes noticeably different from that predicted by the

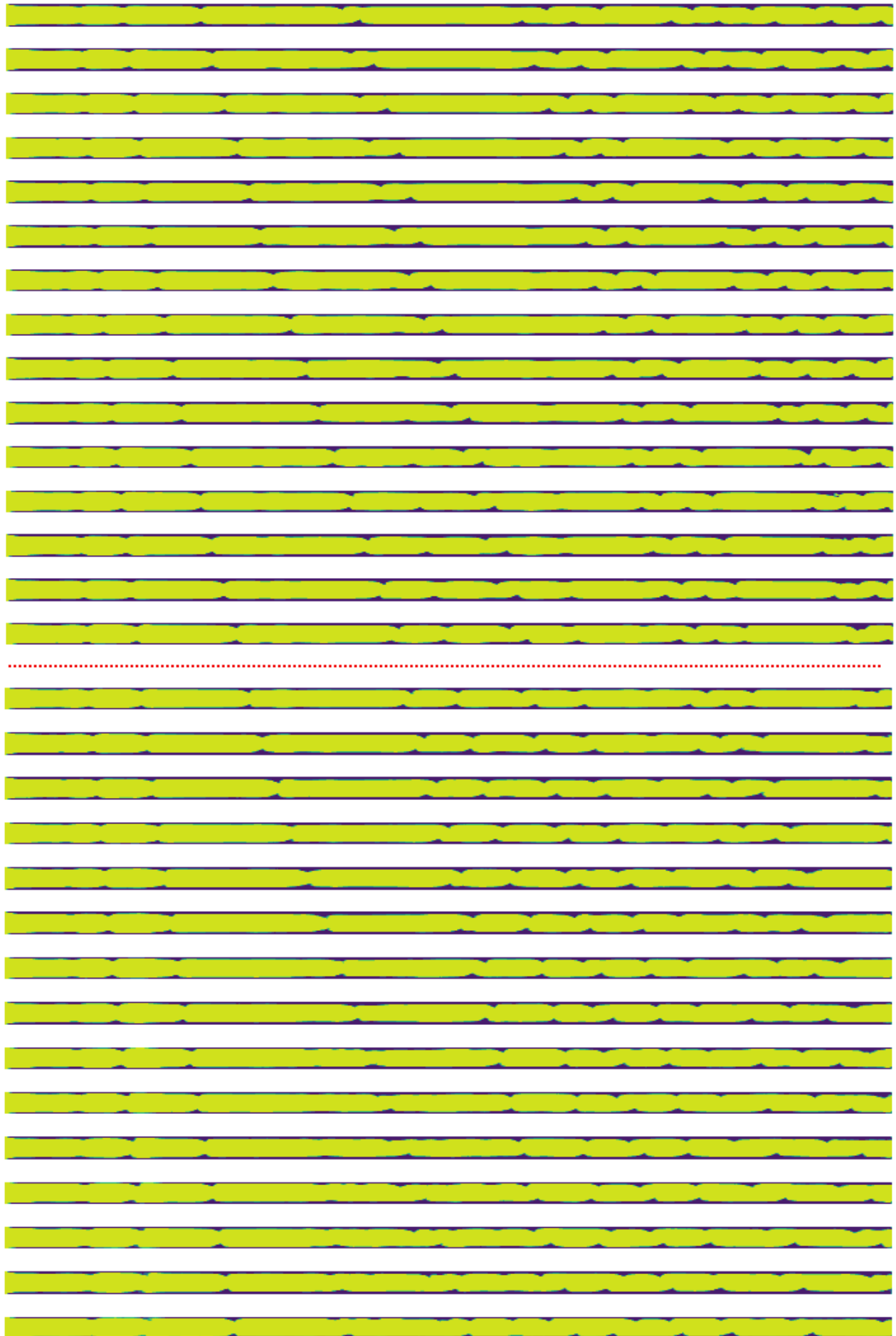


Figure 3.14: Deposit volume fraction in test case 2 obtained from a rollout. Here, and in subsequent figures, the red dashed line represents the transition between training timesteps and rollout steps. Test case 2 is characterised by the same parameters as in Tab. 3.1.

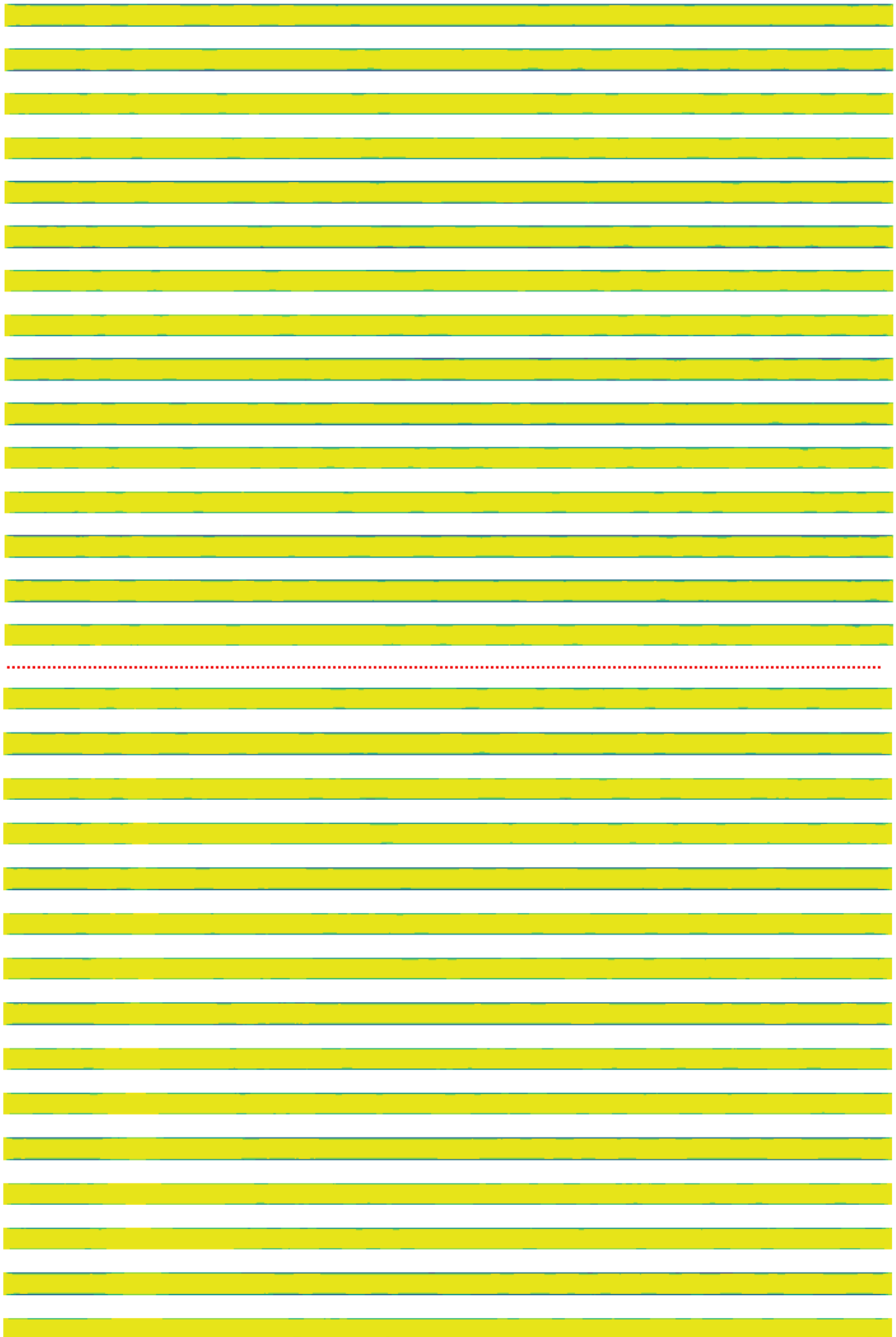
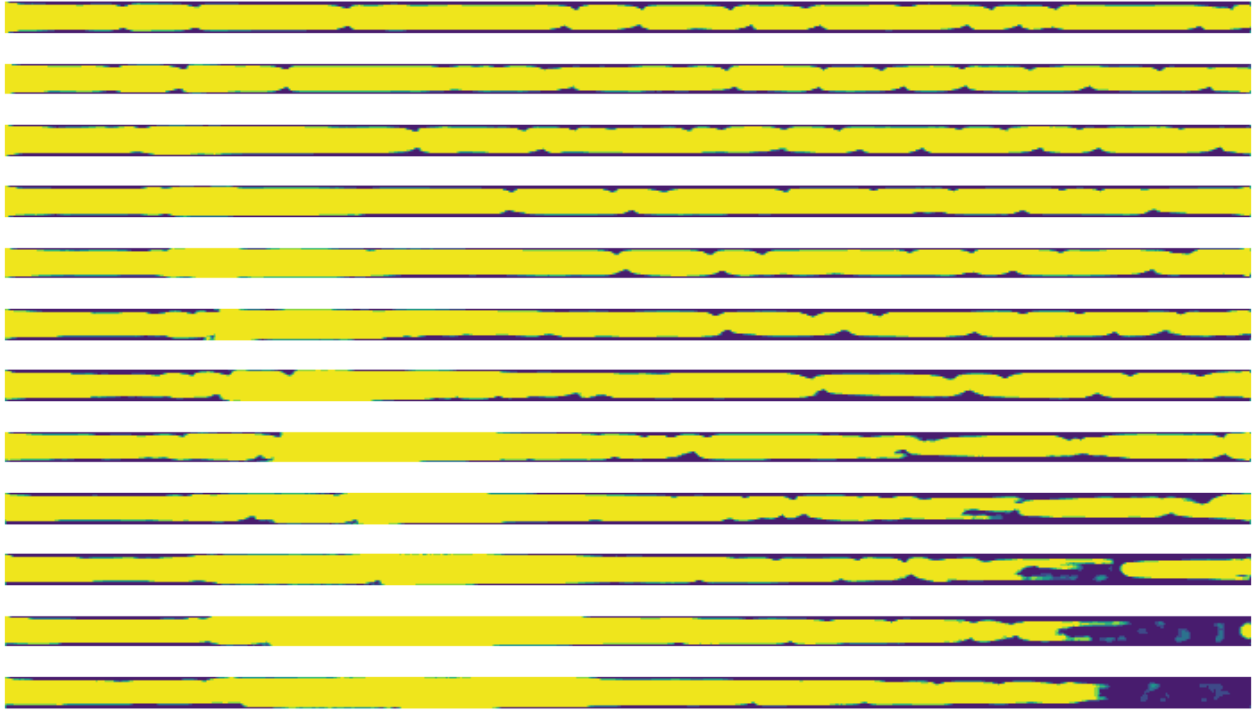


Figure 3.15: Temperature field in test case 2 obtained from a rollout for the same parameters as in Fig. 3.14.

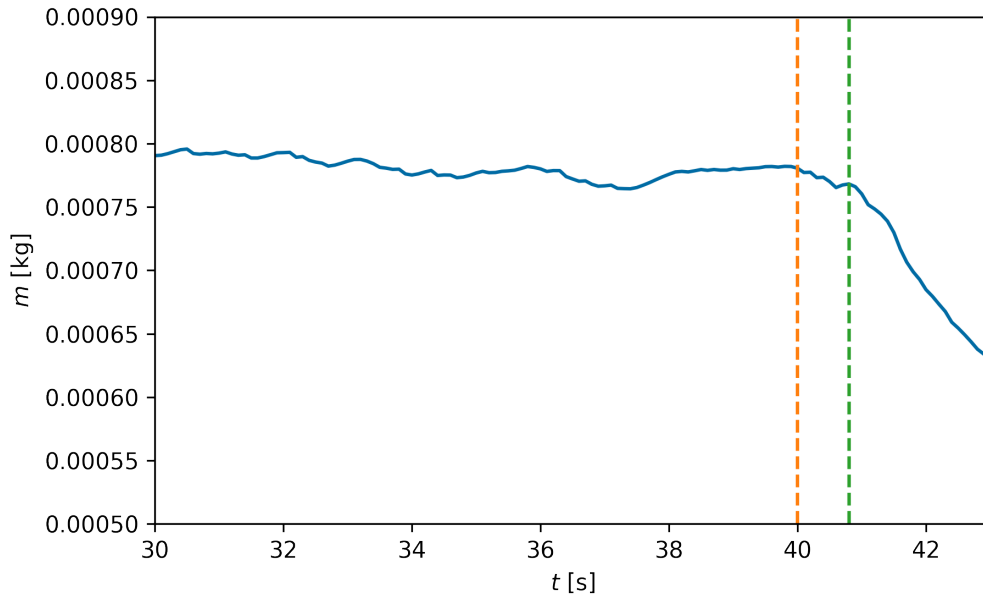
physics-based simulations, which are treated as the ‘ground truth’ in this case, with further catastrophic artifacts of the extrapolation being created near the outlet after 80-90 steps. The temporal evolution of the deposit mass is shown in Fig. 3.16(b) where the red dashed line indicates the moment when the extrapolation begins. The dynamic steady state seems to be maintained until around $t = 40.8\text{ s}$ (viz. the dashed green line in Fig. 3.16(b)) when the amount of deposit begins to decrease sharply.

In order to deal with the deterioration of the accuracy of the extrapolated results, a “hybrid”, multi-fidelity approach can be followed which combines the data-driven, graph-based method for rollouts that can be corrected when the accuracy of the extrapolated solutions dips below a user-defined threshold via brief deployment of the physics-based simulations. This strategy can, in principle, lead to reliable solutions with (a potentially significantly) enhanced computational efficiency provided minimal use of the physics-based simulations is made throughout the computations. This approach involves restarting the simulations, following rollout breakdown, from reconstructed fields obtained from the rollouts associated with a time before the breakdown (chosen when the extrapolated solution is deemed satisfactory). The inaccuracies of these fields are expected to give rise to delays in re-initialising the simulations. Nonetheless, this is not anticipated to provide a major deficiency. One possible way of implementing this hybrid approach would be to utilize loss terms that are based on the governing equations, as in Raissi et al. (2019). Here, instead, we opt for a simpler approach according to which extrapolation and simulations are performed in an alternate way: each cycle consists of 0.3 s of rollout, followed by 0.1 s of simulation. The extrapolation was assumed to start to break down when the value of the deposit mass first went out of the range of variation of the dynamic steady-state observed in the simulation. Although this does not correspond to an automated strategy by which the physics-based simulations are restarted based on the quality of the data-driven rollouts, the adopted methodology will nonetheless provide an illustration of the efficiency of a multi-fidelity approach.

In contrast to the fully data-driven approach, the deposit volume fraction field generated after 20 s using the hybrid multi-fidelity approach of extrapolation-solution cycles is still stable, with no major unphysical issues, as shown in Fig. 3.17(a). Although the wave structures show



(a)



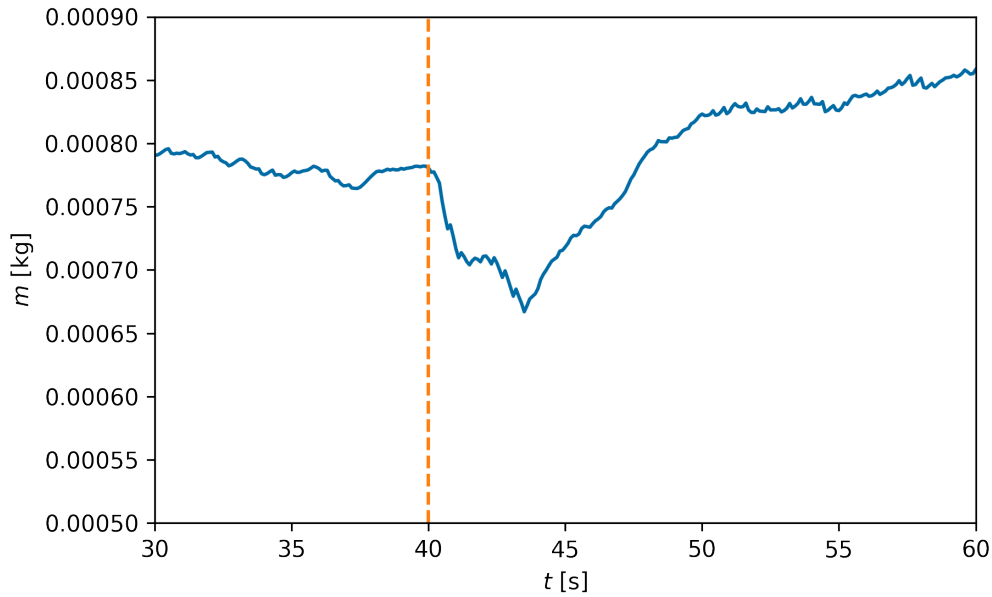
(b)

Figure 3.16: Deterioration of the extrapolated solution accuracy for test case 2: deposit volume fraction, (a), and temporal variation of the deposit mass, (b), for the same parameters as in figure 3.14; each snapshot represents 10 steps of rollout. In (b), the dashed red line represents the beginning of the extrapolation and the dashed green line, at $t = 40.8$ s, indicates the onset of the decline in the extrapolated solution accuracy.

some differences compared to the full solution, notably, wave free regions near the inlet and in the centre, the behaviour of the flow is similar to the one of the full solution. The deposit mass, shown in Fig. 3.17(b), decreases significantly when the extrapolation begins, but seems to nearly stabilize after around 10 s, at a new dynamic steady-state. The final deposit mass is 6% higher than the one obtained with the full solution. The hybrid method also takes around



(a)



(b)

Figure 3.17: Predictions of the hybrid multi-fidelity approach for test case 2 with a cycle consisting of 0.3 s of rollout followed by 0.1 s of physics-based simulation: deposit volume fraction for times $t = 40, 44, 46, 50, 55, 60$ s, (a), and temporal variation of the deposit mass, (b), for the same parameters as in figure 3.14. In (b), the red dashed line indicates the beginning of deployment of the hybrid approach.

30 core hours per second of simulation on 32 cores, a gain of up to 30% in comparison to the fully physics-based solution. The gain is not proportional to the time spent in the extrapolation stages since the solution of the governing equations in the restarted physics-based simulations is slowed down if the initial conditions provided by the extrapolation are not exact, as anticipated

above. Nonetheless, the above results demonstrate that consistent gains can be obtained even with a very simple workflow combining data-driven and physics-based methods.

3.6 Conclusions

The wax model proposed by Magnini and Matar (2019) was successfully re-implemented in an open source platform. It was shown that the choice of numerical implementation procedures can have a significant effect on the variables of interest. The graph based approach proved successful at providing short and medium term extrapolations of the time evolution of the flow. Notably, the deposit interface remains sharp despite the use of a very large Courant number used in the rollout. On long extrapolations, however, the quality of the solution started to deteriorate, with finally non-physical “plugs” of deposit being formed in some regions.

A “hybrid” methodology, alternating a physical solver with short extrapolations, was also proposed, and proved successful in maintaining the stability of the solution for a long time period. In the future, improvements could include the use of a more extensive training database, physical informed network architectures, or dynamic criteria for switching between direct solutions and surrogate models.

Chapter 4

Deposition with thin film model

4.1 Introduction

Here, we propose a simulation methodology based on the full solution of the transport equations for fluid flow, in a three-dimensional, transient setting. The deposit region is modelled with a thin-film simplification, which allows for a simple but realistic description of the deposition and removal physics. Since the model is implemented in a powerful, versatile CFD framework, it can use several of its capabilities for handling of complex geometries and physics as will be illustrated below. The model is validated with data from single-phase and two-phase flow experiments.

The rest of this chapter is organised as follows. In Section 4.2, details of the problem formulation are provided, while in Section 4.3, the solution methodology is presented. A discussion of the results for single-phase and two-phase stratified flows is provided in Section 4.4; a brief set of results for single-phase flow with deposition in an elbow is also provided. Finally, concluding remarks are given in Section 4.5.

4.2 Modelling

Two solution domains are considered: a volumetric domain in the interior of the pipe, where the equations for the gas and liquid phases are solved, and a surface domain at the pipe wall, where the thin film solution is applied. A schematic of the proposed model is shown in Fig. 4.1.

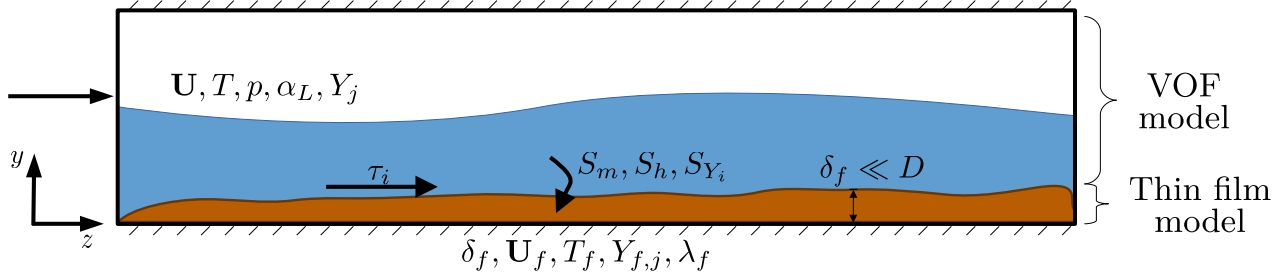


Figure 4.1: Schematic representation of the proposed thin film model employed in the present work.

4.2.1 Bulk region

We assume that the wax deposition takes place inside a control volume that corresponds to a pipe, heat exchanger, or any given process engineering device. The working fluid is assumed to be a liquid or a mixture of gas and liquid. The flow is incompressible and non-isothermal, but the formulation is compatible with a variable density. The continuity equation for transient, variable density flow reads:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0 \quad (4.1)$$

where t is time, ρ is the density of the mixture, and $\mathbf{U}$ is the velocity. The momentum equation is given by:

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot (\rho \mathbf{U} \mathbf{U}) = -\nabla p_d - \nabla \rho \mathbf{g} \cdot \mathbf{x} + \nabla \cdot (\mu_{\text{eff}} \nabla \mathbf{U}) + \sigma \kappa_L \nabla \alpha_L \quad (4.2)$$

where μ_{eff} is the effective viscosity, σ is the surface tension, κ_L is the interface curvature, α_i is the volume fraction of phase i , $\mathbf{g}$ is the gravity vector, and p_d is the total pressure without

the hydrostatic contribution. Note that the effective viscosity considered here may depend on the phase, thermodynamic state or turbulence related variables, depending on the specific situation.

The effective stress tensor $\mathbf{R}_{\text{eff}}$, including laminar and turbulent components, can be calculated as:

$$\mathbf{R}_{\text{eff}} = -\mu_{\text{eff}} \left(\nabla \bar{\mathbf{U}} + \nabla (\bar{\mathbf{U}})^T \right) - \mu_{\text{eff}} \left(\frac{2}{3} \nabla \cdot \mathbf{U} \right) \mathbf{I} \quad (4.3)$$

The following form is used for the energy equation:

$$\frac{\partial \rho c_p T}{\partial t} + \nabla \cdot (\rho c_p \mathbf{U} T) = \nabla \cdot (k_{\text{eff}} \nabla \mathbf{T}) + S_h \quad (4.4)$$

where c_p is the specific heat capacity, T is the temperature, and k_{eff} is the effective thermal conductivity. The equation for the volume fraction of phase i , α_i , is written as:

$$\frac{\partial \rho_i \alpha_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{U} \alpha_i) = S_{m_i} \quad (4.5)$$

where $i(= L, G)$ denotes the phase and ρ_i is the density of phase i .

We also assume that each phase comprises $N_{c,i}$ components, with individual transport equations given by:

$$\frac{\partial \rho_i \alpha_i Y_{i,j}}{\partial t} + \nabla \cdot (\rho_i \mathbf{U} \alpha_i Y_{i,j}) = S_{Y_{i,j}} \quad \text{for } j \in \{1, \dots, N_{c,i}\} \quad (4.6)$$

where $Y_{i,j}$ is the mass fraction of component j in phase i . The source terms on the right-hand-side of Eqs. (4.4) and (4.5) are discussed below.

Finally, turbulence in the bulk region is modelled using the SST k - ω model (Menter et al., 2003), adding a damping term given by Egorov et al. (2004) (*apud* Frederix et al., 2018) in the cases where an interface is present.

4.2.2 Deposit region

The mass equation for the film has the following form:

$$\frac{\partial \rho \delta}{\partial t} + \nabla_s \cdot (\rho \delta \mathbf{U}_f) = S_{s,m} \quad (4.7)$$

where ρ is the film density, δ is the film thickness, ∇_s is the vector differential operator tangential to the surface (wall), and $\mathbf{U}_f$ is the film velocity. The momentum, enthalpy, and species equations for the film have the following forms, respectively:

$$\frac{\partial \rho \delta \mathbf{U}_f}{\partial t} + \nabla_s \cdot (\rho \delta \mathbf{U}_f \mathbf{U}_f) = -\delta \nabla_s p + \mathbf{S}_{s,\mathbf{U}_f} \quad (4.8)$$

$$\frac{\partial \rho \delta h}{\partial t} + \nabla_s \cdot (\rho \delta \mathbf{U}_f h) = S_{s,h} \quad (4.9)$$

$$\frac{\partial \rho \delta Y_{f,j}}{\partial t} + \nabla_s \cdot (\rho \delta \mathbf{U}_f Y_{f,j}) = S_{s,Y_{f,j}} \quad (4.10)$$

where h is the mean enthalpy of the film, and $Y_{f,j}$ is the mass fraction of component j in the film. The source terms $S_{s,m}$, $S_{s,\mathbf{U}_f}$, $S_{s,h}$, and $S_{s,Y_{f,j}}$ couple the solutions of the the pipe interior and pipe wall domains; they will be described in detail on Sec. 4.2.3.

Finally, the effect of ageing is included through the use of a thixotropic model for the film viscosity, μ :

$$\mu = \frac{\mu_\infty}{(1 - K_\lambda \lambda)^2} \quad (4.11)$$

where the so-called ‘structuration’ parameter, λ , is calculated via solution of the following equation:

$$\frac{\partial \lambda}{\partial t} + \nabla_s \cdot (\mathbf{U}_f \lambda) = a_\lambda (1 - \lambda)^{b_\lambda} - c_\lambda \lambda \dot{\gamma}^{d_\lambda} - \frac{\max(S_{s,m}, 0)}{\rho \delta} \lambda \quad (4.12)$$

where $\dot{\gamma}$ represents the second invariant of the rate of deformation tensor, $(\nabla \mathbf{U}_f + \nabla \mathbf{U}_f^T)/2$, and K_λ is given by:

$$K_\lambda = 1 - \sqrt{\frac{\mu_\infty}{\mu_0}} \quad (4.13)$$

wherein μ_∞ and μ_0 are constants. Furthermore, a_λ , b_λ , c_λ , and d_λ denote constants (their values

are listed in Tab. 4.3) that control the structure-building and de-structuring effects which are represented by the first and second terms on the right-hand-sides of Eq. (4.12), respectively.

4.2.3 Source terms

The mass transfer rate for each component is given by (Svendsen, 1993; Magnini and Matar, 2019):

$$S_{s,Y_{f,j}} = \Gamma_m \rho \eta_{L,j} \frac{\nabla \mathbf{T} \cdot \hat{\mathbf{n}}}{T} \quad (4.14)$$

where Γ_m is an average diffusion coefficient and $\hat{\mathbf{n}}$ is the deposit interface normal vector (assumed to be equal to the wall normal). The procedure for calculation of $\eta_{L,j}$, the dimensionless variation of the mass concentration of species i at the liquid state in the mixture per unit temperature, is presented in Svendsen (1993). Additionally, the phase change is assumed to take place exclusively on liquid-wetted regions of the wall, i.e. regions where $\alpha_L > 0$. The total mass transfer rate for an N_Y -component film is, consequently:

$$S_{s,m} = \sum_{j=1}^{N_Y} S_{s,Y_{f,j}} \quad (4.15)$$

The momentum transfer term is given by:

$$\mathbf{S}_{s,\mathbf{U}_f} = \tau_i + \tau_w + \rho \mathbf{U}_f S_{s,m} \quad (4.16)$$

where the terms on the right-hand side can be attributed to the interfacial shear, wall shear and mass transfer, respectively. Similarly to Meredith, Vries, et al. (2011), an analytical streamwise velocity profile is prescribed for the wall-normal direction, y , based on the assumption that the shape is preserved even in the case of wavy film flow. Extending the expression to take into account a fixed shear stress at the interface τ_i imposed by the bulk flow leads to:

$$\mathbf{u}(y) = 3 \left(\mathbf{U}_f - \frac{\tau_i \delta}{2\mu} \right) \left(\frac{y}{\delta} - \frac{y^2}{2\delta^2} \right) + \frac{\tau_i \delta}{\mu} \frac{y}{\delta} \quad (4.17)$$

where τ_i is given by:

$$\tau_i = -\hat{\mathbf{n}} \cdot \mathbf{R}_{\text{eff}}|_s \quad (4.18)$$

where $\mathbf{R}_{\text{eff}}|_s$ represents the value of the effective stress tensor for the bulk flow, evaluated at the deposit surface.

Consequently, the wall shear stress τ_w exerted on the film is given by the following expression:

$$\tau_w = -\mu \frac{3\mathbf{U}_f}{\delta} - \frac{\tau_i}{2} \quad (4.19)$$

The enthalpy transfer is given by:

$$S_{s,h} = \dot{q}_i + \dot{q}_w + hS_{s,m} + \sum_{j=1}^{N_Y} \Delta h_{f,j} S_{s,Y_{f,j}} \quad (4.20)$$

where the right-hand-side terms refer to interfacial and wall heat transfer, mass transfer, and phase change, respectively. Here, $\Delta h_{f,j}$ denote the phase change enthalpy of component j in the film. A similar approach to the one used for the velocity can be adopted for the temperature field in the deposit, assuming that the advection is negligible in relation to the heat conduction. For a heat transfer rate imposed by the bulk flow at the interface $\dot{q}_i$, the wall-normal dependence of the deposit temperature $T_d(y)$ is given by:

$$T_d(y) = T_w + (T_w - T_f) \frac{3y^2}{2\delta^2} + 3(T_f - T_w) \frac{y}{\delta} + \frac{3\dot{q}_i y^2}{4\delta k_f} - \frac{\dot{q}_i y}{2k_f} \quad (4.21)$$

where T_f and T_w denote the interfacial and wall temperatures, respectively, and the heat transfer rate through the interface is:

$$\dot{q}_i = \alpha_{\text{eff}} c_p \nabla T|_s \quad (4.22)$$

Here, α_{eff} is the effective thermal diffusivity of the deposit film, and the heat transfer to the wall, consequently, can be calculated as:

$$\dot{q}_w = \frac{3k_f}{\delta} (T_w - T_f) + \frac{1}{2} \dot{q}_i \quad (4.23)$$

where k_f is the thermal conductivity of the deposit.

Finally, we assume that the transfer between superficial and volumetric domains takes place on the control volume adjacent to the wall. The volumetric and surface source terms S_ϕ and $S_{s,\phi}$ for a variable ϕ can be related by:

$$S_\phi = \frac{A_{w,cell}}{V_{cell}} S_{s,\phi} \quad (4.24)$$

where $\phi = h, m, Y_j$, while V_{cell} denotes the volume of the cell adjacent to the wall, and $A_{w,cell}$ denotes its projected area onto the wall.

4.2.4 Stratified flow

The liquid holdup at the inlet is calculated through the correlation of Spedding and Chen (1984):

$$H_L = \left[1 + 0.45 \left(\frac{U_{SG}}{U_{SL}} \right)^{0.65} \right]^{-1} \quad (4.25)$$

where U_{SG} and U_{SL} denote the superficial gas and liquid velocities, respectively. From H_L , the height of the liquid layer h_L may be calculated numerically from the following geometric relation:

$$H_L = \frac{1}{\pi} \left[\cos^{-1} \left(1 - 2 \frac{h_L}{D} \right) - 4 \left(\frac{1}{2} - \frac{h_L}{D} \right) \sqrt{\frac{h_L}{D} - \left(\frac{h_L}{D} \right)^2} \right] \quad (4.26)$$

in which D is the pipe diameter. The fluid velocity and the volume fraction of liquid at the inlet are given by:

$$U_{inlet} = \begin{cases} \bar{U}_L, & \text{if } y < h_L \\ \bar{U}_G, & \text{else} \end{cases} \quad (4.27)$$

where the average liquid and gas velocities are respectively given by

$$\bar{U}_L = \frac{U_{SL}}{H_L} \quad (4.28)$$

$$\bar{U}_G = \frac{U_{SG}}{(1 - H_L)} \quad (4.29)$$

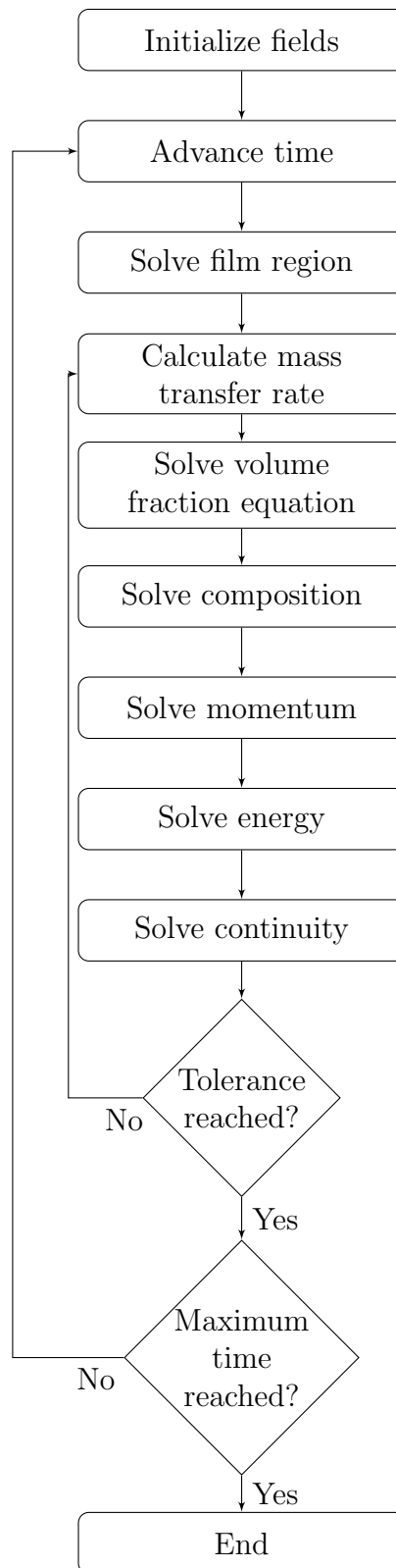


Figure 4.2: Solution algorithm for the wax deposition simulations using the thin film model.

The inlet liquid volume fraction is related to h_L by

$$\alpha_{L,\text{inlet}} = \begin{cases} 1, & \text{if } y < h_L \\ 0, & \text{else} \end{cases} \quad (4.30)$$

The gas phase thermodynamic behaviour was approximated by that of pure methane gas. The density is obtained from the assumption of a perfect gas behaviour. The gas viscosity is calculated with the Sutherland law:

$$\mu_G = \frac{A_s \sqrt{T}}{1 + T_s/T} \quad (4.31)$$

where $A_s = 1.67212 \times 10^{-6} \text{ kg}/(\text{ms}\sqrt{\text{K}})$ and $T_s = 170.672 \text{ K}$. The thermal conductivity is obtained through the Eucken approximation:

$$k_G = \mu_G c_v \left(1.32 + 1.77 \frac{R}{c_v} \right) \quad (4.32)$$

where c_v is the specific heat capacity at constant volume, and R denotes the universal gas constant. The gas specific heat capacity at constant pressure is calculated using the formula from JANAF tables of thermodynamics:

$$c_{p,G} = R(((a_4 T + a_3)T + a_2)T + a_1)T + a_0 \quad (4.33)$$

here, the constants a_i , ($i = 0, \dots, 4$) in this equation are provided in the JANAF tables (Chase, 1998).

4.3 Solution method

The numerical model was implemented within the OpenFOAM v2006 library (OpenCFD, 2020). Second-order schemes were utilized for the discretization of spatial terms, and a first-order implicit Euler scheme for the time. The solution algorithm is presented in Fig. 4.2. First, the

equations described in Sec. 4.2.2 are solved, with the source terms calculated in Sec. 4.2.3. The volumetric source terms S_{m_i} , $\mathbf{S}_{\mathbf{U}_f}$, $S_{Y_{i,j}}$ and S_h are calculated based on the surface values S_{s,m_i} , $\mathbf{S}_{s,\mathbf{U}_f}$, $S_{s,Y_{i,j}}$ and $S_{s,h}$, and Eq. (4.24). With those values, Eqs. (4.5), (4.6), (4.2), (4.4) and (4.1) are solved. Correction loops are then executed until convergence is achieved for each timestep.

The correct calculation of the interface shape is essential for a good prediction of the liquid-wetted area and other related parameters (Duan, Deng, et al., 2018). The geometric reconstruction method *plicRDF* (Scheufler and Roenby, 2019) was used for the description of the interface. This algorithm has been shown to provide lower numerical errors than the traditional compressive scheme utilized in OpenFOAM, at moderate computational costs. The implementation of the turbulence damping model utilized was adapted from Fan and Anglart (2020).

Following Magnini and Matar (2019), we assume that the liquid and deposit phases consist of two pseudo-components, with high and low molecular weights. We refer to the original publication for the details on the lumping procedure utilized. In the case of single-phase deposition, the bulk flow is expected to vary very slowly in time, such that a pseudo steady-state approximation may be used for the solution of the fluid domain. In that case, the limiting timescale in the simulation is given by the dynamics of the deposit region, and the timestep was based solely on the Courant number in the that domain. In the two-phase cases, the maximum between the the Courant number in the bulk and walls regions was utilized. In both situations, a maximum Courant number of 0.5 was prescribed.

The computational domain, boundary, and initial conditions are presented in schematic form in Fig. 4.3. The average velocity of each phase is calculated based on the mass flow rate and the estimated volume fraction. The value obtained is used for the inlet and initial conditions, except for the pipe bend, where the initial velocity is set to zero, since its direction is expected to vary through the domain. Similarly, the volume fraction field is set according to the height h_L as calculated in Sec. 4.2.4. This initialization is utilized in order to achieve a quicker steady state.

The wall boundaries values of velocity and temperature are adjusted dynamically according to

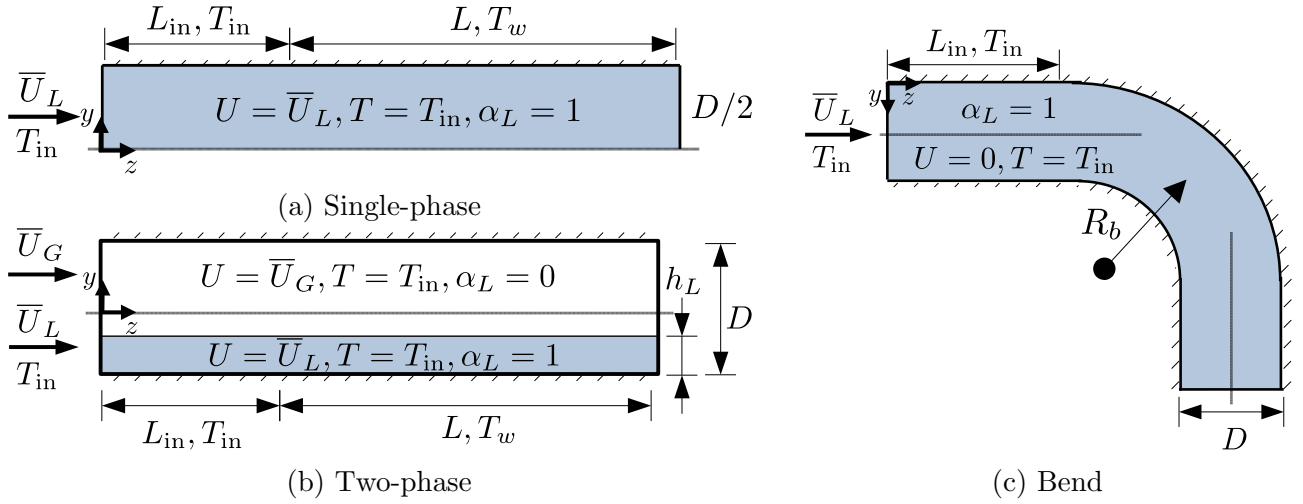


Figure 4.3: Schematics of the computational setups for the test cases associated with single-phase flow in a pipe and a bend, and a two-phase stratified pipe flow. Here, the bend is characterised by a diameter D and radius of curvature $R_b = 5D$, while L_{in} represents the entry length; the remaining variables are defined in the text.

the values obtained for the deposit wetted interface. A prescribed pressure value is assumed for the outlets. All simulations start with a no-deposition condition (i.e. $\Gamma_m = 0$) until a steady-state is established, after which the deposition model is applied. Since gravitational effects are assumed negligible for the liquid-deposit system (Magnini and Matar, 2019), an axisymmetric domain was adopted for the single-phase simulations.

For the stratified flow simulations, the grid utilized is shown in Fig. 4.4. The size of cells in the cross-section directions and in the streamwise direction are $\Delta x/D = \Delta y/D = 0.02$ and $\Delta z/D = 0.2$, respectively. Convergence was achieved upon mesh refinement. For the simulations presented here, the pipe was split into a development section with length $10D$ and a deposition section of length $30D$.

Table 4.1: Parameters utilized for the comparison between the interface capturing and thin film models.

Parameter	Value	Unit
$\bar{U}_L$	0.226	m s^{-1}
D	0.009	m
L	0.18	m
$Y_{1,1,\text{in}}$	0.85	-
$Y_{1,2,\text{in}}$	0.15	-
T_{in}	303.0	K
T_w	275.0	K
ρ_1	850	kg m^{-3}
ρ_2	850	kg m^{-3}
μ_1	4.6×10^{-3}	Pa s
μ_2	4.6×10^{-3}	Pa s
k_1	0.134	$\text{W m}^{-1} \text{K}^{-1}$
k_2	0.134	$\text{W m}^{-1} \text{K}^{-1}$
$c_{p,1}$	1920	$\text{J kg}^{-1} \text{K}^{-1}$
$c_{p,2}$	1920	$\text{J kg}^{-1} \text{K}^{-1}$
M_1	215	kg kmol^{-1}
M_2	530	kg kmol^{-1}
$T_{f,1}$	271.0	K
$T_{f,2}$	349.0	K
$\Delta h_{f,1}$	37.8×10^3	J mol^{-1}
$\Delta h_{f,2}$	105.4×10^3	J mol^{-1}
K_1	1.0	-
K_2	1.0	-
Γ_m	2.76×10^{-7}	$\text{m}^2 \text{s}^{-1}$

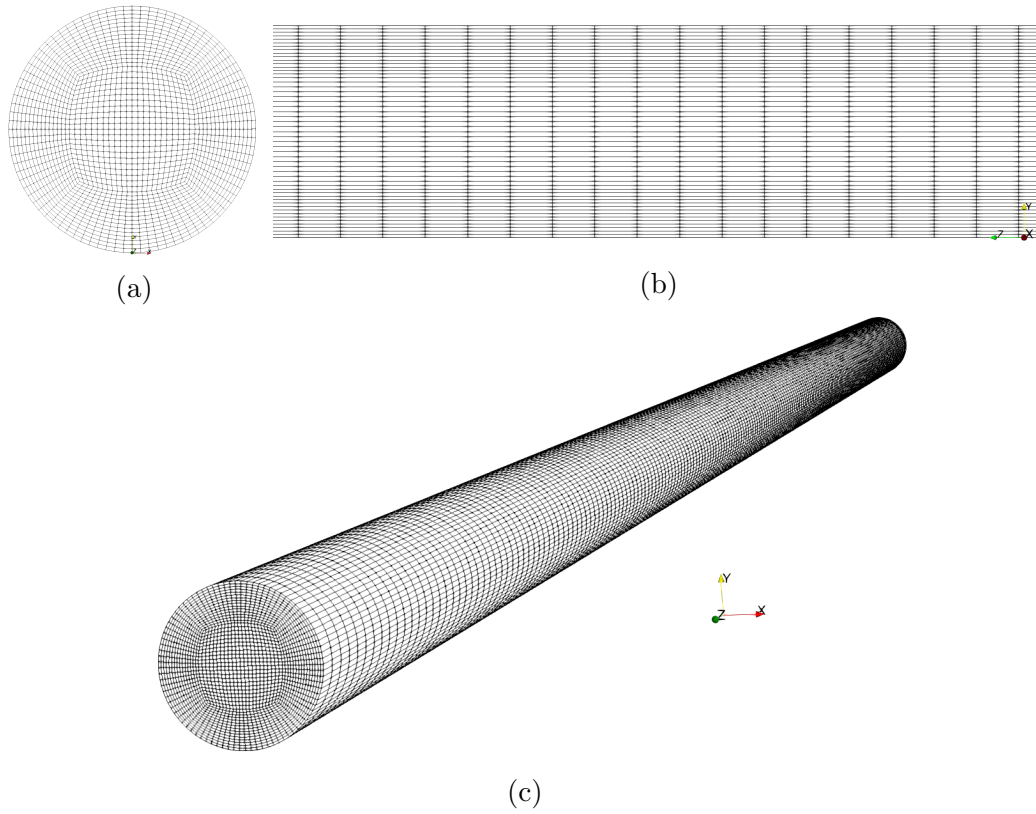


Figure 4.4: The grid utilized for the three-dimensional two-phase flow simulations; side- and front-views are shown in (a) and (b), respectively, and a perspective view is shown in (c).

4.4 Results

4.4.1 Single-phase pipe flow

In order to verify the validity of the assumptions adopted here, the present model is compared to the full interface capturing approach of Magnini and Matar (2019). The benchmark case consists of an axisymmetric pipe flow, with parameters given in Tab. 4.1. Figure 4.5 presents a comparison of the thickness of the deposit layer over time for the VoF and thin film approaches. The quantitative agreement is excellent for deposit thickness lower than 2% of the diameter, after which a discrepancy can be observed, although the qualitative agreement is still satisfactory. The computational cost of the simplified formulation is 3.7 times lower than the one with the full VoF model, even with relatively coarse meshes. In practice, achieving the necessary resolution of the deposit would require a finer mesh near the wall in the full VoF simulations, which would increase the gains of the thin film assumption several fold.

Table 4.2: Parameters utilized for the numerical predictions of single-phase flow test cases of Singh, Panacharoensawad, et al., 2017 using the thin film model.

Parameter	Value	Unit
$\dot{m}$	20, 30, 40, 50	kg min^{-1}
D	16.5×10^{-3}	m
L	0.21	m
$Y_{1,1,\text{in}}$	0.85	-
$Y_{1,2,\text{in}}$	0.15	-
T_{in}	298.0	K
T_w	289.0	K
ρ_1	836	kg m^{-3}
ρ_2	836	kg m^{-3}
μ_1	4.6×10^{-3}	Pa s
μ_2	4.6×10^{-3}	Pa s
k_1	0.134	$\text{W m}^{-1} \text{K}^{-1}$
k_2	0.134	$\text{W m}^{-1} \text{K}^{-1}$
$c_{p,1}$	2008	$\text{J kg}^{-1} \text{K}^{-1}$
$c_{p,2}$	2008	$\text{J kg}^{-1} \text{K}^{-1}$
M_1	213	kg kmol^{-1}
M_2	556	kg kmol^{-1}
$T_{f,1}$	271.0	K
$T_{f,2}$	349.0	K
$\Delta h_{f,1}$	37.8×10^3	J mol^{-1}
$\Delta h_{f,2}$	105.4×10^3	J mol^{-1}
K_1	1.0	-
K_2	1.0	-

Table 4.3: Parameters adjusted with the predictions of single-phase flow test cases of Singh, Panacharoensawad, et al., 2017 using the thin film model.

Parameter	Value	Unit
a_λ	1×10^{-5}	s^{-1}
b_λ	0.0	-
c_λ	5.0	s
d_λ	1.0	-
μ_∞	4.6×10^2	Pa s
Γ_m	1.5×10^{-10}	$\text{m}^2 \text{s}^{-1}$

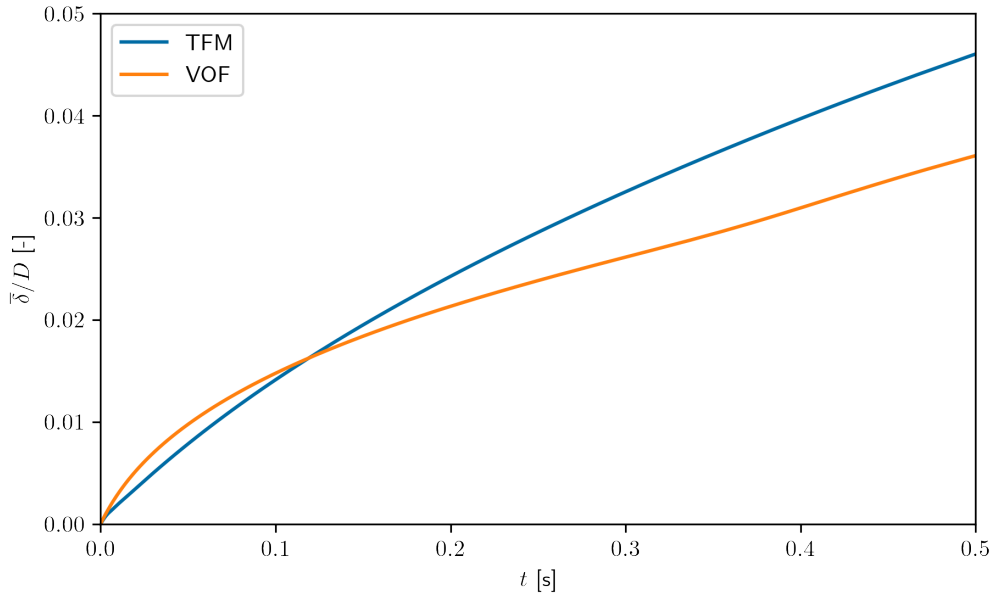


Figure 4.5: Comparison of the predictions provided by the thin film model with those from the interface-capturing volume-of-fluid approach employed by Magnini and Matar, 2019 for the temporal evolution of the average deposit thickness. The parameter values are presented in Tab. 4.1.

The first test cases are based on the experimental setup of Singh, Panacharoensawad, et al. (2017) for single-phase flow. The authors performed a set of experiments with Garden Banks condensate, different mass flow rates, and a maximum test duration of 24 h. The test section consisted of a section of copper piping of length 84 cm and internal diameter 0.651 in. The authors provide measurements of the fluid properties, deposit thickness, and composition as a function of operational conditions, as well as fitting equations. Four mass flow rates, $\dot{m}$, were simulated: 20, 30, 40 and 50 kg min⁻¹. The complete list of parameters utilized in these simulations is presented in Tab. 4.2. Following the procedure of Magnini and Matar (2019), in order to reproduce the long-term trends of the deposit growth, the rheological constants were adjusted to the deposit thickness data, leading to the parameters shown in Tab. 4.3. The diffusivity constant, Γ_m , was also decreased slightly from its original value of 1.97×10^{-10} m² s⁻¹ to compensate for shear stress and thermodynamics mechanisms which have not been fully accounted for in the proposed closure relations.

The comparison between predicted and measured deposit thickness for single-phase flow over time is presented in Fig. 4.6. During the initial stages of deposition, the thickness grows linearly

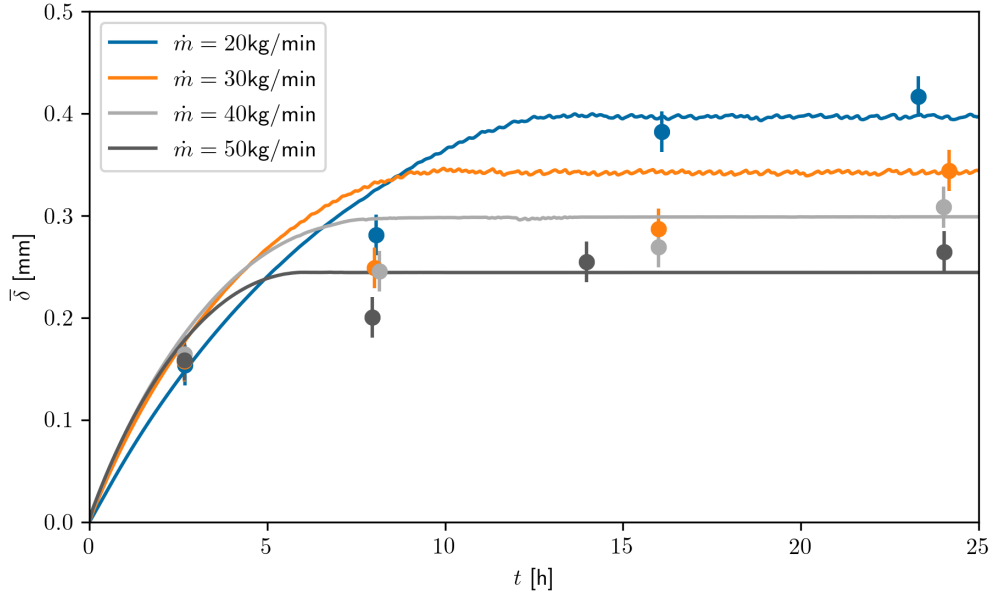


Figure 4.6: Variation of the average deposit thickness over time for the single-phase cases characterised by the parameters in Tab. 4.2: the thin film model predictions and the experimental data of Singh, Panacharoensawad, et al., 2017 are shown by Continuous lines and symbols, respectively.

as the source term does not depend directly on δ . However, as the deposit layer becomes thicker, three phenomena begin to influence the growth rate: (i) the heat transfer between the wall and the liquid is inhibited, resulting in a decrease of the growth rate; (ii) the shear removal gains in influence, controlling the increase in thickness; and (iii) the ageing of the deposit results in a increase of the deposit viscosity, retarding, and eventually preventing further removal of the deposit material.

The proposed thin film model is also capable of simulating time intervals that are compatible with the experimental observations, which are orders of magnitude larger than those that can be explored with interface-capturing methodologies such as the ones based on VoF. As can be seen clearly in Fig. 4.6, the model captures successfully all relevant stages of the temporal evolution of the deposit including its late stages in which a quasi-steady thickness is reached spanning a period of 24 hours.

Fig. 4.7(a,b) shows profiles of the thickness and streamwise velocity component along the axial direction after 24 h of deposition. Similarly to what was observed with the interface-capturing simulations by Magnini and Matar, 2019, interfacial waves are formed in the deposit which

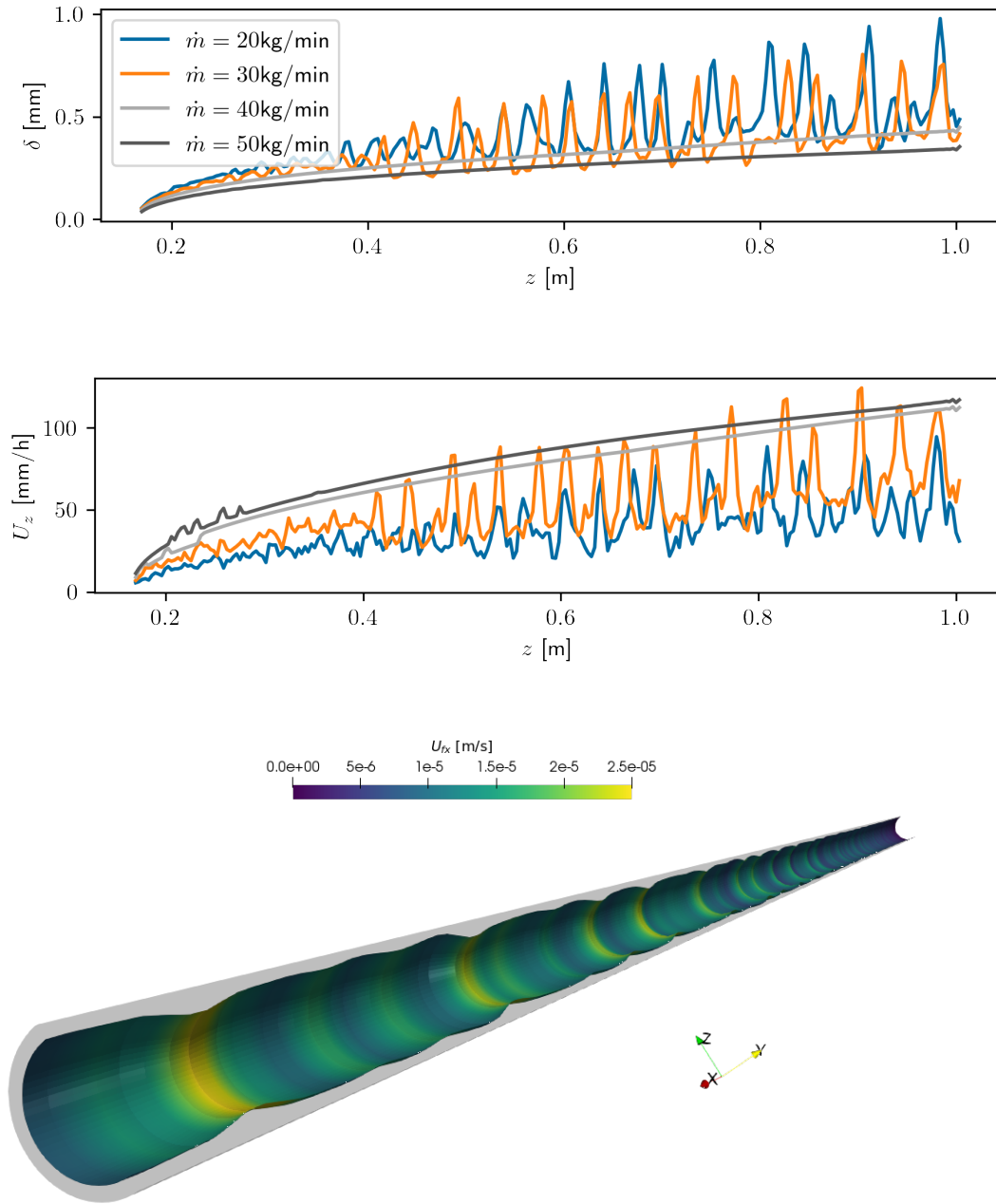


Figure 4.7: Axial profiles in the pipe longitudinal section after 24 hours of the deposit thickness, (a), and axial velocity component, (b), for the single-phase cases characterised by mass flow rates of 20 kg min^{-1} - 50 kg min^{-1} and the parameters presented in Tab. 4.2; also shown in (c) is a perspective view of the deposit layer for 20 kg min^{-1} and 24 hours. Note that the elevation has been multiplied by a factor of 3 in (c) to aid visualisation.

Table 4.4: Parameters utilized for the numerical predictions of two-phase stratified flow test cases of Chi et al. (2019) using the thin film model.

Parameter	Value	Unit
U_{SL}	0.1	m s^{-1}
U_{SG}	1.5, 3.0	m s^{-1}
D	52.5×10^{-3}	m
L	1.56	m
$Y_{1,1,\text{in}}$	0.85	-
$Y_{1,2,\text{in}}$	0.15	-
T_{in}	299.85	K
T_w	294.25	K
ρ_1	836	kg m^{-3}
ρ_2	836	kg m^{-3}
μ_1	4.6×10^{-3}	Pa s
μ_2	4.6×10^{-3}	Pa s
k_1	0.134	$\text{W m}^{-1} \text{K}^{-1}$
k_2	0.134	$\text{W m}^{-1} \text{K}^{-1}$
$c_{p,1}$	2008	$\text{J kg}^{-1} \text{K}^{-1}$
$c_{p,2}$	2008	$\text{J kg}^{-1} \text{K}^{-1}$
M_1	213	kg kmol^{-1}
M_2	556	kg kmol^{-1}
M_G	16.04	kg kmol^{-1}
$T_{f,1}$	271.0	K
$T_{f,2}$	349.0	K
$\Delta h_{f,1}$	37.8×10^3	J mol^{-1}
$\Delta h_{f,2}$	105.4×10^3	J mol^{-1}
K_1	1.0	-
K_2	1.0	-
Γ_m	1.97×10^{-10}	$\text{m}^2 \text{s}^{-1}$

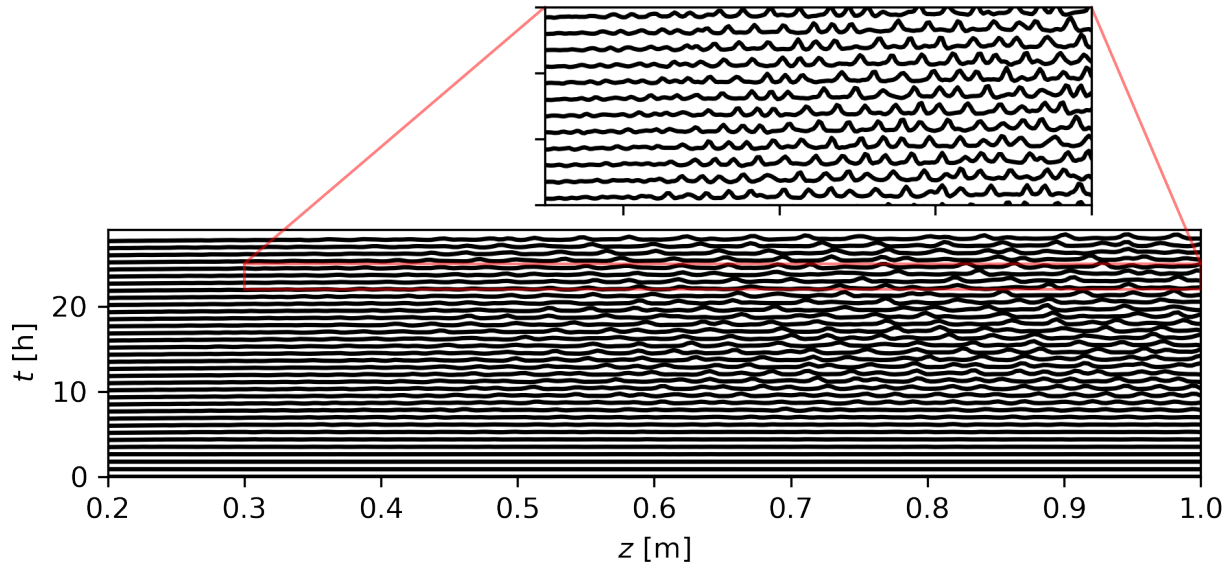


Figure 4.8: Space-time plot of the deposit thickness for flowrate of 20 kg min^{-1} and the rest of the parameters remain unchanged from those listed in Table 4.2. An enlarged view is shown for $0.3 \leq z \leq 1$ and $20 \leq t \leq 25$.

may contribute to the mass transfer in the axial direction. The amplitude of the waves grows with axial distance from the inlet as they develop into highly nonlinear waves that interact as they travel downstream towards the outlet. Figure 4.7(c) also shows an illustrative example of the deposit interface profile obtained for the mass flowrate of 20 kg min^{-1} . The wavy deposit profile is very similar to the ones observed in the simulations of Magnini and Matar (2019). As can also be seen in Fig. 4.7, the waves are virtually absent in the case of the higher mass flow rates considered (e.g., 40 and 50 kg min^{-1}) for which the average deposit thickness is smaller (see also Fig. 4.6).

In order to provide a more complete picture of the complex interfacial dynamics accompanying the flow and deposition process, we present a space-time plot of the deposit thickness in Fig. 4.8 for $\dot{m}=20 \text{ kg min}^{-1}$ with the rest of the parameters remaining unaltered from those listed in Tab. 4.2. We observe that wave activity gains in prominence after $t \approx 10 \text{ s}$ and for $z \approx 0.45 \text{ m}$ for the set of parameters used to generate Fig. 4.8. A dynamic steady-state is then established, which seems to persist indefinitely characterised by large-amplitude waves that travel along the pipe undergoing complex interactions with their neighbouring waves downstream; these interactions manifest themselves through wave coalescence to form larger waves that travel faster than their

original, smaller constituents, leading to additional coalescence events further downstream. These complex dynamics are characteristic of thin films driven by pressure gradients, and body forces, e.g., gravity, centrifugation, and electric fields (Craster and Matar, 2009), and similar to those that accompany crude-oil fouling (Sileri et al., 2011).

Since the formation of waves in this case depends on both space and time coordinates, wavelet transforms can be a useful tool to analyze the evolution of wave lengths with the axial coordinate. A wavelet transform was applied to the thickness profile with a complex Morlet wavelet, using PyWavelets Lee et al. (2019). The resulting amplitude spectrum is shown in Fig. 4.9. The spectrum highlights the existence of important waves on the length range of 20 mm to 50 mm, with amplitudes of around 0.2 mm, for the cases of low flowrates. No significant frequencies are identified for flow rates of 40 kg min^{-1} and 50 kg min^{-1} .

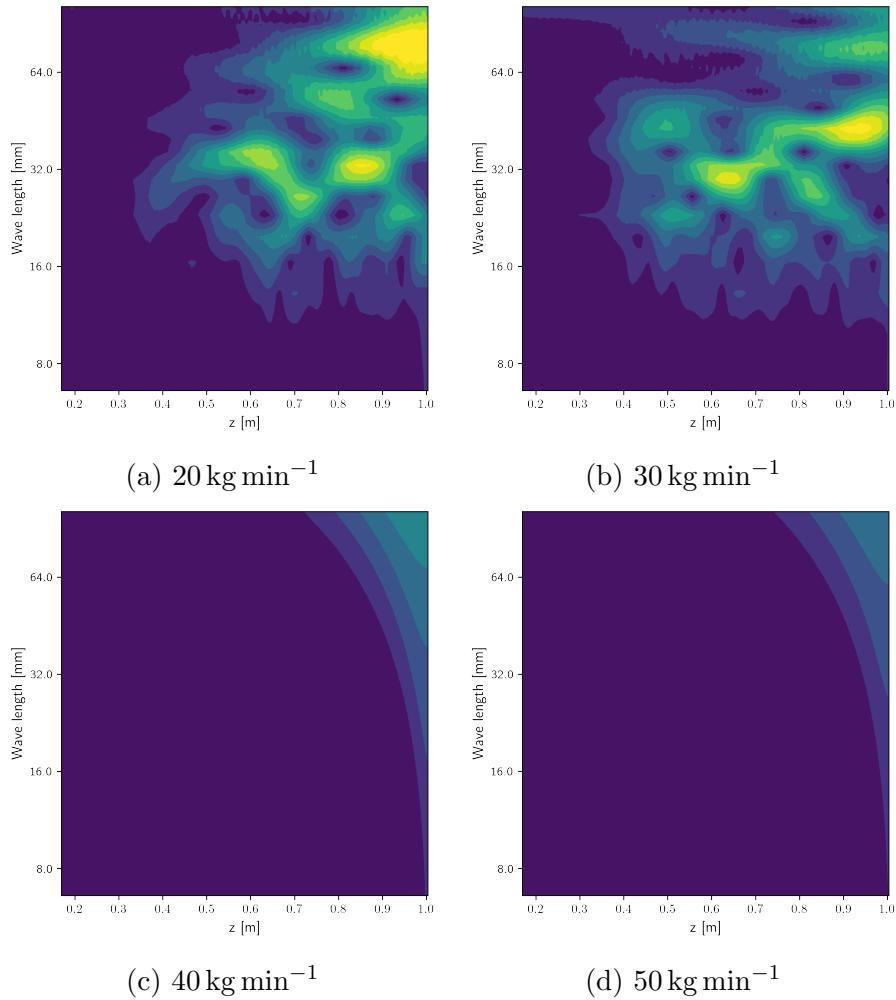


Figure 4.9: Amplitude spectrum density for the thickness profile via a wavelet transform for various mass flow rates and the parameters listed in Tab. 4.2 for single-phase flow.

4.4.2 Two-phase stratified pipe flow

Next, we use the thin film model to tackle a problem involving two-phase stratified flow and deposition. The simulation conditions for the gas-liquid deposition cases are based on the experimental setup of Chi et al. (2019). The experiments utilized Garden Banks condensate and natural gas at the pressure of 2.41 MPa as working fluids. The stratified mixture flowed through a long section for development of the hydraulic and thermal profiles, before entering the measurement area. The main test-section consisted of a 52.5 mm internal diameter, 7.43 m length copper pipe, where local deposit thickness and composition were measured in several positions. In these experiments, the authors observed a significant variation of the deposit thickness over the azimuthal direction, with maximum values being measured at the bottom of the pipe. They also noticed the presence of a region where the deposit roughness was high, close to the gas-liquid interface, in the cases characterised by high gas superficial velocity.

The case initialization followed the procedure described in Sec. 4.3: the liquid height and phase velocities were set according to the holdup estimate, and the flow was resolved without deposition until a steady-state was obtained, after which statistics were collected. In the stratified flow measurements, the deposit growth is linear, indicating a small effect for the shear removal. To prevent significant movement of the deposit, the simulations were run with a constant, high deposit viscosity of $\mu = 4.6 \times 10^6$ Pa s.

Figure 4.10(a) shows the comparison between the simulation and experimental data for the deposit mass over time for two stratified flow cases characterised by superficial gas velocities, $U_{SG} = 1.5$ and 3 m s^{-1} with the remaining parameters unaltered from those in Tab. 4.4. The numerically predicted and experimental observed trends are in good qualitative and quantitative agreement. In particular, the model correctly captures the increase in deposit mass over time with increasing gas superficial velocity. Figure 4.10(b) shows the azimuthal dependence of the deposit thickness. As also observed in the experiments, the thickness is strongly dependent on position within the pipe with the deposit being significantly thicker at the bottom of the pipe and decreasing when approaching the interface. Here, a peak is observed also just below the interface itself, due to the high levels of turbulence generated by the gas shear. As mentioned

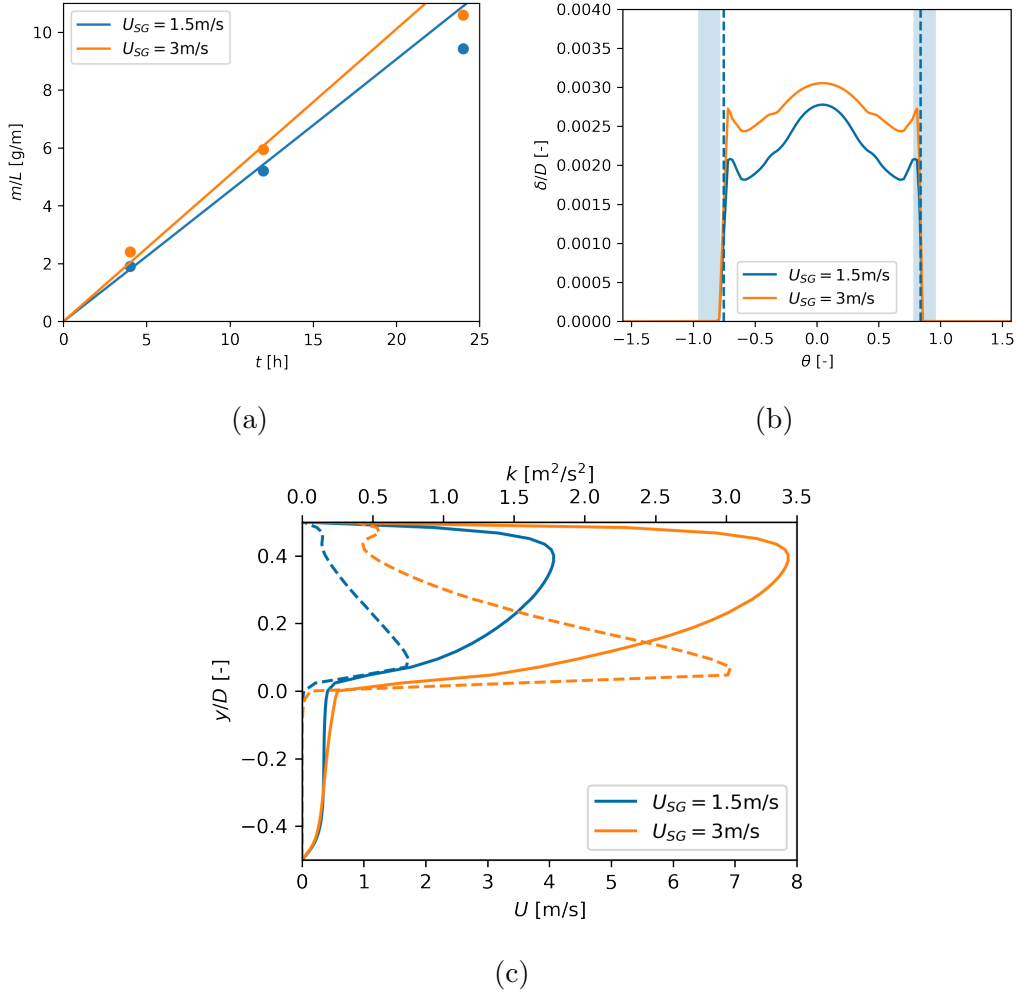


Figure 4.10: Deposit characteristics for two-phase stratified flow: temporal variation of deposit mass, (a), and predicted azimuthal variation of the deposit thickness (the interface position is indicated by a dashed line, and the rough deposit region observed in the experiments, by a solid background), (b), for gas superficial velocities of $U_{SG} = 1.5$ and 3 m s^{-1} with the rest of the parameters remaining unchanged from Table 4.4; in (a), the simulation and experimental data are shown using lines and symbols, respectively. In (c), the cross-stream variation of the axial velocity component and turbulent kinetic energy are shown using continuous and dashed lines, respectively, for $U_{SG} = 1.5$ and 3 m s^{-1} . Profiles are taken at $z = 0.5 \text{ m}$

above, experiments by Chi et al. (2019) included the observation of a well defined region of rough deposit, also just below the interface, which is highlighted in the figure, for the lowest gas flow rate, with a blue background.

The velocity and turbulent kinetic energy profiles are shown in Fig. 4.10(c) to further illustrate the effect of the gas flow on the mass transfer dynamics. The profiles are qualitatively similar to the channel flow data of Fabre et al. (1987). In this operating condition, the deposit (not shown) is restricted to the regions which are wetted by the liquid; the shear removal is very small, and the interfacial waves observed in the single-phase cases have a negligibly small amplitude here.

In this type of two-phase flow, the deposition is heavily dependent on the wall wetted area and local heat transfer along the perimeter. These are governed mainly by the velocity and holdup of the gas and liquid, which in turn depend on the flowrates and thermophysical properties of both phases. The interaction between these factors is not trivial to model, and a detailed simulation is a useful tool in order to make predictions for specific operating conditions.

4.4.3 Single-phase flow in an elbow

The effect of pipe geometry on the characteristics of deposit formation was also investigated with the addition of an elbow of radius of curvature $R_b = 5D$ to the single-phase pipe flow case described previously, as shown in Fig. 4.3; the rest of the parameters remain unchanged from those listed in Tab. 4.2. This case is chosen as a prototypical example of a complex geometry that illustrates the versatility of the model we have developed in the present work.

The deposit thickness profile is shown in Fig. 4.11a. The simulation reproduces qualitatively the effect observed by Makwashi (2020): the deposition is enhanced on the inside wall of the bend, due to the low shear stress in that region, a specific characteristic of the deposition in bends which is not modelled in industry-leading one-dimensional pipe simulators (Makwashi, 2020). The shear stress applied to the deposit is shown in Fig. 4.11b and reinforces this observation: high stresses are observed in most of the elbow region, except for the inner part of the bend. Figure 4.12 also shows a comparison between deposit thickness for the straight pipe and the

bend. After 1.5 h the average thickness is around 60% higher for the bend compared to the straight pipe. This further underscores the fact that bends are more susceptible to deposition than straight pipes primarily due to the stress distribution profile highlighted above.

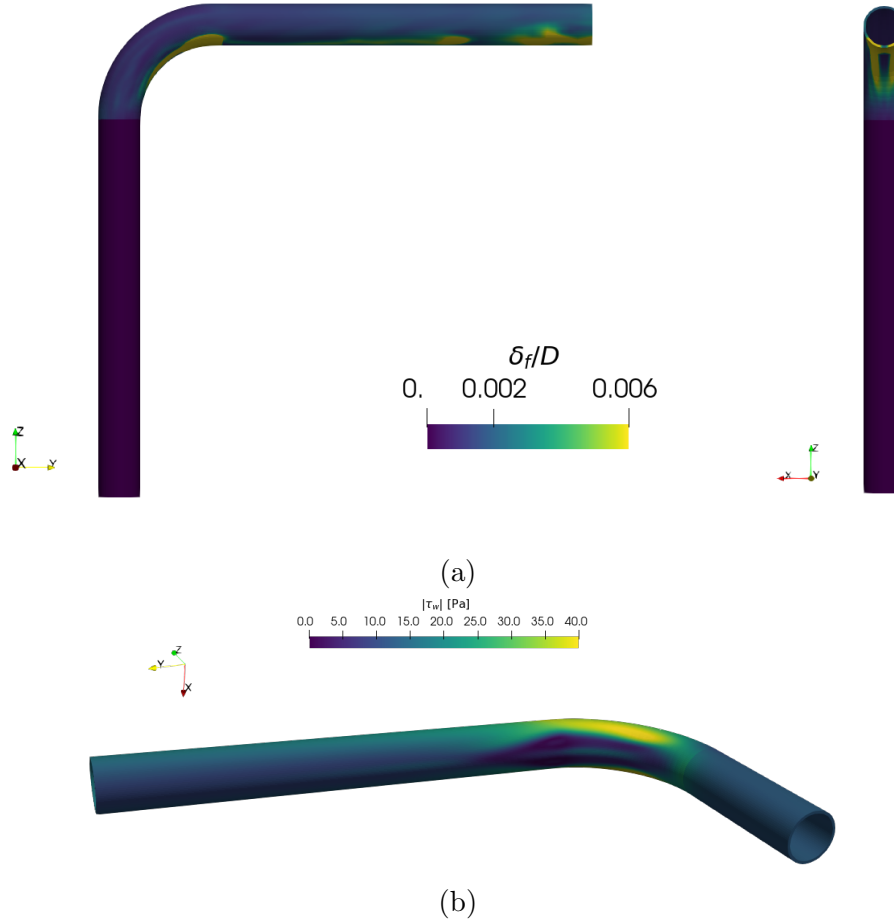


Figure 4.11: Simulation of single-phase flow with deposition in an elbow of radius of curvature $R_b = 5D$: deposit thickness (a), and shear stress, (b), with $\dot{m} = 20 \text{ kg min}^{-1}$ and the same parameters as in Tab. 4.2.

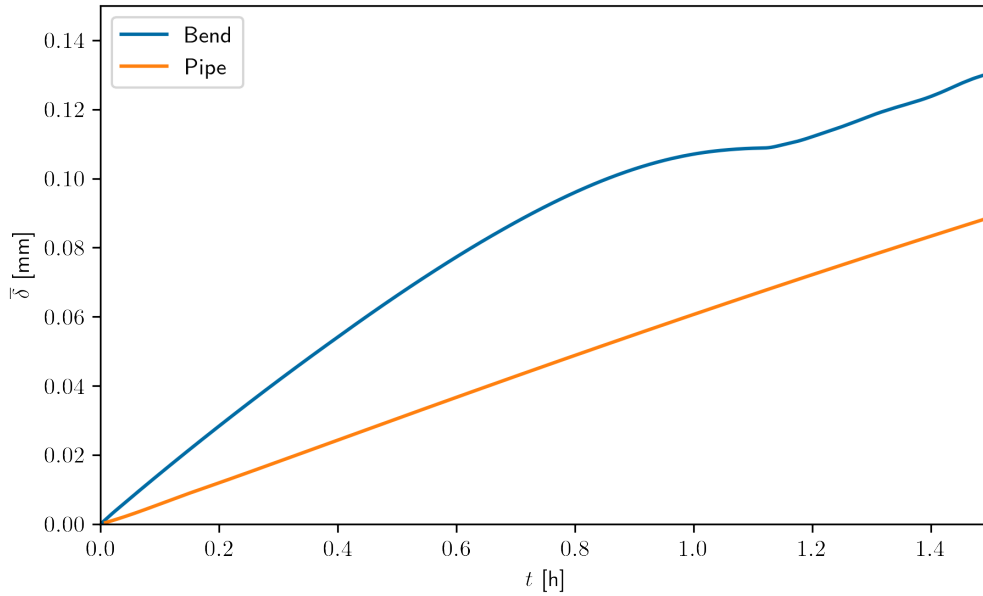


Figure 4.12: Average thickness over time for a straight pipe and bend with $R_b = 5D$, for $\dot{m} = 20 \text{ kg min}^{-1}$ and the same parameters as in Tab. 4.2.

4.5 Conclusions

We have created an efficient model to simulate single- and two-phase flows in arbitrary geometries along with the formation of wall deposits. This versatile model couples equations of mass, momentum, and energy conservation in the bulk to those in the deposit, which is taken to be a thin film region. The model, which is implemented within the open-source environment OpenFOAM, accounts for heat and mass transfer between the deposit and the bulk as well as turbulence in the bulk phase; deposit ageing is also taken into account. The predictions of the thin film model are compared to those obtained from a volume-of-fluid (VoF)-based model data yielding good agreement. It is worth highlighting that the thin film model is significantly more efficient than its interface-capturing VoF counterpart.

The thin film model results were validated against data generated from single-phase and two-phase stratified flow experiments in terms of temporal evolution of the deposit thickness. Very good agreement is obtained over time scales of practical relevance by adjusting the rheological characteristics the deposit using a similar approach to that followed by Magnini and Matar, 2019. Results are also obtained for single-phase flow in an elbow geometry which demonstrate that the deposition is enhanced in elbows relative to straight pipes due to the lower shear stress

on the inner region of the bend. These results further illustrate the versatility of the model in being able to handle complex flow geometries.

The detailed local information provided by the thin film model can be used to obtain insights into fundamental phenomena, e.g., wave propagation in the deposit, or applied engineering information, e.g., deposition in pipe fittings. These, in turn, could be used for design and optimization of process equipment characterised by complex geometries which is beyond the capability of simple low-dimensional models.

Chapter 5

Deposition with mechanistic formulation

5.1 Introduction

Despite the usefulness of detailed computational fluid dynamics (CFD) simulations for the understanding of fundamental phenomena and specific design considerations, in many engineering applications, the computational cost of these CFD analyses is prohibitive and the main tools are based on simplified models, utilizing mechanistic insights or data-driven approaches. A more practically implementable mechanistic model for gas-liquid pipe flow with heat and mass transfer will be presented in this chapter with all the relevant conservation equations and closure relations. A specific sub-model for wax deposition will also be discussed. Finally, validation will be performed with experimental data of hydrodynamic quantities for steady and transient flows and deposit thickness measurements. The simulation results will be utilized for the creation of a surrogate model for deposit thickness under conditions of gas-liquid flow, demonstrating a possible technique for design and parameter exploration of operating conditions.

The rest of this chapter is organised as follows. In Section 5.2, we present details of the equations governing the flow, heat transfer, wax deposition and removal, ageing, and flow regime

transitions. Concise descriptions of the numerical method used to carry out the computations, and of the technique used to generate surrogate models, are also provided in this section. In Sec. 5.3, we provide a discussion of our results which include detailed comparisons against experimental data. Finally, concluding remarks are provided in Sec. 5.4.

5.2 Problem formulation

The model proposed in this chapter is based on a two-fluid formulation with a unit-cell, such as that presented in the studies of De Henau (1992), Bendiksen and Maines (1991), and Bendiksen, Malnes, et al. (1996). The main equations are presented next.

5.2.1 Main equations

Assuming a one-dimensional flow in the x -direction, for a mass concentration $Y_{i,k}$ of component i in phase k , the conservation equation has the following form:

$$\frac{\partial \rho_k \alpha_k Y_{i,k}}{\partial t} + \frac{1}{A} \frac{\partial}{\partial x} (\rho_k A \alpha_k Y_{j,k} U_k) = \sum_{j \neq k} \psi_{i,jk} \quad (5.1)$$

where ρ_k , α_k , and U_k are the density, volume fraction, and velocity of phase k , respectively, A is the cross-sectional area, t denotes time, and $\psi_{i,jk}$ is the mass transfer of Y_i from phase j to phase k . For each phase k ($= L, G, D$, liquid, gas, or deposit), therefore, the following mass conservation equation is valid:

$$\frac{\partial \rho_k \alpha_k}{\partial t} + \frac{1}{A} \frac{\partial}{\partial x} (\rho_k A \alpha_k U_k) = \sum_{j \neq k} \psi_{jk} \quad (5.2)$$

where ψ_{jk} is the mass transfer from phase j to phase k . The equations for each phase can be combined into a continuity equation for the mixture:

$$\left[\sum_k \alpha_k \beta_{T,k} \right] \frac{\partial p}{\partial t} = \sum_k \frac{1}{\rho_k A} \frac{\partial}{\partial x} (\rho_k A \alpha_k U_k) + \sum_k \sum_{j \neq k} \frac{1}{\rho_k} \psi_{jk} \quad (5.3)$$

where p is the pressure and $\beta_{T,k}$ denote the compressibility of phase k .

Similarly, the momentum conservation equation for each phase is given by:

$$\begin{aligned} \frac{\partial \rho_k \alpha_k U_k}{\partial t} + \frac{1}{A} \frac{\partial}{\partial x} (\rho_k A \alpha_k U_k^2) = & -g \rho_k \alpha_k \sin(\phi) - \alpha_k \frac{\partial p}{\partial x} \\ & - F_{w,k} + \sum_{j \neq k} F_{j,k} + \sum_{j \neq k} \psi_{jk} U_{\psi,jk} \end{aligned} \quad (5.4)$$

where g is the gravity acceleration, ϕ is the inclination, $F_{w,k}$ is the momentum transfer between the phase k and the wall, and $F_{j,k}$ is the momentum transfer from phase j to phase k .

An energy equation is also formulated for the mixture:

$$\begin{aligned} \frac{\partial}{\partial t} \left[\sum_k \rho_k \alpha_k \left(e_k + \frac{1}{2} U_k^2 + gz \right) \right] + \frac{\partial}{\partial x} \left[\sum_k \rho_k \alpha_k U_k \left(e_k + \frac{p}{\rho_k} + \frac{1}{2} U_k^2 + gz \right) \right] \\ = h_S + q_{w,m} \end{aligned} \quad (5.5)$$

where the terms h_S and $q_{w,m}$ represent sources of enthalpy and heat transfer through the wall, respectively, and the enthalpy of phase k is given by

$$e_k = \int_{T_{\text{ref}}}^{T_k} c_{v,k}(T) dT + e_{k,\text{ref}} \quad (5.6)$$

in which T_k and T_{ref} denote the temperature of phase k and a reference temperature, respectively, for which the corresponding enthalpy is $e_{k,\text{ref}}$, $c_{v,k}$ is the heat capacity for phase k , and z denotes the elevation.

5.2.2 Gas-liquid unit cell model

The unit-cell model (Dukler and Hubbard, 1975) for gas-liquid pipe flow has been the object of numerous studies over several decades (Nicholson et al., 1978; Taitel and Barnea, 1990; Bendiksen, Malnes, et al., 1996; Cook and Behnia, 2000). The formulation presented here is based on the work of Zhang, Wang, et al. (2003) and Orell (2005). We consider that each

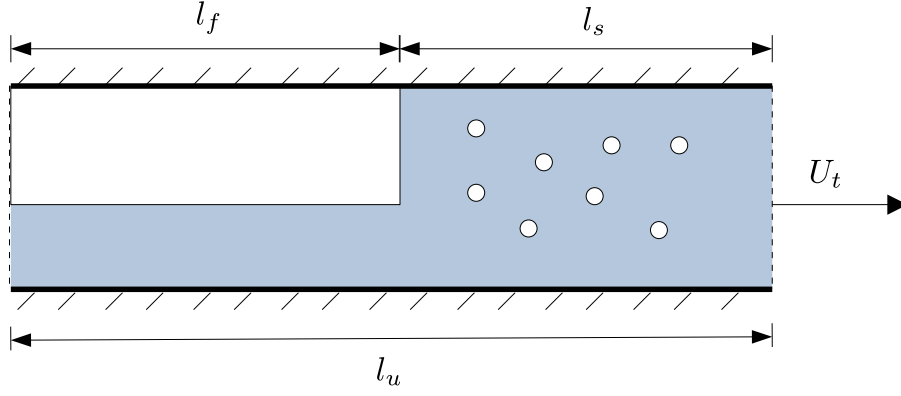


Figure 5.1: Schematic diagram of the slug unit cell. Here, l_u , l_f , and l_s represent the lengths of the unit, the film and slug regions, respectively, and U_t is the translation velocity.

computational point contains a sequence of identical cells that consist of a slug and a film region translating with velocity U_t (see Fig. 5.1). The subscripts f , s , b , and u are used respectively to designate the film, slug, bubble, and unit-cell. Importantly, the model can also describe stratified/annular flow, by assuming that the length of the slug region is zero, or bubbly flow, by assuming that for the film region instead.

A mass balance on the liquid phase in the unit cell yields:

$$U_{SL} = U_{Ls}\alpha_{Ls}(1 - l_f^*) + U_f\alpha_f l_f^* \quad (5.7)$$

where $l_f^* = l_f/l_u$ and l_f and l_u are defined in Fig. 5.1, while another mass balance on the gas phase gives

$$U_{SG} = U_{Gs}(1 - \alpha_{Ls})(1 - l_f^*) + U_f(1 - \alpha_f)l_f^* \quad (5.8)$$

A similar mass balance, in a stationary frame of reference, leads to the following expression:

$$(U_t - U_f)\alpha_f = (U_t - U_{Ls})\alpha_{Ls} \quad (5.9)$$

Assuming that there may be slip between the phases in the slug, the velocity of the gas and

liquid phases are given, respectively, by:

$$U_{Gs} = K_{\text{slip}} \frac{U_m + (1 - \alpha_s)U_{0s}}{1 + \alpha_s(K_{\text{slip}} - 1)} \quad (5.10)$$

$$U_{Ls} = \frac{U_m - \alpha_s K_{\text{slip}} U_{0s}}{1 + \alpha_s(K_{\text{slip}} - 1)} \quad (5.11)$$

where the mixture velocity U_m is:

$$U_m = U_{SL} + U_{SG} \quad (5.12)$$

in which U_{SG} and U_{SL} correspond to the gas and liquid superficial velocities, respectively.

Following Bendiksen, Malnes, et al. (1996), the slip velocity U_{0s} and coefficient K_{slip} are:

$$U_{0s} = 1.18 \left[\frac{g\sigma(\rho_L - \rho_G)}{\rho_L^2} \right]^{1/4} \sqrt{(1 - \alpha_s)|\sin \phi|} \quad (5.13)$$

$$K_{\text{slip}} = \frac{1 - \alpha_s}{0.95 - \alpha_s} \quad (5.14)$$

in which σ is the interfacial tension.

For the slug translational velocity U_t , the following expression is used Nicklin et al. (1962) and Bendiksen (1984):

$$U_t = C_{t,0}U_m + C_{t,1}\sqrt{gD} \quad (5.15)$$

where D is the diameter, and the coefficients $C_{t,0}$ and $C_{t,1}$, following Bendiksen (1984), are given by:

$$C_{t,0} = \begin{cases} 1.05, & Fr < 3.5 \\ 1.2, & Fr \geq 3.5 \end{cases} \quad (5.16)$$

and

$$C_{t,1} = \begin{cases} 0.54, & Fr < 3.5 \\ 0, & Fr \geq 3.5 \end{cases} \quad (5.17)$$

where $Fr = U_{Ls}/\sqrt{gD}$ is the Froude number.

The mixture velocity U_m is given by:

$$U_m = U_{SL} + U_{SG} \quad (5.18)$$

The liquid holdup in the slug is given by the correlation of Andreussi and Bendiksen (1989) as shown in Andreussi, Minervini, et al. (1993):

$$\alpha_{Ls} = 1 - \frac{U_m/\sqrt{gD} - F_0}{U_m/\sqrt{gD} + 2400Bo^{-3/4}} \quad (5.19)$$

where we define the Bond number Bo as:

$$Bo = \frac{(\rho_L - \rho_G)gD^2}{\sigma} \quad (5.20)$$

and the factor F_0 is expressed by

$$F_0 = 2.6 \left[1 - 2 \left(\frac{D_0}{D} \right)^2 \right] \quad (5.21)$$

with $D_0 = 0.025$ m.

A momentum balance on the film region leads to:

$$\tau_f S_f A_G - \tau_G S_G A_L - \tau_i S_i A + (\rho_L - \rho_G)g \sin \phi A_G A_L = 0 \quad (5.22)$$

Here, τ_f , τ_G , and τ_i are the shear stresses of the liquid and gas phase with the wall, and on the interface, respectively, given by

$$\tau_f = \frac{1}{2} f_f \rho_L U_f |U_f| \quad (5.23)$$

$$\tau_G = \frac{1}{2} f_G \rho_G U_b |U_b| \quad (5.24)$$

$$\tau_i = \frac{1}{2} f_i \rho_G (U_b - U_f) |U_b - U_f| \quad (5.25)$$

The friction factor between the phases and the wall is:

$$f_k = \begin{cases} 0.0055 \left[1 + \left(2 \times 10^4 \cdot \frac{\epsilon}{D} + \frac{10^6}{Re_k} \right)^{\frac{1}{3}} \right], & Re_k \geq 2000 \\ 16/Re_k, & Re_k < 2000 \end{cases} \quad (5.26)$$

in which ϵ is the wall roughness. The interfacial friction factor is given by the expression of Andritsos and Hanratty (1987):

$$\frac{f_i}{f_G} = 1 + 15 \left(\frac{\delta_{fL}}{D} \right)^{0.5} \left(\frac{U_b}{U_{b,t}} - 1 \right) \quad (5.27)$$

with

$$U_{b,t} = 5 \text{ m s}^{-1} \sqrt{\frac{\rho_{G0}}{\rho_G}} \quad (5.28)$$

where ρ_{G0} is the gas density at atmospheric pressure, and δ_{fL} is the height of the liquid film.

The slug density and Reynolds number are given by:

$$\rho_s = \alpha_s \rho_G + (1 - \alpha_s) \rho_L \quad (5.29)$$

$$Re_s = \frac{\rho_s D U_{Ls}}{\mu_s} \quad (5.30)$$

where μ is the dynamic viscosity. The slug viscosity is given by Einstein's equation:

$$\mu_s = \mu_L (1 + 2.5 \alpha_s) \quad (5.31)$$

We assume that the film geometry can be described by the double-circle geometry proposed by

Chen et al. (1997), or an annular geometry, leading to:

$$S_i = D\theta_i \left(\xi_s \frac{\sin \theta}{\sin \theta_i} + (1 - \xi_s) \sqrt{1 - \alpha_f} \right) \quad (5.32)$$

$$S_f = D\theta \quad (5.33)$$

$$S_G = D(\pi - \theta) \quad (5.34)$$

$$S = D\pi \quad (5.35)$$

$$A_f = A\alpha_f \quad (5.36)$$

$$A_G = A(1 - \alpha_f) \quad (5.37)$$

where S is the cross-section perimeters, θ_i is the wetted wall fraction angle, and ξ_s is an indicator function that has the value of unity for a stratified geometry and zero for an annular film.

Although the value of θ_i can be obtained by the following implicit equation, from geometric considerations,

$$\theta_i = \left(\frac{\sin \theta_i}{\sin \theta} \right)^2 \left(\theta + \frac{\sin^2 \theta}{\tan \theta_i} - \frac{\sin 2\theta}{2} - \pi\alpha_f \right) \quad (5.38)$$

instead, we propose the following approximation:

$$\theta_i \approx 1.6 \arctan \left(\frac{\theta}{\sin^2 \theta} - \frac{1}{\tan \theta} - \frac{\pi\alpha_f}{\sin^2 \theta} \right) \quad (5.39)$$

Fig. 5.2 shows the comparison between the exact and approximate expression proposed for θ_i . The comparison is limited to $\theta < 0.9\pi$, since after this threshold an annular film is assumed instead.

The wetted wall fraction angle is given by the correlation of Grolman and Fortuin (1997)

$$\frac{\theta}{\pi} = \frac{\theta_0}{\pi} \left(\frac{\sigma_{\text{water}}}{\sigma} \right)^{0.15} + \frac{\rho_G}{\rho_L - \rho_G \cos \phi} \frac{1}{\left(\frac{\rho_L U_{SL}^2 D}{\sigma} \right)^{0.25}} \left(\frac{U_{SG}^2}{(1 - \varepsilon_L)^2 g D} \right)^{0.8} \quad (5.40)$$

where θ_0 is the flat wetted angle given by the explicit expression Biberg (1999):

$$\theta_0 = \pi\alpha_f + \left(\frac{3\pi}{2} \right)^{(1/3)} \left[1 - 2\alpha_f + \alpha_f^{(1/3)} - (1 - \alpha_f)^{(1/3)} \right]. \quad (5.41)$$

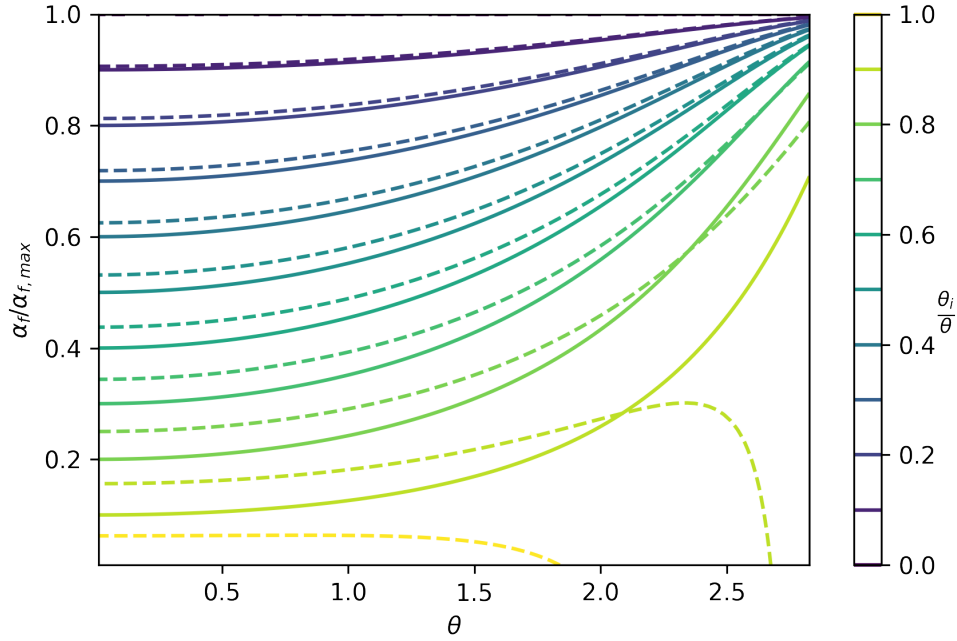


Figure 5.2: Comparison between exact (continuous lines) and approximate (dashed lines) expressions for the wetted angle θ_i .

Equations (5.7), (5.8), (5.9), and (5.22) must be solved simultaneously for U_f , U_b , α_f and l_f^* , and the pressure drop is calculated as:

$$\frac{dp}{dx} = 2 \frac{f_s}{D} \rho_s U_{Ls}^2 (1 - l_f^*) + \frac{\tau_f S_f - \tau_i S_i}{A_f} l_f^* \quad (5.42)$$

Based on the slug properties obtained, the source terms in the momentum equation, Eq. (5.4), can be linearized as:

$$F_{w,G} = F_{GG} U_G + F_{GL} U_L + C_G \quad (5.43)$$

$$F_{w,L} = F_{LL} U_L + F_{LG} U_G + C_L \quad (5.44)$$

$$F_{G,L} = \alpha F_{w,L} - (1 - \alpha) F_{w,G} - \alpha(1 - \alpha) g(\rho_L - \rho_G) \sin \phi \quad (5.45)$$

where the forms of the coefficients (F_{GG} , F_{GL} , F_{LL} , F_{LG} , C_G , C_L , $F_{w,L}$ and $F_{w,G}$) are presented in Bendiksen, Malnes, et al. (1996).

5.2.3 Flow pattern transition criteria

The definition of the gas-liquid flow patterns can vary considerably between different works in the literature. Here, we adopt the division of bubbly, annular, stratified, and intermittent, although most of the discussion will be focused on the latter two regimes. The criteria for existence of bubbly flow is taken to be (Bendiksen and Maines, 1991):

$$\alpha_s > \frac{U_{SG}}{U_{Gs}} \quad (5.46)$$

The film region is treated as an annular flow ($\xi_s = 0$) when the wetted fraction is greater than 90% of the perimeter (Zhang, Wang, et al., 2003):

$$\frac{\theta}{\pi} > 0.9 \quad (5.47)$$

The flow is considered to be in the intermittent regime when the following two conditions are satisfied (Bendiksen and Espedal, 1992):

$$U_b|_{\text{stratified}} > U_{b,\text{crit}}|_{\text{stratified}} \quad (5.48)$$

and

$$\alpha|_{\text{slug}} > \alpha|_{\text{stratified}} \quad (5.49)$$

where, following Taitel and Dukler (1976):

$$U_{b,\text{crit}} = (1 - h^*) \sqrt{\frac{(\rho_L - \rho_G)}{\rho_G} g \cos(\phi) D \frac{(1 - \alpha_{Lb})}{\sqrt{1 - (2h^* - 1)^2}}} \quad (5.50)$$

and h^* is expressed by

$$h^* = \frac{1 - \cos \theta_0}{2} \quad (5.51)$$

5.2.4 Heat transfer

The heat transfer model for the unit cell is based on the one proposed by Meziou et al. (2019).

The average heat transfer coefficient over the slug unit is:

$$h_u = l_f^* h_s + (1 - l_f^*) h_f \quad (5.52)$$

This expression is applicable to constant temperature boundary conditions for both horizontal and vertical flows, as derived in Dong et al. (2021) and Dong et al. (2022).

Here, the heat transfer coefficient h_s is given by:

$$h_s = \frac{Nu_s k_s}{D} \quad (5.53)$$

while the heat transfer coefficient in the film region is calculated as (Kaminsky, 1999):

$$h_f = \frac{k_L \sqrt{\rho_L}}{10 \mu_L} \left[S_f D \left(\frac{dp}{dx} \right)_f \right]^{1/2} \quad (5.54)$$

The Nusselt number for turbulent flow in the slug region, Nu_s , is given by the correlation of Gnielinski (1975):

$$Nu_s = \frac{\left(\frac{f_s}{8}\right) (Re_s - 1,000) Pr_s}{1.07 + 12.7 \sqrt{\frac{f_s}{8}} (Pr_s^{2/3} - 1)} \quad (5.55)$$

where the Prandtl number Pr_s is defined by:

$$Pr_s = \frac{\mu_L c_{ps}}{k_s} \quad (5.56)$$

and the slug average heat capacity and thermal conductivity are given by:

$$c_{ps} = \alpha_s \frac{\rho_G}{\rho_s} c_{pG} + (1 - \alpha_s) \frac{\rho_L}{\rho_s} c_{pL} \quad (5.57)$$

$$k_s = 0.25 \left\{ (2 - 3\alpha_{Ls}) k_G + (3\alpha_{Ls} - 1) k_L + \sqrt{[(2 - 3\alpha_{Ls}) k_G + (3\alpha_{Ls} - 1) k_L]^2 + 8k_L k_G} \right\} \quad (5.58)$$

where c_{pG} and c_{pL} , and k_G and k_L denote the heat capacities and thermal conductivities of the gas and liquid phases, respectively.

For laminar flow, Meziou et al. (2019) suggest:

$$Nu_s = \begin{cases} 1.86 \left[\left(\frac{D}{L} \right) Re_s Pr_s \right]^{1/3} \left(\frac{\mu_{L,b}}{\mu_{L,w}} \right)^{0.14}, & \text{if } Gz_s \leq 20 \\ 3.657 + \frac{0.0668 \left(\frac{D}{L} \right) Re_s Pr_s}{1 + 0.04 \left[\left(\frac{D}{L} \right) Re_s Pr_s \right]^{2/3}}, & \text{if } Gz_s \leq 20 \text{ and } Pr > 5 \\ 3.657, & \text{if } Gz_s \leq 20 \text{ and } Pr < 5 \text{ and } T_w = \text{constant} \\ 4.364, & \text{else} \end{cases} \quad (5.59)$$

where

$$Gz_s = \frac{Re_s Pr_s}{L/D} \quad (5.60)$$

The heat transfer coefficients described in this section, h_u , h_s and h_f , are used for computation of the mass transfer (through the temperature and temperature gradient at the deposit interface), as well as for the calculation of the overall heat transfer (Sec. 5.2.5)

5.2.5 Wax deposition

It is assumed here that the wax is composed of a single component, denoted by the subscript w . Its mass fraction in the liquid and deposit phases, $Y_{w,L}$ and $Y_{w,D}$, are given by Eq. (5.1), while the gas phase is considered to be free of wax.

The main mechanisms of mass transfer between the liquid and deposit in two-phase gas-liquid flow are represented in Fig. 5.3. In slug flow conditions, the presence of a thin film at the top of the pipe in the bubble region has been shown to have a significant effect on heat transfer (Fershtman et al., 2019) and wax deposition (Rittirong, 2014). The total mass and wax mass transfers are then given by a combination of the contributions of the slug, bubble and film

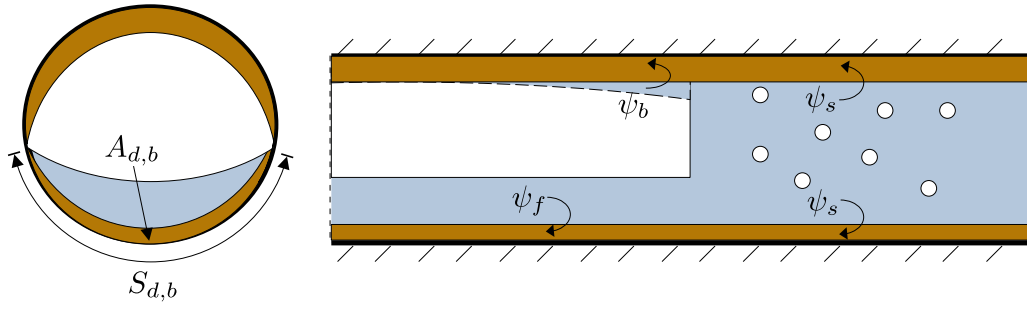


Figure 5.3: Schematic diagram of the deposition mechanisms in two-phase flow.

zones:

$$\psi_{LD} = K [(1 - l_f^*)\psi_s + l_f^*(\psi_b + \psi_f)] \quad (5.61)$$

$$\psi_{w,LD} = K [(1 - l_f^*)\psi_{w,s} + l_f^*(\psi_{w,f} + \psi_{w,b})] \quad (5.62)$$

The deposition rate ψ in each region is treated essentially in the same way, although the wetted area, temperature gradient and shear stresses are adjusted in the calculation of the respective terms. The multiplicative factor K was included to take into account non-linear interactions between film and slug, in the slug flow cases; it is set to unity otherwise. The source term ψ_{LD} is used in the mass transport Eqs. (5.2) and (5.3), and $\psi_{w,LD}$, in the conservation equation given by Eq. (5.1). For the momentum equation of the deposit, a sink term is set such that the deposit remains immobile; alternatively, a creeping flow of the deposit could also be considered.

For slug flow, the deposition layer at the bottom of the pipe has a different thickness from the one at the top. One may assume that the film wetted perimeter delineates the division between the two zones, and track the fraction of the deposition that is concentrated in the lower area (see Fig. 5.3):

$$\dot{A}_{D,b} = \frac{K [S(1 - l_f^*)\psi_s + l_f^*\psi_f]}{\psi_{LD}} A \quad (5.63)$$

$$S_{D,b} = S_f \quad (5.64)$$

Assuming that the mass diffusion controls the process of deposition, the mass transfer rate of

wax between liquid and deposit can be written as (Svendsen, 1993):

$$\psi_{w,LD}^{\text{deposition}} = \Gamma_{wo} \left. \frac{dC_w}{dT} \right|_i \left. \frac{dT}{dy} \right|_{i,L} \frac{A_p}{V_p} \quad (5.65)$$

where y is the direction normal to the interface, A_p is the interface area and V_p is the volume. The molecular diffusivity coefficient can be calculated, for example, with a correlation such as that provided by (Hayduk and Minhas, 1982):

$$\Gamma_{wo} = 1.33 \times 10^{-11} \text{ T}^{1.47} (1000\mu_o)^\gamma V_a^{-0.71} \quad (5.66)$$

$$V_a = 1000 \frac{M}{\rho_o} \quad (5.67)$$

$$\gamma = \frac{10.2}{V_a} - 0.791 \quad (5.68)$$

The concentration gradient at the interface should be between the limiting values of a process in thermodynamic equilibrium or one with independent heat and mass transfer (Lee, 2008; Singh, Panacharoensawad, et al., 2017). For the former, the following applies:

$$\left. \frac{dC_w}{dT} \right|_i = \left. \frac{dC_w}{dT} \right|_{\text{eq}} \quad (5.69)$$

where the equilibrium precipitation curve can be obtained with the simplified two-component methodology of Svendsen (1993) or with a full multicomponent calculation with SP-Wax (Shahdi and Panacharoensawad, 2019). Here, we assume thermodynamic equilibrium throughout, although an independent heat and mass transfer process would also be compatible with the formulation. The wax phase equilibrium depends on the temperature of the interface, and both the deposition and ageing expressions depend on temperature gradients. Sections 5.2.5 and 5.2.5 will discuss the calculation of these values for the different regions of the unit cell.

The mechanism proposed by Singh, Venkatesan, et al. (2000) is also adopted in the calculations and the internal diffusion of wax particles in the deposit, responsible for the increase in wax

fraction over time, is given by:

$$\psi_{\text{diff}} = D_e \left. \frac{dC_w}{dT} \right|_i \left. \frac{dT}{dy} \right|_{i,D} \frac{A_p}{V_p} \quad (5.70)$$

where D_e is given by

$$D_e = \frac{D_m}{1 + \alpha_c^2 Y_{w,D}^2 / (1 - Y_{w,D})} \quad (5.71)$$

where $Y_{w,D}$ is the mass fraction of wax in the deposit, and the crystal aspect ratio α_c is (Singh, Venkatesan, et al., 2000):

$$\alpha_c = 1 + k_\alpha Y_{w,D} \quad (5.72)$$

with $k_\alpha = 1$ (Panacharoensawad, 2012). The total mass transfer between liquid and deposit phases is then given by:

$$\psi_{LD}^{\text{deposition}} = \frac{\psi_{w,LD}^{\text{deposition}} - \psi_{\text{diff}}}{Y_{w,D}} \quad (5.73)$$

Shear removal

The effect of shear removal may be taken into account by modifying the deposition rate with an empirical coefficient, similarly to Panacharoensawad (2012). Assuming that this coefficient is a function of shear stress and deposit properties, the following is valid:

$$\psi_i = F_i(\tau_w, \tau_y, \delta_d, \mu_L, \rho_L) \psi_{LD}^{\text{deposition}} \quad (5.74)$$

where the index $i = s, f, b$ represents a specific region of the unit cell and the yield stress τ_y is calculated with the correlation of Zhang, Huang, et al. (2021).

Assuming that the deposit thickness is uniform along the circumferential direction, the following relation between volumetric fraction and deposit thickness at the bottom is obtained:

$$\frac{\delta_d}{D} = \frac{1 - \sqrt{1 - K_b \alpha_D}}{2} \quad (5.75)$$

with $K_b = A_{d,b} S / (A S_{d,b})$. This thickness is also utilized in the calculation of the deposit's

thermal resistance.

The area and diameter of the cross section, utilized in the unit-cell model, are modified according to:

$$A = \frac{A_0}{(1 - \alpha_D)} \quad (5.76)$$

$$D = \frac{D_0}{\sqrt{1 - \alpha_D}} \quad (5.77)$$

with the subscript 0 indicating the initial values, for a clean pipe.

Heat transfer in bubble region

We present here an approach based on the one proposed by Sun et al. (2004) for calculation of the heat transfer in the bubble region. Coney (1974) integrated the wall-normal velocity profiles to obtain the following forms for the non-dimensional thickness b and velocity ω of the film as it drains:

$$\begin{aligned} (f_1 - 1) \omega \frac{dt}{db} - \frac{b^2}{2} \left(\frac{7}{10} - \frac{293}{630} \omega \right) \frac{d\omega}{db} &= \frac{b}{2} \omega \left(\frac{74\omega}{630} - \frac{3}{10} \right) \\ f_2 \frac{dt}{db} - \frac{7}{10} b \frac{d\omega}{db} &= \frac{7}{10} \omega - 1 \end{aligned} \quad (5.78)$$

The initial conditions, b_0 and ω_0 , represent non-dimensional thickness and velocity of the film as it leaves the slug region and enters the bubble region, and the integration time, $t_{\max}$, represents the time required for the film to cross the latter. These can be calculated based on the velocities and lengths of the different parts of the unit cell. We have solved the system (5.78) for the range of initial values and integration time that occur in the experimental conditions. From this, we determine the following approximations for the average non-dimensional thickness and

velocity, $\bar{b}$ and $\bar{\omega}$, respectively:

$$\begin{aligned}\bar{b} = & 0.140 + 0.192b_0 - 9.80 \times 10^{-4}t_{\max} \\ & + 4.49 \times 10^{-6}t_{\max}^2 - 0.0849\omega_0\end{aligned}\quad (5.79)$$

$$\begin{aligned}\bar{\omega} = & 0.00137 + 0.00173b_0 - 4.33 \times 10^{-5}t_{\max} \\ & + 3.06 \times 10^{-7}t_{\max}^2 - 6.07 \times 10^{-4}\omega_0\end{aligned}\quad (5.80)$$

Once $\bar{b}$ and $\bar{\omega}$ have been calculated, the film Reynolds number is given by:

$$Re_{fb} = \frac{4\delta_{fb}U_{fb}\rho_L}{\mu_L} \quad (5.81)$$

where δ_{fb} and U_{fb} are the film thickness and velocity, respectively.

The heat transfer coefficient h_b is:

$$h_b = \frac{C_{pL}(\rho_L\tau_{fb})^{0.5}}{T^+} \quad (5.82)$$

where the shear stress τ_{fb} is given by:

$$\tau_{fb} = \frac{1}{\rho_L} \left(\frac{\delta^+\rho_L\mu_L}{\delta_{fb}} \right)^2 \quad (5.83)$$

with the following expressions for T^+ and δ^+ :

$$T^+ = \begin{cases} \delta^+ Pr_L & \text{for } \delta^+ \leq 5 \\ \{Pr_L + \ln[1 + Pr_L(\delta^+/5 - 1)]\} & \text{for } 5 \leq \delta^+ \leq 30 \\ 5 \left\{ Pr_L + \ln[1 + 5Pr_L] + \frac{1}{2} \ln \frac{\delta^+}{30} \right\} & \text{for } \delta^+ > 30 \end{cases} \quad (5.84)$$

$$\delta^+ = \begin{cases} 0.7071 Re_{fb}^{0.5} & \text{for } Re_{fb} \leq 50 \\ 0.6323 Re_{fb}^{0.5286} & \text{for } 50 \leq Re_{fb} \leq 1483 \\ 0.0504 Re_{fb}^{0.875} & \text{for } Re_{fb} > 1483 \end{cases} \quad (5.85)$$

With the heat transfer coefficient h_b , the temperature gradient in the bubble region can be calculated.

Heat transfer across the deposit

The temperature gradients in the slug, film and bubble regions are given, respectively, by:

$$\left. \frac{dT_s}{dy} \right|_{i,L} = \frac{h_s}{k_o}(T - T_i) \quad (5.86)$$

$$\left. \frac{dT_f}{dy} \right|_{i,L} = \frac{h_f}{S_f k_o}(T - T_i) \quad (5.87)$$

$$\left. \frac{dT_b}{dy} \right|_{i,L} = \frac{h_b}{k_o}(T - T_i) \quad (5.88)$$

and the interface temperature is given by:

$$T_i = \frac{hTR_d + T_w}{hR_d + 1} \quad (5.89)$$

The heat transfer coefficients are obtained from Eqs. (5.53), (5.54) and (5.82).

The extra thermal resistance due to a layer of thickness δ_d of deposit is:

$$R_d = -\frac{2(1 - 2\delta_d/D) \log(1 - 2\delta_d/D)}{k_d D} \quad (5.90)$$

The temperature gradient across the deposit is:

$$\left. \frac{dT}{dy} \right|_{i,D} = \frac{1}{R_d}(T_i - T_w) \quad (5.91)$$

Finally, the heat transfer coefficient obtained for the gas-liquid flow can be corrected with the effect of the deposit using the following expression:

$$h_{\text{eff},d} = \frac{h_u}{1/h + R_d} \quad (5.92)$$

leading to the following heat transfer through the wall, in the energy equation Eq. (5.5):

$$q_{w,m} = h_{\text{eff},d}(T_w - T) \quad (5.93)$$

5.2.6 Numerical method

The numerical solution of the aforementioned equations is performed on a staggered grid, using a finite differences discretization. The advective terms are discretized with a upwind scheme, and an implicit Euler method is used for the transient components. Firstly, the subgrid model in Sec. 5.2.2 is used in each computational cell and the source term coefficients are calculated with Eq. (5.43). Equations (5.3) and (5.4) are then solved simultaneously for the pressure and phase velocities with a sparse supernodal LU factorization as implemented in Guennebaud, Jacob, et al. (2010). Next, Eqs. (5.2), (5.5), and (5.1) are solved sequentially with the tridiagonal matrix algorithm for the volume fractions, temperature and concentrations, respectively. This process is repeated until the normalized residuals in the mass and momentum conservation equations are lower than 1×10^{-6} ; following that, the time advances and the steps are repeated until the end of the simulation is reached. The time-step is prescribed with a maximum value of the Courant number, C_{max} . For the wax model, the precipitation curve is automatically obtained for the range of temperatures expected in the simulations with a module based on SP-Wax (Shahdi and Panacharoensawad, 2019) and cached to a file. During the simulations, the data are interpolated from the stored table.

5.2.7 Surrogate model

The methodology for development of the surrogate model follows the approach of Gonçalves et al. (2020). The base model receives a vector of inputs $\mathbf{p}$ (e.g. flowrates, diameter, fluid properties) and generates an output $f(\mathbf{p})$ (e.g. pressure drop, drag, heat/mass transfer coefficient), both of which are defined according to the problem of interest. The surrogate model is defined as a function $f^*(\mathbf{p})$ that aims to reproduce the original model results, based on a

limited number of samples. Here, a random forest is utilized for the regression of the data points, since it is a proven robust technique that can deal with discontinuities.

The output of a random forest is given by an average of the predictions of individual decision trees, which can be trained with the whole dataset or with random sub-samples of the available points. The technique can be used for regression or classification tasks, and can scale well to multiple dimensions.

The simulation conditions $\mathbf{p}_s$ to be run are picked with a greedy criterion (Wu et al., 2019):

$$\mathbf{p}_s = \operatorname{argmax}_{\mathbf{p}_i} d_{\mathbf{p}}(\mathbf{p}_i) d_f(\mathbf{p}_i) \quad (5.94)$$

where the distances in input and output spaces are given by:

$$d_{\mathbf{p}}(\mathbf{p}_i) = \min_j \|\mathbf{p}_i - \mathbf{p}_j\| \quad (5.95)$$

$$d_f(\mathbf{p}_i) = \min_j |f^*(\mathbf{p}_i) - f(\mathbf{p}_j)| \quad (5.96)$$

where the minimum values are calculated over the previous simulation conditions.

After each simulation is run, the surrogate model is updated and the sampling procedure is repeated, until the limit number of iterations has been reached.

5.3 Results

5.3.1 Validation of hydrodynamic model

The steady-state unit cell model was validated with a large database consisting of several experimental datasets from the open literature (Tab. 5.1). These experiments were performed with a variety of different fluids, in small and large diameter pipes, horizontal and vertical flow, and intermittent and stratified regimes. The comparison of experimental and predicted pressure drop values is presented in Figs. 5.6 and 5.4 for intermittent and stratified flows, respectively.

The model has a good performance for all databases, with most predictions being within $\pm 20\%$ of the actual measurements. The worst performance is observed for the high velocity cases of Reid et al. (1957), where Orell (2005) also observed larger deviations. In general, there is no clear systematic trend of under- or over-estimation of the pressure drop values. A flow pattern map predicted with the hydrodynamic model is also presented in Fig. 5.5. The boundaries are qualitatively very similar to the ones observed in the literature, e.g. Mandhane et al. (1974), Taitel and Dukler (1976), and Spedding and Spence (1993).

Table 5.1: Databases utilized for validation of the unit cell model

Reference	Flow pattern	Inclination
Reid et al. (1957)	Intermittent	Horizontal
Griffith and Wallis (1961)	Intermittent	Vertical
Akagawa et al. (1971)	Intermittent	Vertical
Stanislav et al. (1986)	Intermittent	Horizontal
Ottens et al. (2001)	Stratified	Horizontal
Marruaz et al. (2001)	Intermittent	Horizontal
Gonçalves, Baungartner, et al. (2018)	Intermittent	Horizontal
Bhagwat and Ghajar (2017) ($Re_{SL} = 10000$)	Intermittent	Horizontal

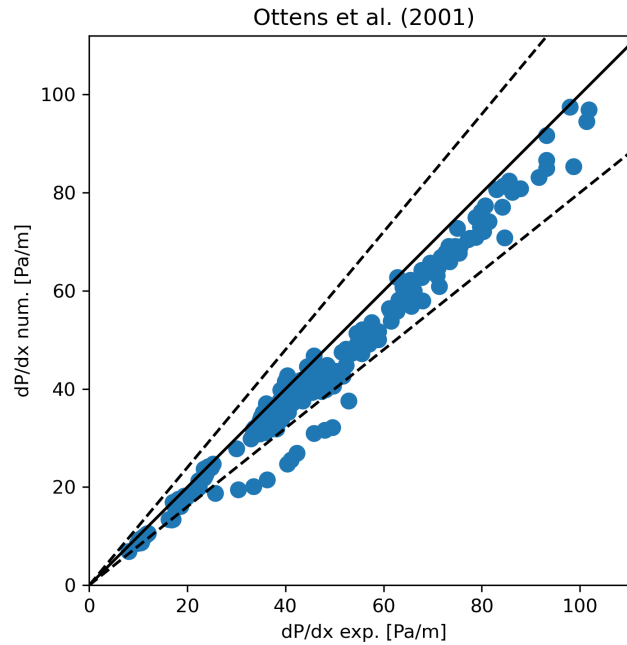


Figure 5.4: Comparison of the model predictions of the pressure drop against the experimental data of Ottens et al. [2001] for stratified flows. The data source is indicated in the panel and the dashed lines represent a $\pm 20\%$ error band.

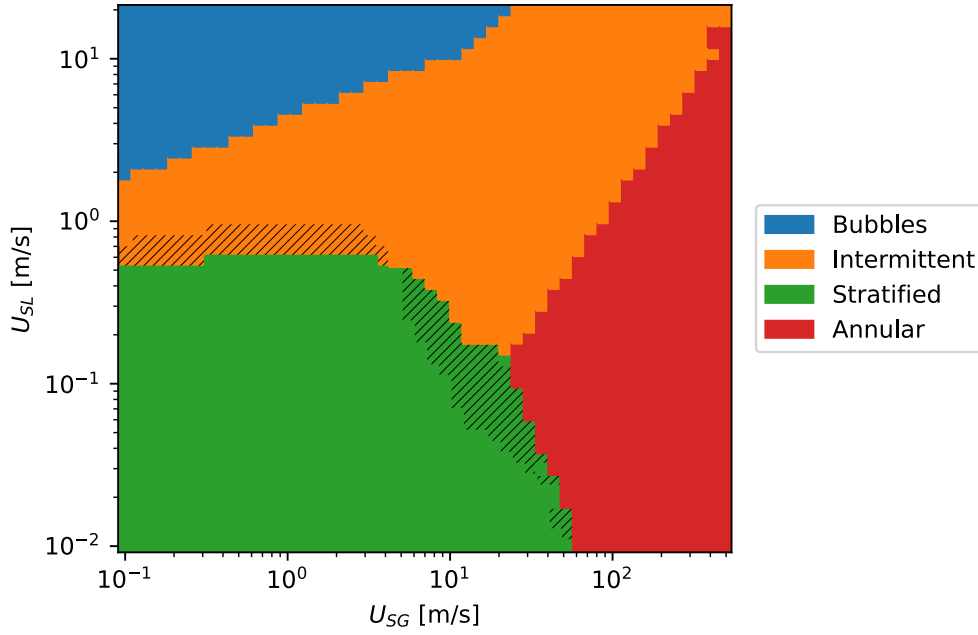


Figure 5.5: Flow pattern map for air-water flow in a horizontal pipe with diameter of 50 mm. The dashed region corresponds to parameters for which the use of a different interfacial friction factor (Petalas and Aziz, 1998) changes the classification.

The validation of the transient model utilized the experimental data obtained by Caussade et al. (1989). The test section consists of a 90 m pipe, with internal diameter of 53 mm. Initially, the flowrates are set such that $U_{SL} = 1.03 \text{ m s}^{-1}$ and $U_{SG} = 1.12 \text{ m s}^{-1}$, in the slug flow region. The superficial gas velocity is then increased with a step change of $\Delta U_{SG} = 0.36 \text{ m s}^{-1}$, followed by a similar step change down. The simulations here were performed with $C_{\max} = 1$ and $\Delta z = 1 \text{ m}$. The liquid flowrate at the outlet was measured, and is compared to the results of the numerical calculations in Fig. 5.7. The trend of the curve is very well predicted, both in terms of total amplitude of the perturbation and the response time. It is important to note, however, that the large frequency oscillations are not reproduced and the solution suffers from some numerical damping, which can be attributed to the use of a coarse grid and an averaged subgrid model. Next, we turn our attention to the validation of our numerical predictions in the presence of deposition.

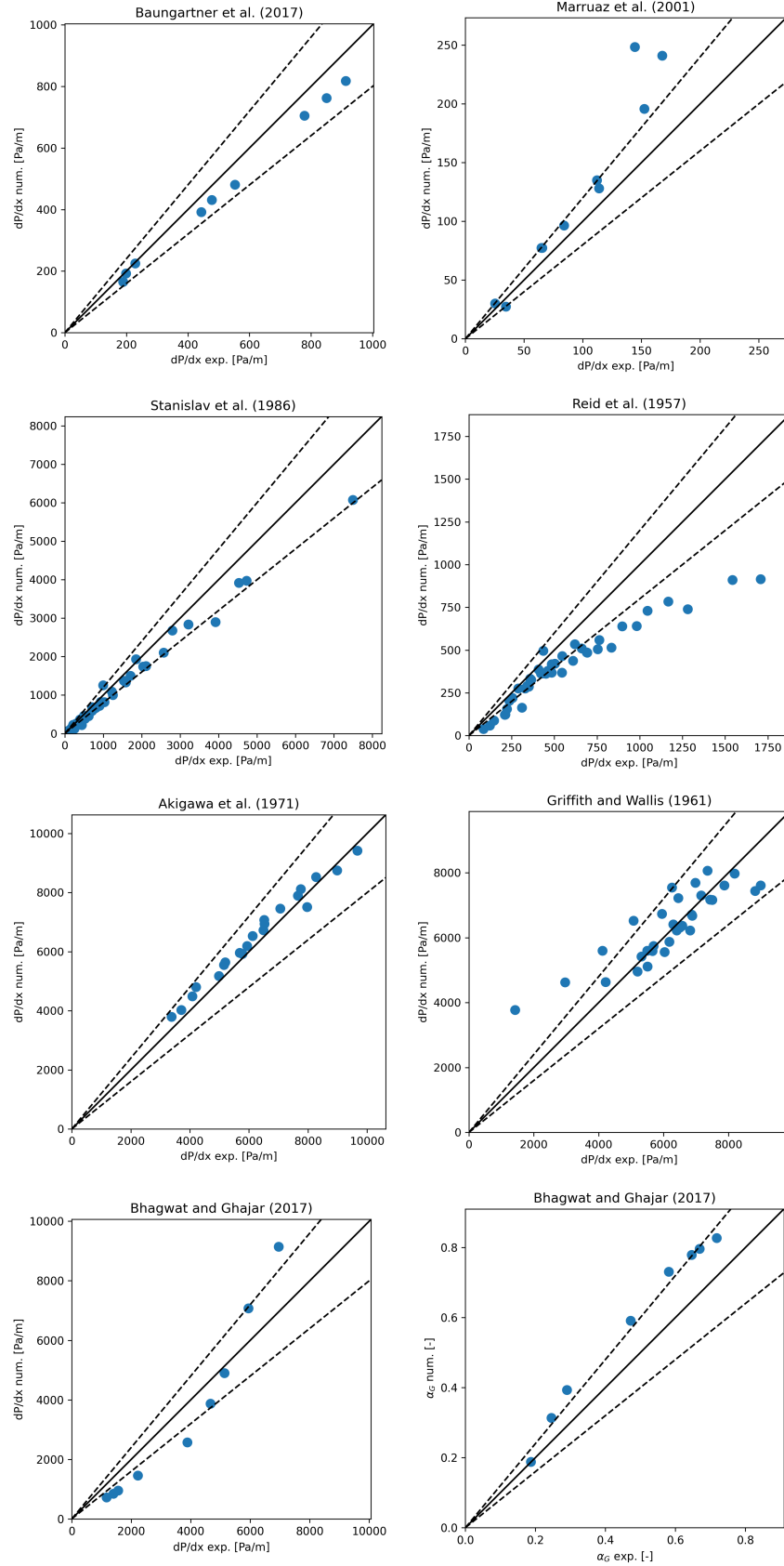


Figure 5.6: Comparison of the model predictions of the pressure drop against experimental data for intermittent flows. The data sources are indicated in the panels and the dashed lines represent a $\pm 20\%$ error band.

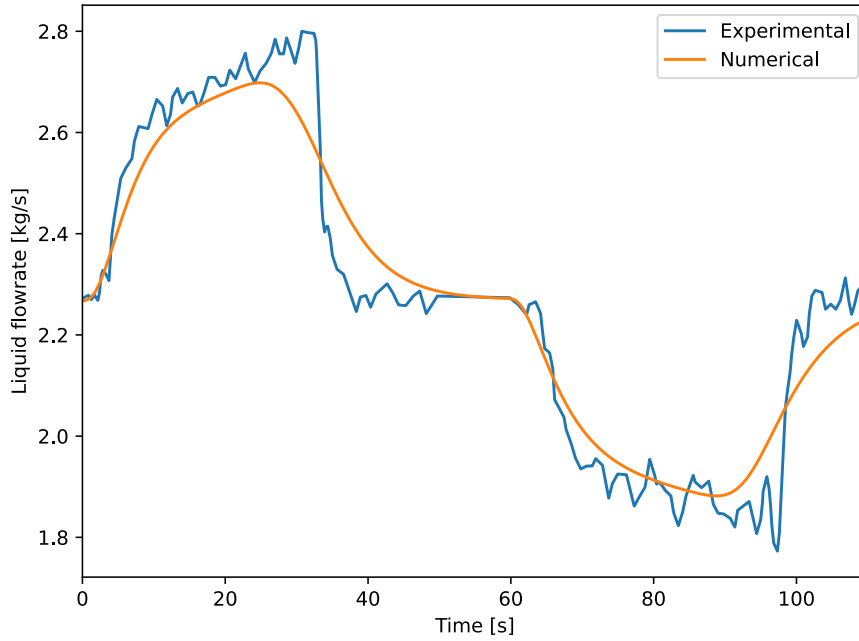


Figure 5.7: Liquid flowrate at the outlet of a 90 m pipe of internal diameter 53 mm used in the experimental study of Caussade et al., 1989 in which the superficial gas velocity was varied from $U_{SG} = 1.12 \text{ m s}^{-1}$ by step changes of $\Delta U_{SG} = 0.36 \text{ m s}^{-1}$ with the liquid superficial velocity set to $U_{SL} = 1.03 \text{ m s}^{-1}$. The experimental data are compared with the numerical predictions obtained by solving the transient model.

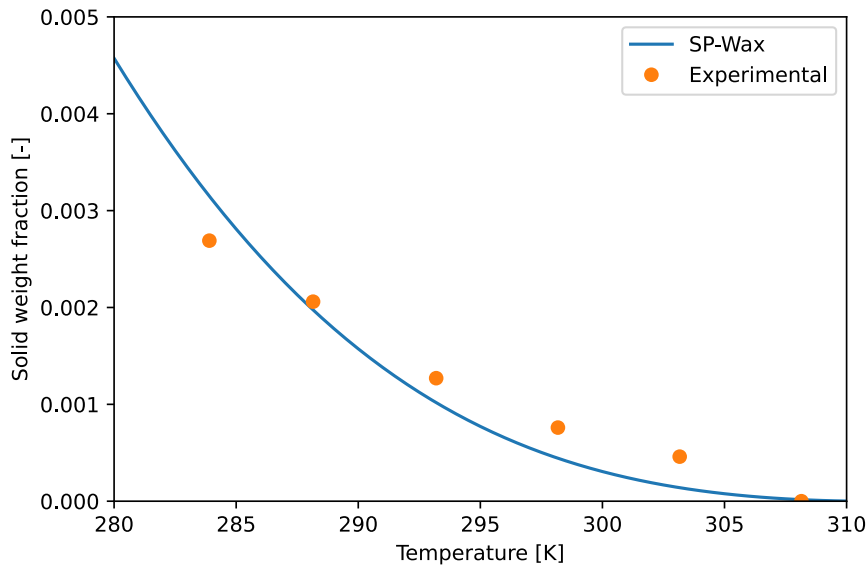


Figure 5.8: Solid weight fraction of Garden Banks condensate for the experiments of Rittirong (2014) and predictions by SP-Wax (Shahdi and Panacharoensawad, 2019).

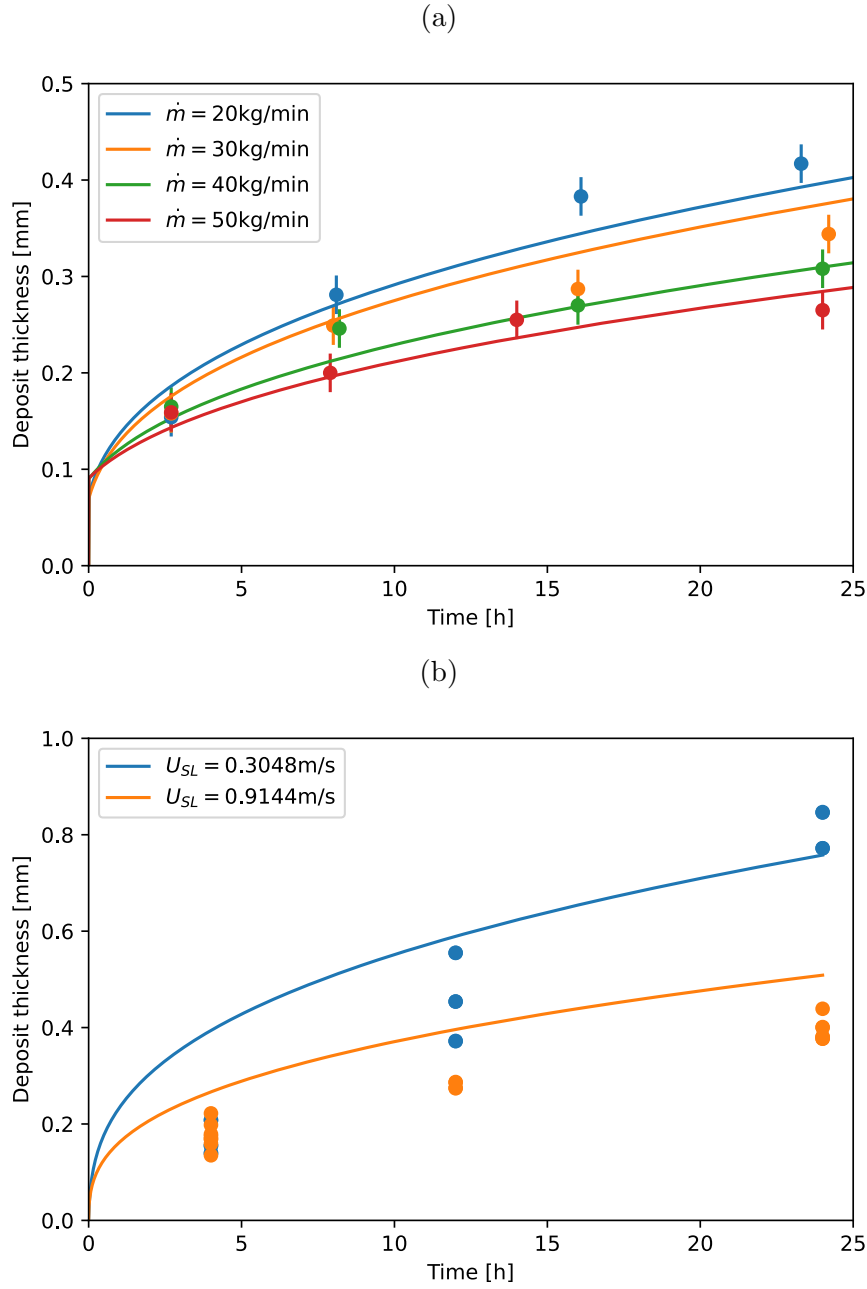


Figure 5.9: Variation of the deposit thickness with time obtained from the single-phase flow experiments of Singh, Panacharoensawad, et al. (2017), (a), and Rittirong et al. (2017), (b), and the numerical predictions represented by symbols and lines, respectively.

5.3.2 Validation of wax model

The accurate prediction of the precipitation curve (i.e. the equilibrium weight fraction of solids in the mixture, for given operating conditions) is essential for any kind of simulation of wax deposition. As such, for completeness, the validation performed by Shahdi and Panacharoensawad (2019) for the working fluid of Rittirong (2014) is reproduced here. The fraction of solid material as a function of temperature is shown Fig. 5.8. The agreement with the experimental data is excellent, and the wax appearance temperature (WAT) is estimated very well.

Single-phase flow

The first analysis of single phase deposition simulations is performed with the experimental data of Singh, Panacharoensawad, et al. (2017). In the original work, the author noted that the growth rates could not be explained purely through the deposition rate due to mass diffusion unless a term such as that associated with the shear effect is included; this is because the growth rates decrease with time and the temporal variation of the deposit thickness adopts a power law-like behaviour. For deposition in single-phase flow, we therefore propose the following functional form for the shear stress correction:

$$F_s(\tau_w, \tau_y, \delta_d, \mu_L, \rho_L) = \frac{1}{1 + a_s \left(\frac{\tau_w}{\tau_y} \frac{\delta_d \sqrt{\tau_w \rho_L}}{\mu_L} \right)^{b_s} \left(\frac{\delta_d \sqrt{\tau_w \rho_L}}{\mu_L} \right)^{c_s}} \quad (5.97)$$

This form is based on the ones proposed by Matzain (1999) and Edmonds et al. (2008), and was designed such as to avoid numerical singularities and maintain dimensional consistency. The coefficient values of $a_s = 0.156$, $b_s = 0.302$ and $c_s = 1.867$ were obtained with a least-squares fit to the experiments. The resulting curves are shown in Fig. 5.9. The model introduced here is capable of capturing very well the trends of the curves over time, as well as the dependence on the flow rate. The validation of the single-phase deposition model was also performed with the independent experiments of Rittirong et al. (2017) and it is shown in Fig. 5.9. The quantitative agreement is excellent, with the discrepancy being consistent with the uncertainty associated

with the experimental data in Rittirong et al. (2017).

Two-phase flow

For the two phase flow cases, we utilize the data associated with the stratified flow experiments of Chi et al. (2019) and the slug flow work of Rittirong et al. (2017). Based on the stratified flow data, we propose that $F_f(\tau_w, \tau_y, \delta_d, \mu_L, \rho_L) = 0.1$. The results for these calculations are shown in Fig. 5.10. In contrast to the single-phase flow results shown in Fig. 5.9, the deposit growth rate does not appear to decrease with time, instead remaining approximately constant for the time duration considered in the experiments. This indicates that there is indeed a difference in the effects of the shear term in the two-phase flow case. Furthermore, the good agreement between the experimental data and numerical predictions observed for the lowest and intermediate values of the gas superficial velocity, U_{SG} , deteriorates for the highest value of U_{SG} studied.

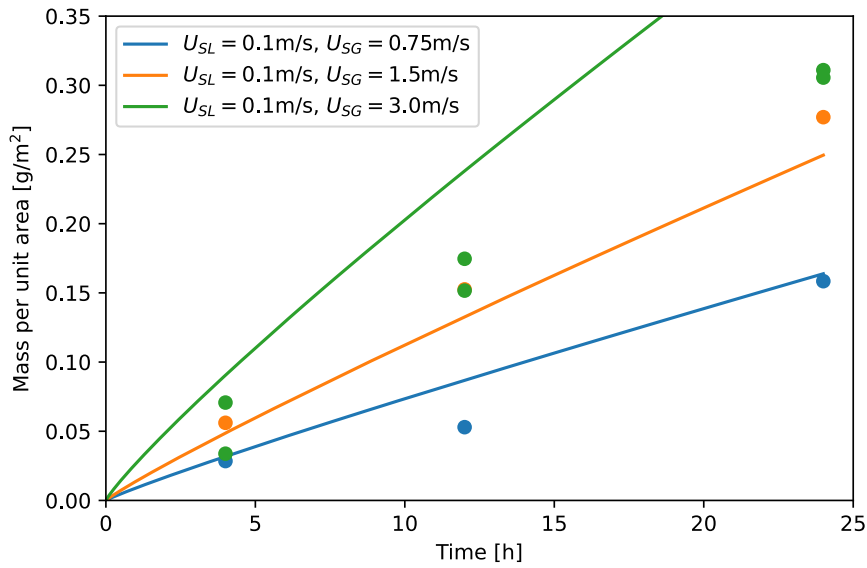


Figure 5.10: Variation of the mass per unit area of the deposit with time for the stratified flow experiments of Chi et al. (2019); the experimental data and numerical predictions are represented by symbols and lines, respectively.

The validation of the slug flow model is shown in Fig. 5.11 where deposit thickness at the top and bottom of the pipe are presented. For these curves, the values of F_b and K were determined

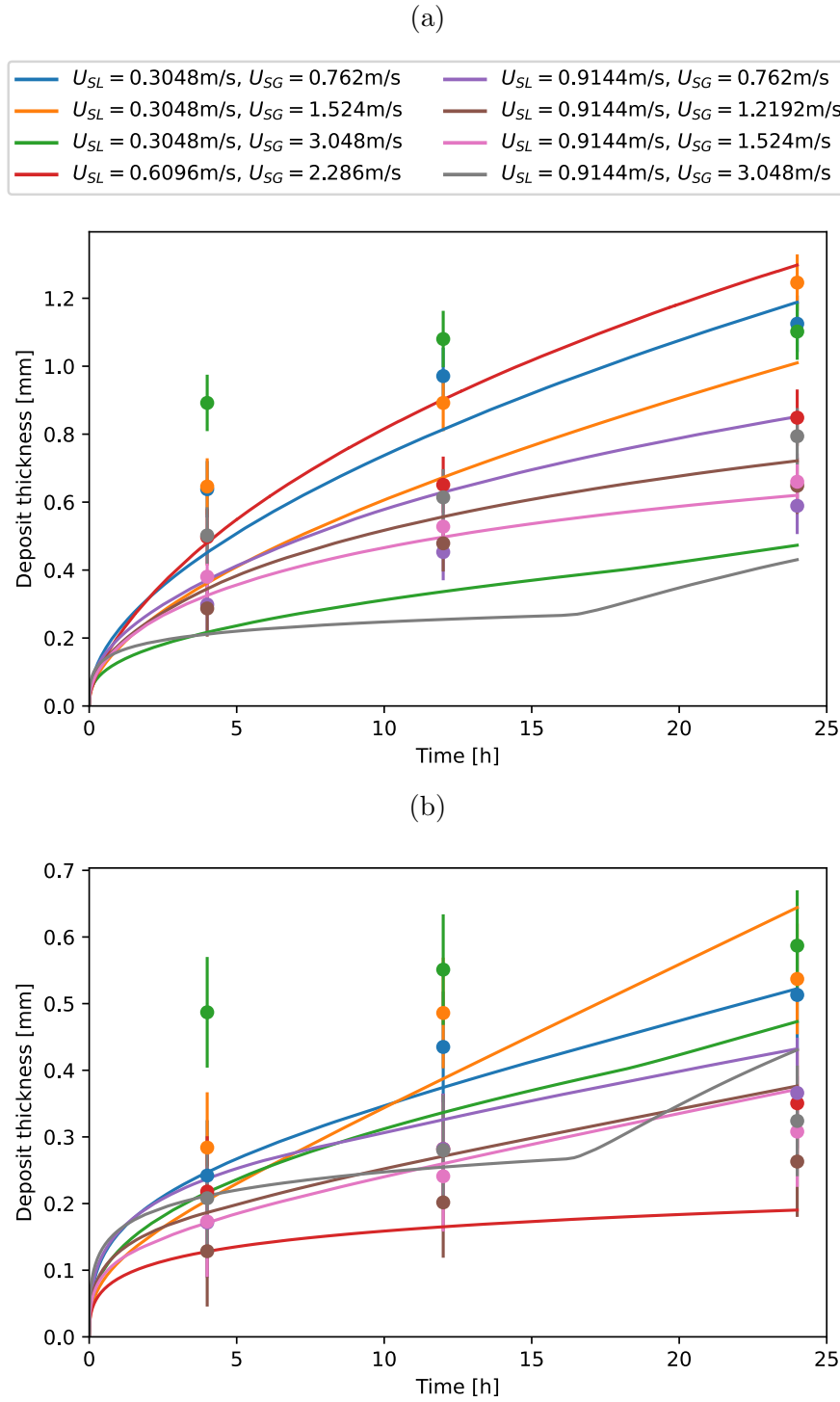


Figure 5.11: Variation of the top and bottom deposit thicknesses with time for the slug flow experiments of Rittirong et al. (2017); the experimental data and numerical predictions are represented by symbols and lines, respectively.

to be:

$$F_b(\tau_w, \tau_y, \delta_d, \mu_L, \rho_L) = 0.02 \quad (5.98)$$

$$K = \begin{cases} 30.0, & S_f/S = 1 \\ 2.5, & \text{otherwise} \end{cases} \quad (5.99)$$

The parameter K assumes two different values since the film region may have a stratified or annular geometry, with different dynamics occurring in each case. We utilized the dispersion of the single-phase flow measurements, where several repetitions were performed, to estimate the uncertainty of the data. The model correctly predicts the trend of the curves over time, and seems able to account for the influence of the liquid flowrate. The worst predictions are observed for the cases of high gas superficial velocity, where possibly the effects of interfacial waves and liquid entrainment could have been underestimated. The mean absolute errors for top and bottom regions were 32% and 25%, respectively, which can be considered acceptable for engineering purposes, considering the complexity of the problem.

5.4 Conclusions

A comprehensive model for the hydrodynamics and thermodynamics of gas-liquid pipe flow in the presence of wax deposition was presented. The model was thoroughly validated using a large database of experimental data obtained from the open literature. The pressure drop predictions for steady-state flows in the stratified and slug flow regimes were excellent, with the large majority of them being within a 20% deviation of experimental measurements. Similarly, the model can reproduce satisfactorily the liquid flow rate over time in a transient experiment.

The predictions of wax deposit thickness were adequate, although the performance depends on the specific flow regime being evaluated. The single phase simulations had excellent agreement with the experimental data, showing that the shear removal correlation proposed is adequate for quantitative predictions. In the cases of stratified and slug flow, predictions generally followed

the right trends and were mostly within experimental uncertainty, although the model was less accurate at high gas velocities.

The algorithm proposed here was designed with physical completeness and computational efficiency in mind, in order to be adequate for industrial needs. In the future, it should be tested with field data and more complex conditions, such as longer pipelines and larger periods of time.

Chapter 6

Data-driven surrogate modelling

6.1 Introduction

In the present work, a methodology for generation of surrogate models based on CFD simulations is explored and evaluated with a set of test cases from the literature. The library developed for benchmarking is available on GitHub¹ under an MIT Licence, which allows users to freely “use, copy, modify, merge, publish, distribute, sublicense, and/or sell copies of the software”. This includes functions for selecting between different strategies, preparing and extracting results from CFD cases and calculating errors, as well as case setups and plotting scripts.

The remainder of this chapter is organised as follows: in Sec. 6.2, the surrogate model development algorithm will be presented, along with the specific regression and sampling techniques which were evaluated. Following that, Sec. 6.3 will introduce the test cases used in the present work and Sec. 6.5.1 will detail the methodology used for comparison between methods. Finally, Sec. 6.5.2 will present the results of the analysis, along with general conclusions and recommendations for the engineering applicability of the methodology.

¹https://github.com/ImperialCollegeLondon/al_cfd_benchmark.

6.2 Surrogate modelling framework

The objective of the surrogate model approach is to develop computationally inexpensive statistical model which, following a systematic calibration can reproduce key predictions of a complete CFD simulation at a fraction of the computational cost. Mathematically, the aim is to find a regressor $f^*(\mathbf{x})$ that approximates a function $f(\mathbf{x})$ for the domain $\mathbf{x} \in [\mathbf{x}_{\min}, \mathbf{x}_{\max}]$, based on a limited number N_s of function evaluations $\{f(\mathbf{x}_i)\}, i \in [1, N_s]$. Since the toolbox is designed generically to evaluate the sampling criterion and choose from a discrete *pool* of parameters, the domain is divided into a fine grid of possible simulation conditions.

An initial set of working conditions $\{\mathbf{x}_i\}, i \in [1, N_0]$ is chosen with a fixed initialization strategy, and the respective simulations are performed in order to obtain a set of initial responses. A regression model is built based on these results. Following that, a sampling algorithm selects a new operating condition (e.g. from the available *pool*) to be evaluated. This is repeated until N_s simulations have been performed. This workflow is shown in Fig. 6.1. Alternatively the

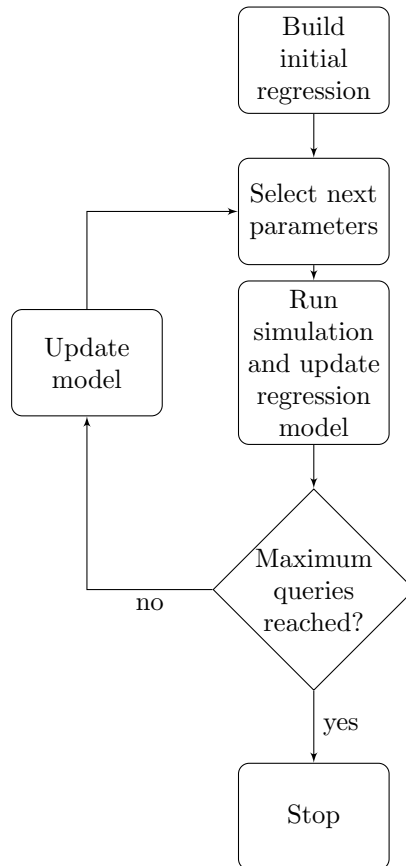


Figure 6.1: Workflow utilized for building the surrogate models for CFD simulations through the active learning methodology

stopping criterion could be defined based on some measure of estimated uncertainty. For benchmarking purposes, however, the procedure presented here seems more appropriate, allowing for a direct comparison between different methods given a fixed number of simulations.

6.2.1 Regression techniques

Five regression techniques of varying complexity were chosen for evaluation. The key concepts will be introduced here; for details on each model we refer the reader to Hastie et al. (2009). The implementations were provided in the *scikit-learn* package (Pedregosa et al., 2011). Most of these techniques depend on *hyperparameters* — parameters the values of which are set before the training process begins. These need to be adjusted through empirical rules and systematic testing. In order to keep the procedure of this work simple and relevant to engineering applications, we forfeited fine-tuning of default parameters whenever possible, restricting the analysis to the defaults provided by the software. These settings have been shown to work well across a wide range of problem domains and have hence been recommended as defaults in the popular software implementations. As such, they would also be the default choice to a user applying such active learning techniques to a new CFD model with minimal prior insight regarding the choice of hyperparameters. Therefore, the results of each method should not be seen as best case scenarios, but instead as a typical results.

Linear regression

The most basic kind of regression is a linear model, given by:

$$f^*(\mathbf{x}) = \mathbf{a} \cdot \mathbf{x} + b \quad (6.1)$$

where $\mathbf{a}$ and b are coefficients to be adjusted based on observations.

Linear regression can often describe the behaviour of functions over small ranges, but eventually becomes too limited to describe data from real systems. It is included here as a baseline for

comparison to more sophisticated models.

Gaussian process regression

Gaussian process (GP) regression is a non-parametric Bayesian technique, which provides the regression as a distribution over functions. As such, predictions are also characterized by a mean value and a standard deviation. The mean values of the predictions are given by:

$$f^*(\mathbf{x}) = \sum_{i=0}^{N_t} w_i k(\mathbf{x}_i, \mathbf{x}) \quad (6.2)$$

where $\mathbf{x}_i$ are the parameters used for training and N_t is the total number of observations. The weights w_i can be calculated with the knowledge of the kernel function $k(\mathbf{x}_i, \mathbf{x}_j)$ and the responses $f(\mathbf{x}_i)$. A kernel function $k(\mathbf{x}_i, \mathbf{x}_j)$ must be chosen to generate the covariance matrix, which defines the smoothness of the regression function. Here, three alternatives will be compared: the radial-basis function (RBF), Matérn, and cubic kernels (Rasmussen and Williams, 2005). The RBF kernel is a popular choice for GP models, given by:

$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{1}{2}d(\mathbf{x}_i/l, \mathbf{x}_j/l)^2\right) \quad (6.3)$$

where d is the Euclidean distance between the vectors and l is a length-scale hyperparameter, which should be strictly positive. The Matérn kernel is a generalization of the RBF kernel. It is defined by an additional parameter ν_M . In the particular case of $\nu_M = 5/2$, the obtained functions are twice differentiable, and the kernel is given by:

$$k(\mathbf{x}_i, \mathbf{x}_j) = \left(1 + \sqrt{5}d(\mathbf{x}_i/l, \mathbf{x}_j/l) + \frac{5}{3}d(\mathbf{x}_i/l, \mathbf{x}_j/l)^2\right) \exp\left(-\sqrt{5}d(\mathbf{x}_i/l, \mathbf{x}_j/l)\right) \quad (6.4)$$

In the present models, the initial length scale l was set to 0.1. The cubic kernel is given by:

$$k(\mathbf{x}_i, \mathbf{x}_j) = (\sigma_0^2 + \mathbf{x}_i \cdot \mathbf{x}_j)^3 \quad (6.5)$$

where σ_0 is a hyperparameter. The parameter estimation was performed using an optimization algorithm (L-BFGS-B, a variation of the Limited-memory Broyden–Fletcher–Goldfarb–Shanno algorithm (Zhu et al., 1997)).

Random forest regression

In a random forest regression, the response is obtained from a combination of the predictions of several decision trees, which are trained on random subsets of the complete dataset. The technique has become very popular for nonlinear regression, scaling well to many input parameters and large amounts of data. It also allows for an inspection of the importance of individual features in the results, which can be useful for interpretability. The number of trees was set to 10.

Support vector regression

Support vector regression relies on projecting the input data onto a reproducing kernel Hilbert space (RKHS), where a linear regression is then performed. Here, the frequently adopted RBF kernel (Eq. 6.3) was used.

Multilayer perceptron

A multilayer perceptron is a type of neural network composed of a sequence of layers of neurons. A series of linear operations and nonlinear activation functions is applied to the input vector as it passes through the network, until a single output vector is obtained. Since data are scarce in the cases considered here, a single hidden layer with 10 neurons was used. The stochastic optimization algorithm *Adam* (Kingma and Ba, 2014) was used for weight adjustment.

Summary

A summary of the total number of adjustable parameters for each technique, with the configurations presented before, is shown in Tab. 6.1. Here, N_f is the number of features in the input vector. In a situation of scarce data, as examined here, the computational cost of fitting the parameters is negligible in comparison to the data collection. In scenarios of abundant data, on the other hand, the scalability of each method in respect to N_t may be a matter of concern.

Table 6.1: Number of fitting parameters used in each regression technique.

Method	Number of parameters
Linear	N_f coefficients, 1 intercept
GP	N_t coefficients, 1 hyperparameter
Random forest	10 decision trees, variable number of leaves
Support vector	N_t coefficients, 1 intercept
Multilayer perceptron	$10(N_f + 1)$ weights, 11 intercepts

6.2.2 Sampling strategies

Five sampling strategies were compared: random sampling, three variations of greedy sampling presented by Wu et al. (2019) and a strategy based on the estimation of prediction variance, specific to GP models. The active learning strategies were implemented using the *modAL* Python package (Danka and Horvath, 2018).

Random sampling

Random sampling is commonly used as a base reference for comparing against other methodologies. Since it does not require any kind of modelling, it has negligible computational overhead, and is readily parallelizable. However, the fact that it neglects the underlying structure of the response space means that for complex functions it might require a very large number of

function evaluations to converge. Samples are randomly chosen from the pool:

$$\{\mathbf{x}_i\} \xrightarrow{R} \mathbf{x}_s \quad (6.6)$$

Greedy sampling on the inputs

Greedy sampling on the inputs seeks to sample the locations which maximize the exploration of the input space, ignoring outputs. It is not dependent on a regression model for estimation of outputs, which means that the computational overhead is low. The distance d in feature space of an unlabeled instance $\mathbf{x}_i$ to the already labeled positions $\mathbf{x}_j$ is given by:

$$d_{\mathbf{x}}(\mathbf{x}_i) = \min_j \|\mathbf{x}_i - \mathbf{x}_j\| \quad (6.7)$$

For greedy sampling on inputs, each sample is selected according to:

$$\mathbf{x}_s = \operatorname{argmax}_{\mathbf{x}_i} d_{\mathbf{x}}(\mathbf{x}_i) \quad (6.8)$$

This methodology can be characterized as a passive sampling scheme, since the selection does not require values of the output variables, meaning that it shares some of the same advantages of the random scheme. As the points are added gradually, the distribution of points generates a hierarchical grid somewhat similar to the one generated by a grid search.

Greedy sampling on the output

In contrast to the previous strategy, greedy sampling on the output aims to find the unlabeled instance that maximizes the distance of estimated responses to the previously observed function values. The distance of an unlabeled instance in output space is given by:

$$d_f(\mathbf{x}_i) = \min_j |f^*(\mathbf{x}_i) - f(\mathbf{x}_j)| \quad (6.9)$$

The next sample is selected according to:

$$\mathbf{x}_s = \operatorname{argmax}_{\mathbf{x}_i} d_f(\mathbf{x}_i) \quad (6.10)$$

This strategy will lead to a large number of samples in the regions where the response function varies rapidly, but potentially small exploration of the parameter space. In the case of multimodal functions, for example, this could lead to important features being missed in the sampling procedure.

Greedy sampling on both inputs and output

The greedy algorithm based on inputs and outputs is a combination of the previous criteria. The distances in both feature and response spaces are combined. The next sample is selected according to:

$$\mathbf{x}_s = \operatorname{argmax}_{\mathbf{x}_i} d_{\mathbf{x}}(\mathbf{x}_i) d_f(\mathbf{x}_i) \quad (6.11)$$

The distances in input and output spaces are calculated as shown before. The product of distances is used here instead of a weighted sum so that the resulting function is independent of the scales of the inputs and output.

Variational sampling

In the case of GP regressors, the standard deviation σ^* of the predictive distribution may be used as a criterion for choosing sampling locations. In this case, the sample is chosen with:

$$\mathbf{x}_s = \operatorname{argmax}_{\mathbf{x}_i} \sigma^*(\mathbf{x}_i) \quad (6.12)$$

The standard deviation does not depend directly on the response values obtained at the training stage, which is a characteristic of the Gaussian distribution (Rasmussen and Williams, 2005). However, these values are still utilized for the optimization of the kernel's hyperparameters, which affect in turn the expected covariance.

6.3 Benchmark cases for computational fluid dynamics

6.3.1 Computational fluid dynamics simulations

In order to quantify the performance of the systems analyzed here, the flow field inside the domain of interest has to be characterized. Engineering quantities such as pressure and shear stresses, for example, can be obtained from the knowledge of velocity and pressure fields, along with the fluid properties. The core equations to be solved are the continuity and momentum balance equations (Batchelor, 2000). The continuity equation for incompressible flows is given by:

$$\nabla \cdot \mathbf{u} = 0 \quad (6.13)$$

while the momentum equation is expressed by:

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) - \nabla \cdot (\nu_{\text{app}} \nabla \mathbf{u}) = -\nabla p \quad (6.14)$$

where $\mathbf{u}$ is the velocity, p is the static pressure divided by the constant fluid density, ν_{app} is the apparent kinematic viscosity, and t denotes time; gravitational forces have been neglected. We consider, for generality, that the apparent kinematic viscosity follows a power law $\nu_{\text{app}} = k|\dot{\gamma}|^{n-1}$, where k is the consistency and n is the flow index. The Newtonian behaviour of the fluid, as assumed in test Cases 1 and 2, can be recovered by setting the value of n to unity in which case we set $k \equiv \nu$, a constant. In non-dimensional form, Eqs. (3.1) and (3.2) may be rewritten as:

$$\nabla \cdot \mathbf{u}^* = 0 \quad (6.15)$$

and

$$\frac{\partial \mathbf{u}^*}{\partial t} + \nabla \cdot (\mathbf{u}^* \otimes \mathbf{u}^*) - \frac{1}{Re} \nabla \cdot \left(\frac{\nu_{\text{app}}}{\nu_{\text{ref}}} \nabla \mathbf{u}^* \right) = -\nabla p^* \quad (6.16)$$

where $Re (= UL/\nu_{\text{ref}})$ is a Reynolds number in which L and U represent characteristic length and velocity scales, the choice of which is case dependent; here, t and p were scaled on L/U and ρU^2 , respectively, wherein ρ denotes the fluid (constant) density. The reference viscosity

is taken to be $\nu_{\text{ref}} = k(U/L)^{n-1}$.

In the case of turbulent flows, two-equation models based on the turbulent viscosity are used such as the k - ϵ model (Launder and Spalding, 1974). The simulations were performed with OpenFOAM-6 with two-dimensional setups, except for the last test case, which is fully three dimensional. In the case of axisymmetric flows (Cases 1 and 2), the geometry is defined as a wedge of small angle and thickness of a single cell in the out-of-plane direction. All simulations utilized second-order discretization schemes for the spatial terms, and steady state was assumed. If the mixing performance is to be evaluated (as in test Case 1), a transport equation for a passive scalar c can also be solved:

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c) - \nabla \cdot \left(\frac{\nu_{\text{eff}}}{Sc} \nabla c \right) = 0, \quad (6.17)$$

where the turbulent viscosity, ν_{eff} , is provided by the turbulence model and the Schmidt number, Sc , is taken to be unity.

6.3.2 Case 1: flow through a static mixer

Industrial high efficiency vortex (HEV) static mixers are commonly used for turbulent mixing along pipelines (Eissa, 2009; Thakur et al., 2003). The first case in this study aims to model the geometry of such a mixer. The fluid enters the domain through the leftmost boundary, where a passive scalar is inserted in part of the domain. As it goes across the device, turbulent mixing takes place, eventually leading to a nearly uniform concentration of the tracer on the cross-section. To evaluate the mixing performance of the device, Eq. (6.17) was solved along with the flow equations, as mentioned previously. The two-dimensional geometry of the static mixer is shown in Fig. 6.2. For the surrogate model, we mainly focus on two of the parameters: blade length to diameter ratio (L/D) from 0.2 to 0.3, and blade angle (θ) from 0.8 to 1.57 rad. The Reynolds number, Re ($= UD/\nu$), is kept constant at 1×10^5 , where U is the constant speed of the fluid that enters the mixer from the left boundary, where a uniform velocity profile is imposed; note that here we consider the fluid to be Newtonian with a constant kinematic

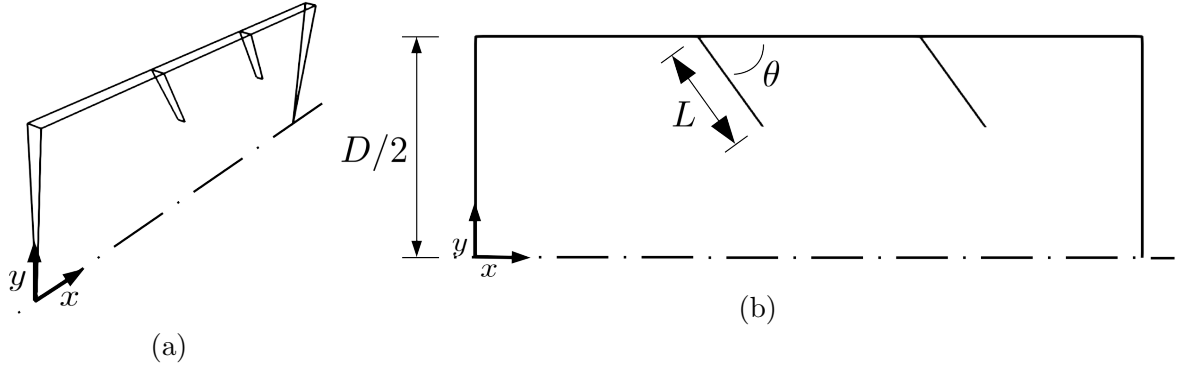


Figure 6.2: Schematic representation of the static mixer geometry used in Case 1 with side- and front-views shown in (a) and (b), respectively

viscosity, ν . For all the walls in contact with the fluid (e.g. upper wall of the wedge, and blade walls), a no-slip condition is imposed. For scalar transport, the tracer injection at the inlet is set as a step profile similar to the one presented by (Eissa, 2009). The turbulence model used is the standard k - ϵ (Launder and Spalding, 1974), and a turbulence intensity of 5% was set for the inlet. To determine the mixing performance, c_v at the outlet is calculated, which corresponds to the variance of the tracer concentration at the outlet:

$$c_v = \frac{\sqrt{\overline{(c - \bar{c})^2}}}{\bar{c}} \quad (6.18)$$

where the average concentration, $\bar{c}$, is computed over the outlet area.

In order to assure that the results were valid in a wide range of conditions, the wall boundary conditions utilized for ϵ , k and ν_t were set to, respectively *epsilonWallFunction*, *kLowReWallFunction*, *nutUSpaldingWallFunction*, which automatically switch between low- and high-Reynolds number formulations as needed.

Fig. 6.3 shows the non-dimensional velocity magnitude, turbulent kinetic energy, and concentration fields obtained for a geometry similar to the one presented by Eissa (2009), with an angle of $\theta = \pi/4$. Despite the fact that the current results were generated using a two-dimensional formulation, they are nonetheless in qualitative agreement with the results of Eissa (2009) and Bakker and Laroche (2000). One major discrepancy with the work by Eissa (2009) is the cross-sectional vortices generated at the blade tips. In order to reproduce those more accurately it

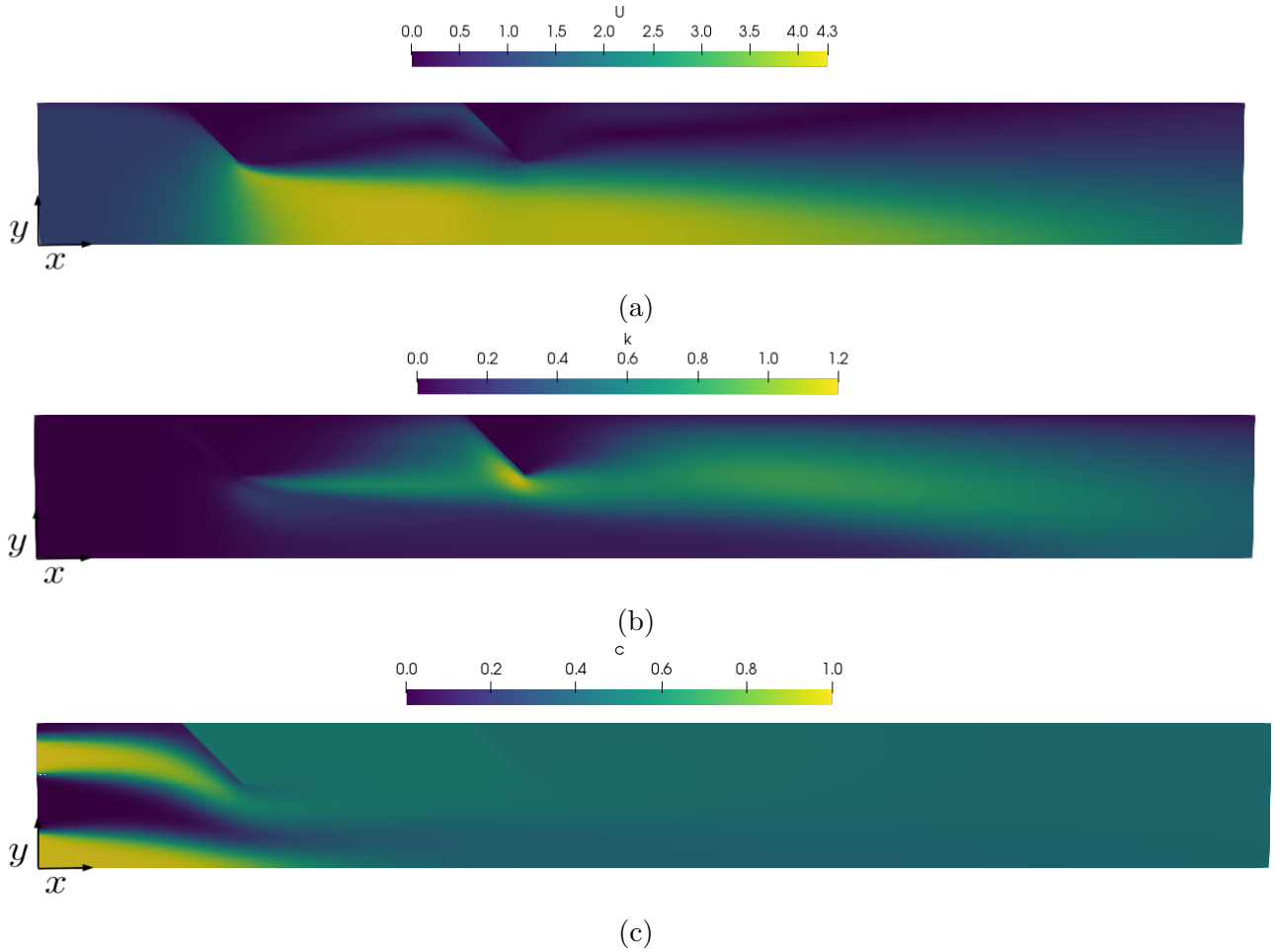


Figure 6.3: Computational fluid dynamics simulation of turbulent scalar transport through a static mixer using the k - ϵ model (Launder and Spalding, 1974) for Case 1 showing steady, two-dimensional non-dimensional velocity magnitude, (a), turbulent kinetic energy, (b), and scalar concentration, (c), fields, generated with $Re = 10^5$, $L/D = 0.3$ and $\theta = \pi/4$. The scale bars represent the magnitude of the fields depicted in each panel

is possible for us to deploy more sophisticated turbulence models, or large eddy simulations, to better capture these phenomena, but this is not the focus of the present work.

6.3.3 Case 2: orifice flow

Flow through an orifice is a common occurrence in industry with applications that include pipeline transportation of fluids, and flow in chemical reactors and mixers wherein orifice flows are used for the purpose of flow rate measurement and regulation. Here, pressure drop across the orifice as a function of system parameters is investigated. As the shape is symmetrical in both the radial and axial directions, the computational domain is a pipe sector, as shown in Fig. 6.4. A uniform velocity profile is considered for the inlet boundary, and no slip conditions are applied

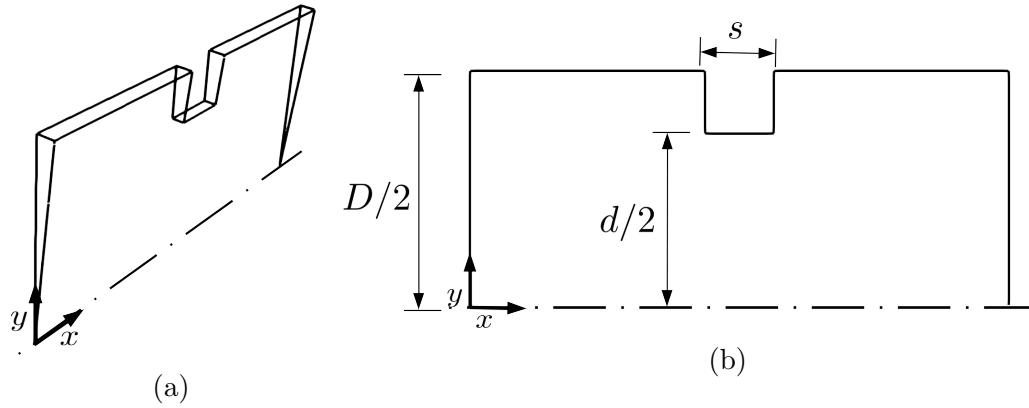


Figure 6.4: Schematic representation of the orifice geometry used in Case 2 with side- and front-views shown in (a) and (b), respectively

for the wall. At the outlet, a constant pressure is assumed. When creating the surrogate model, the geometry of the orifice is allowed to vary, such that each configuration is defined by the area ratio $(d/D)^2$ and length to diameter ratio s/d . The Reynolds number Re , given here by UD/ν , is taken to be constant and equal to 1×10^5 . The flow field simulated in OpenFOAM is using the SST $k-\omega$ model (Menter et al., 2003). A turbulence intensity of 2% was assumed for calculation of turbulent kinetic energy at the inlet, and this value was used along with a prescribed mixing length for definition of the specific turbulence dissipation value. The chosen mesh resolution resulted in a total of 5.1×10^4 cells for a setup with area ratio $(d/D)^2 = 0.54$ and length to diameter ratio $s/d = 0.2$ (see Fig. 6.4b). Mesh refinement is utilized to increase the mesh

density close to wall while reducing computational cost simultaneously. A mesh-refinement study has been conducted to prove that the solutions obtained are mesh-independent. The difference in pressure drop across the *vena contracta* between 2.5×10^4 cells and 5.1×10^4 cells is less than 2% as well as the difference between 5.1×10^4 cells and 1.0×10^5 ; thus the setup for 5.1×10^4 cells was deemed to produce simulation results that are unaffected by mesh resolution.

Since the change in geometry is expected to have an impact on the mesh requirements for the wall, the boundary conditions for ω , k and ν_t were set to, respectively *omegaWallFunction*, *kLowReWallFunction*, *nutUSpaldingWallFunction*, which are able to deal with low- and high-Reynolds number scenarios as needed.

In Fig. 6.5, we compare our results with the of experimental data of Fossa and Guglielmini (2002) for the local pressure drop across the orifice as a function of the flow Reynolds number. Inspection of Fig. 6.5 reveals excellent agreement — with maximum deviations of 7.9% — which inspires confidence in the reliability of the present numerical predictions.

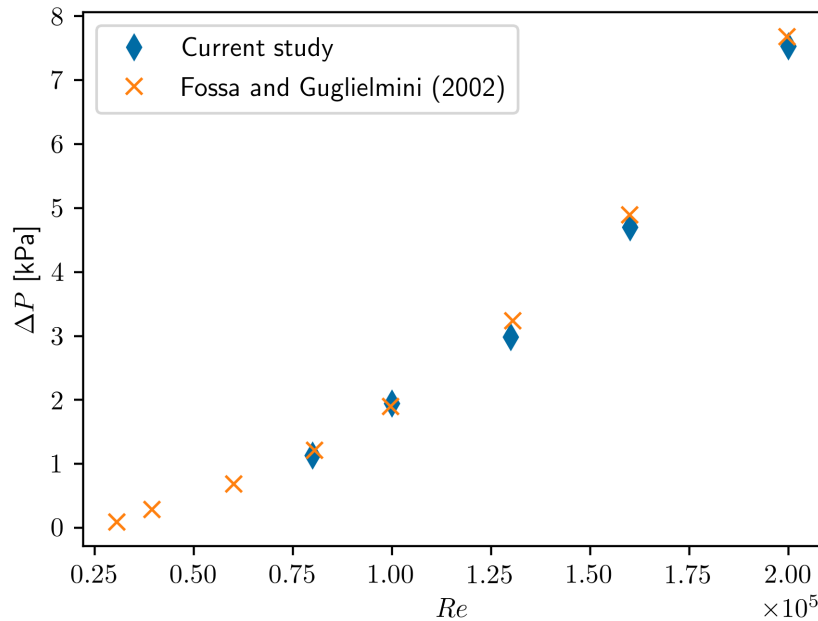


Figure 6.5: A comparison of the current predictions of pressure drop across the orifice as a function of the local Reynolds number with the experimental data of Fossa and Guglielmini (2002) with $(d/D)^2 = 0.54$, and $s/d = 0.20$ (see Fig. 6.4b)

6.3.4 Case 3: flow in an inline mixer (2D)

The third case is representative of flow of Newtonian and power-law fluids in an inline mixer reported by Vial et al. (2015). This setup utilizes a two-dimensional geometry, neglecting the effect of the flow in the axial direction. The geometry and key variables are shown in Fig. 6.6. The impeller rotates in the counter-clockwise direction around the z -axis, while the outer tank wall is kept fixed. For further efficiency gains in the simulation, a periodic symmetry is prescribed in the tangential direction. For this system, the power number (per non-dimensional length L_e/d) $N_{p,2D}$ is chosen as the main variable of interest. It is given by:

$$N_{p,2D} = \frac{2\pi T_{2D}}{N^2 d^4} \quad (6.19)$$

where T_{2D} is the torque applied per fluid mass and N is the rotation speed. Through dimensional analysis, it can be shown that this value is a function of the Reynolds number, Re ($= d2\pi N^{(2-n)}d^2/k$), non-dimensional gap between rotor and stator α ($= (D-d)/D$), flow index n , and number of blades N_b .

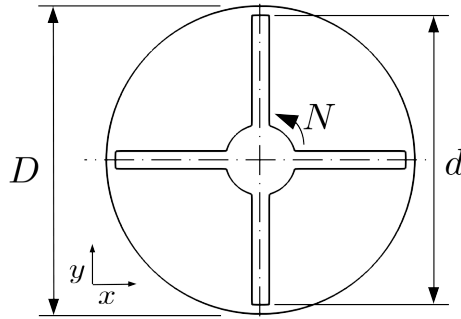


Figure 6.6: Schematic representation of the geometry used in Case 3, two-dimensional flow in an inline mixer

The simulations performed were two-dimensional. Vial et al. (2015) reported that this simplification was adequate to describe the behavior of the system as long as the flow was in the laminar regime and the non-dimensional gap between rotor and stator was kept below 0.2. Thus, these restrictions were considered in the choice of parameter ranges. Similarly to the original study, the computational domain consisted of a single blade, and cyclic boundaries were applied for the tangential direction. No-slip conditions were considered for the walls, and

the rotation effect was included through the Single Reference Frame (SRF) model. Further details about the SRF methodology can be found in Wilhelm (2015).

All computations were performed with a quadrilateral mesh with circumferential resolution $\Delta s/D_s = 0.005$ and radial resolutions $\Delta r_i/D_s = 0.005$ and $\Delta r_o/D_s = 0.002$ at the rotor and stator regions, respectively. The difference in the power number obtained with a finer mesh, with double the resolution, was 0.3%. Table 6.2 shows the comparison of the power coefficient k_p ($= N_{p,2D} Re L_e/d$) calculated here and the results obtained by Vial et al. (2015) through experiments and two-dimensional simulations. The agreement is very good.

Table 6.2: Comparison between present results for power coefficient, α , and those reported by Vial et al. (2015).

α	Exp. (Vial et al., 2015)	Vial et al. (2015) - 2D	Present - 2D	Present - 3D
0.057	3100 ± 400	3000	2950	3030
0.2	2000 ± 300	1680	1690	1800

6.3.5 Case 4: flow in an inline mixer (3D)

The final test case is a three-dimensional version of the inline mixer presented before. Here, besides the rotation around the z -axis, we also take into account the flow along that direction, as well as the finite length of the blades. The newly introduced variables are illustrated along with the general geometry in Fig. 6.7.

Besides the parameters defined before, this setup introduces two new parameters to the input: the axial Reynolds number Re_{ax} ($= dUN^{(1-n)}d/k$), and the nondimensional length L_e/D , for a total of 6 parameters. The mesh utilized for the 3D case was less refined than for the two-dimensional setup, with circumferential resolution $\Delta s/D_s = 0.01$, radial resolutions $\Delta r_i/D_s = 0.01$ and $\Delta r_o/D_s = 0.005$ at the rotor and stator regions, respectively, and axial resolution $\Delta z/D_s = 0.01$. The power number difference to a mesh with double the resolution was 1.2%. The power coefficient numbers obtained with this setup and the comparison to the experimental values are shown in Table 6.2. The values are well within the experimental uncertainty of the measurements.

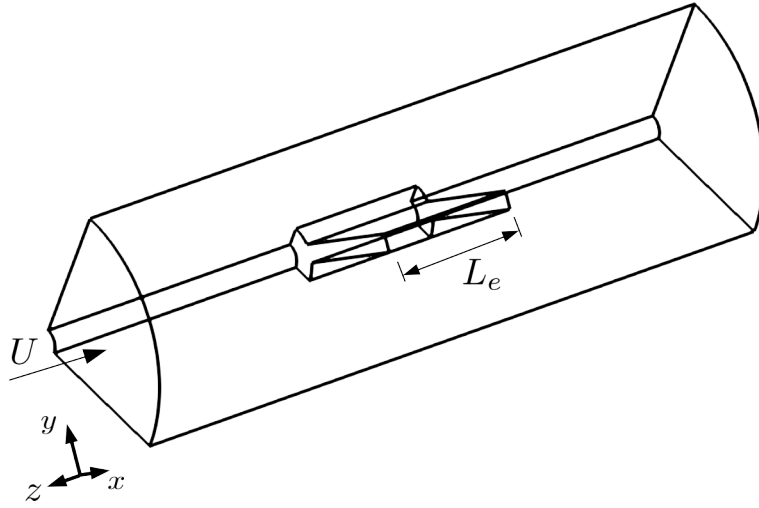


Figure 6.7: Schematic representation of the geometry used in Case 4, three-dimensional flow in an inline mixer

6.3.6 Summary of regression variables

Table 6.3 shows a summary of the parameters considered for the surrogate models, along with the respective output variables. Note that all variables are nondimensional, in order to enforce similarity constraints. The variables that could vary over several orders of magnitude were represented in logarithmic form.

Table 6.3: Features and responses utilized in each of the three test cases.

Case	1	2	3	4
x_1	L/D	$(d/D)^2$	$\log Re$	$\log Re$
x_2	θ	s/D	α	α
x_3	-	-	n	n
x_4	-	-	N_b	N_b
x_5	-	-	-	Re_{ax}
x_6	-	-	-	L_e/D
$f(\mathbf{x})$	$\log c_v$	$\frac{\Delta P}{\rho U^2}$	$\log N_{p,2D}$	$\log N_{p,2D}$

Table 6.4 presents the comparison between the average computational costs of the test cases, including the time to both generate the parameterized mesh as well as to calculate the solution of the flow. The values range from a few minutes to one hour, and are directly related to the size of the grid that is required.

Table 6.4: Typical computational cost of individual simulations of each test case.

Case	Number of cores	Time [s]
1	1	260
2	1	1070
3	1	1020
4	192	3430

6.3.7 Mesh study of Cases 1 and 2

For Case 1, the effect of mesh resolution on the concentration field along the symmetry axis is presented in Fig. 6.8. The chosen resolution proves sufficient for capturing the solution accurately without requiring excessive time for computation. For the base case, the mesh adopted had an average y^+ of 38.7 and 22.3 and maximum of 80.8 and 67.4 for walls and blades, respectively, which is adequate for the high-Reynolds model.

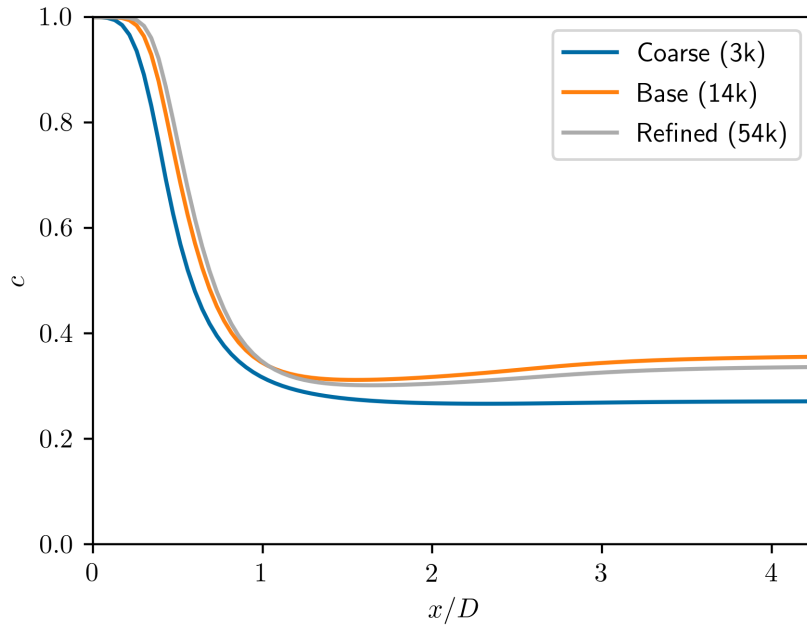


Figure 6.8: Effect of mesh resolution on concentration profile along the symmetry axis.

For Case 2, the pressure profiles along the symmetry axis for different mesh resolutions are presented in Fig. 6.9. The results are nearly indistinguishable between the three meshes.

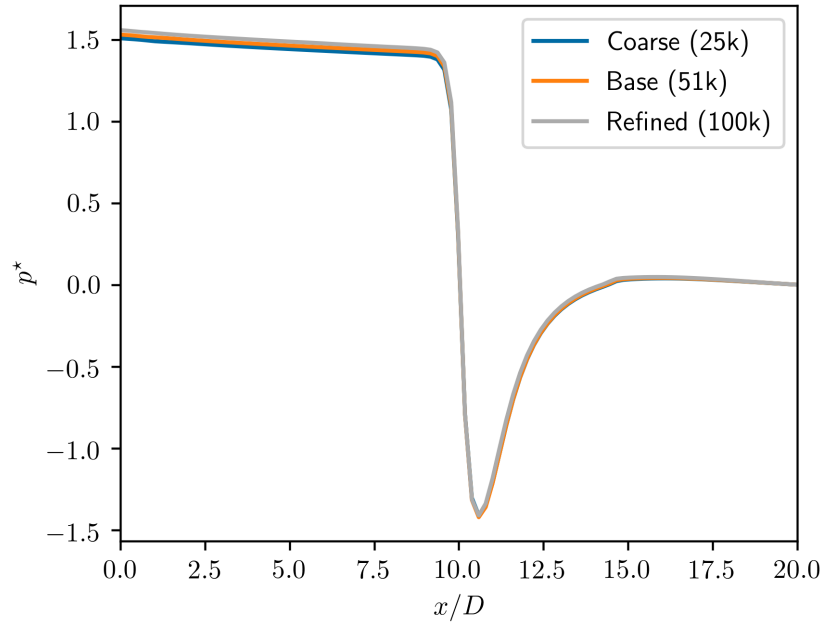


Figure 6.9: Effect of mesh resolution on pressure profile along the symmetry axis.

6.4 Surrogate model for wax deposition simulator

The regression and active learning algorithms analysed here can also be applied to simulators such as the one presented in Chap. 5. This allows for simpler surrogate models that could be used in parametric analysis, optimization or uncertainty quantification.

We propose a test case based on the experimental cases utilized before for validation of the wax deposition model. For a fixed oil precipitation curve (Garden-Banks condensate) and fixed geometry (based on Rittirong et al. (2017), and presented before in Sec. 5.3.2), we predict wax thickness after a period of time as a function of temperature and gas and liquid flowrates (i.e., $\mathbf{p} = [\log U_{SG}, \log U_{SL}, T]$ and $f(\mathbf{p}) = \delta_d$).

6.5 Results and discussion

6.5.1 Performance evaluation methodology

Before the active-learning techniques are employed, an initial version of the regression model must be calibrated. All methods are initialized with the procedure proposed by Wu et al. (2019): the first point is located at the centroid of the parameter space, followed by $N_0 - 1$ locations selected with the passive strategy of greedy sampling on inputs. We set the total number of initial simulations N_0 to be equal to $4N_{\text{features}}$ in Cases 1 and 2, $2N_{\text{features}}$ in Case 3 and 6 in Case 4.

In order to quantify the global interpolation performance of each algorithm, a set of N_e simulations with parameters $\mathbf{x}_i$ is performed, independent of the ones used in the development of the surrogate model, to be used as “ground truth”. The average relative error is given by Eq. (6.20):

$$\epsilon^* = \frac{1}{N_e} \sum_{i=0}^{N_e} \frac{|f(\mathbf{x}_i) - f^*(\mathbf{x}_i)|}{|f(\mathbf{x}_i)|} \quad (6.20)$$

The positions $\mathbf{x}_i$ for error estimations were chosen randomly, with the total number of simulations N_e set to 100. Additionally, for the techniques that are stochastic — either due to the regression or sampling methods — 10 repetitions were performed. Results are presented in the form of a mean value and a confidence interval of 95% based on the t -distribution. Due to the very high computational cost of the full 3D computations, we have utilized a single repetition of each for Case 4, such that no confidence bars are provided.

6.5.2 Discussion

Fig. 6.10 presents a qualitative comparison of the interpolation obtained for Case 1 using the regression techniques presented in Sec. 6.2.1. In order to better isolate effects, a fixed sampling method was used for these results: in this case, greedy I/O, based on the recommendation of Wu et al. (2019). The predictions of all methods are found to be qualitatively very similar. The notable outlier is the random forest regression - although the predicted values are reasonable,

the surface is non-smooth, since the values originate from a combination of decision trees. It is important to highlight that, despite using the same sampling strategy, the sampling locations for each regression method may be different, since they also depend on the predicted values provided by the regression.

In Fig. 6.11, a qualitative visual comparison between sampling strategies for case 1 is presented. Based on preliminary performance tests which indicated it performed well in quantitative tests, the fixed regression strategy chosen here was a Gaussian process with the Matérn 5/2 kernel. A good sampling strategy should be able to adapt to both the situation of “effect sparsity” — where only some of the parameters significantly affect the solution — as well as the situation where all inputs have equal importance (Morris and Mitchell, 1995). As such, sampling positions should be spread out enough so as to fully capture the main features of the response surface, while simultaneously avoiding unnecessary computations in regions of low gradient. The greedy input and variational methods provide a uniform coverage of the domain, while the greedy output sampling is heavily biased towards the center and top right regions. The greedy I/O, as a mix of two criterion, has a somewhat attenuated bias.

Fig. 6.12 presents the calculated interpolation error for each regression strategy. The relative errors are high for Case 2 since the response function has values close to zero in a large part of the domain, but the trends are somewhat consistent between all cases. Since it has very few degrees of freedom, the strategy employing linear regression rapidly stagnates after a small number of simulations. Similarly, the performance of the multilayer perceptron does not improve significantly as samples are added; most likely, this can be attributed to overfitting due to the quite limited number of data points. The Gaussian process regression performs well in all three cases, while Support Vector regression has mixed results: the performance is satisfactory for Cases 1 and 3 but poor for Case 3. Finally, it is noticeable that, in general, the curves are non-smooth and non-monotonic, meaning that there is room for significant optimization with the choice of sampling quantity and locations.

Fig. 6.13 show the progress of the estimated error as the number of simulations increases, for different sampling strategies. For cases 1 and 2, most of the examined strategies had perfor-

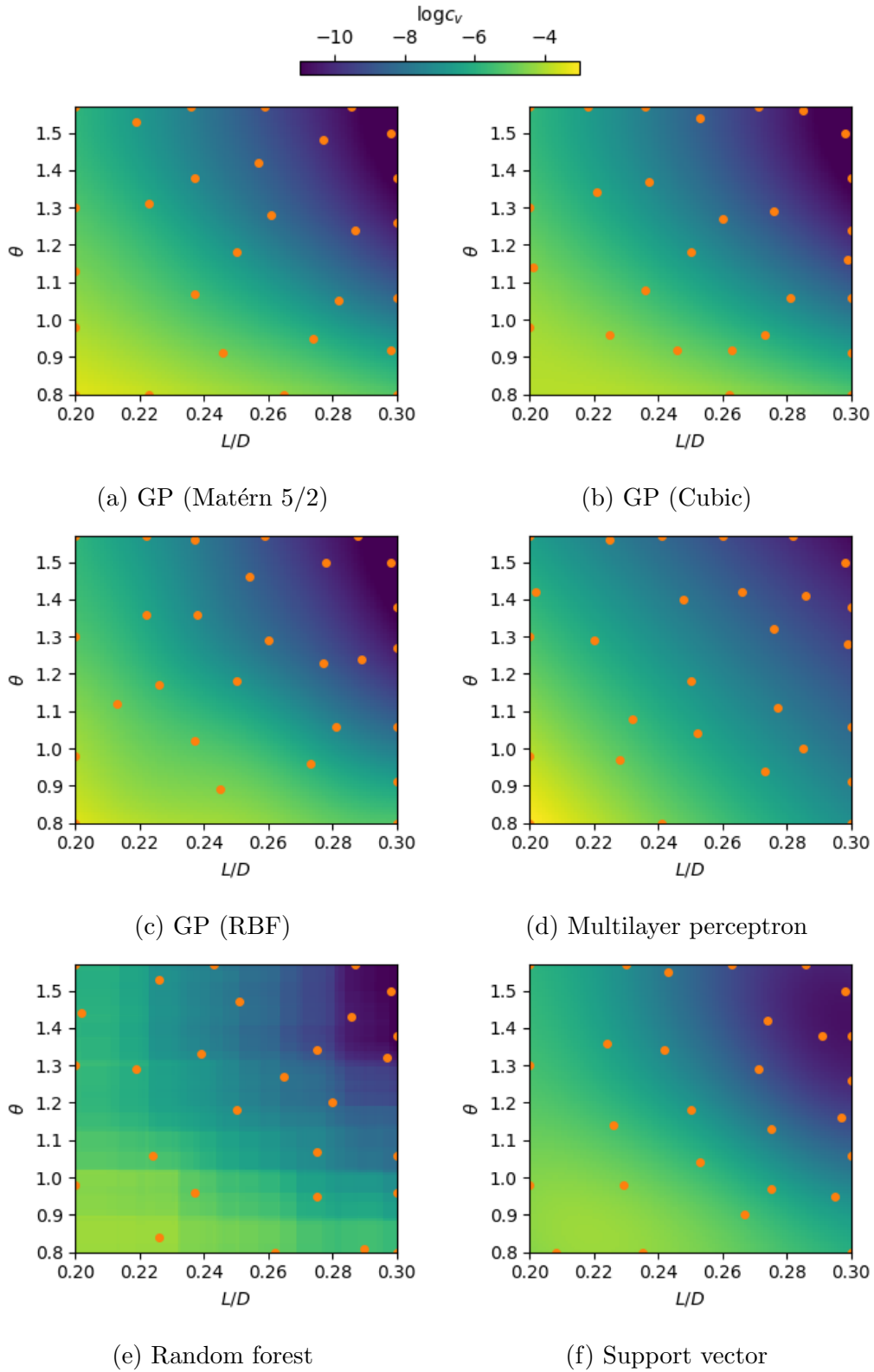


Figure 6.10: Comparison between regressions for case 1, with 20 samples. Circles indicate sampling locations

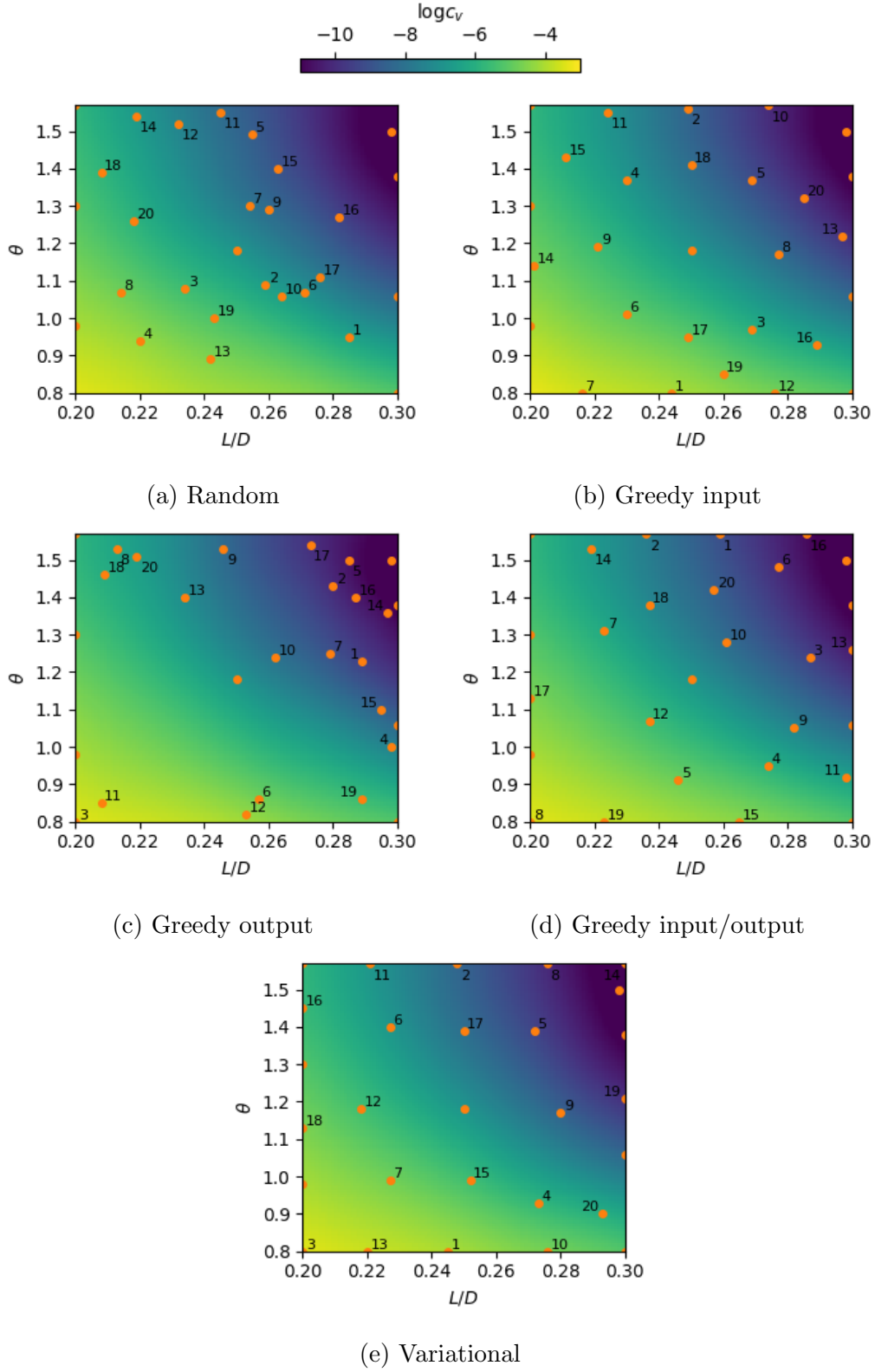


Figure 6.11: Comparison between sampling strategies for case 1, with 20 samples. Circles indicate sampling locations and numbers indicate the sampling order (positions used for initialization are unlabeled)

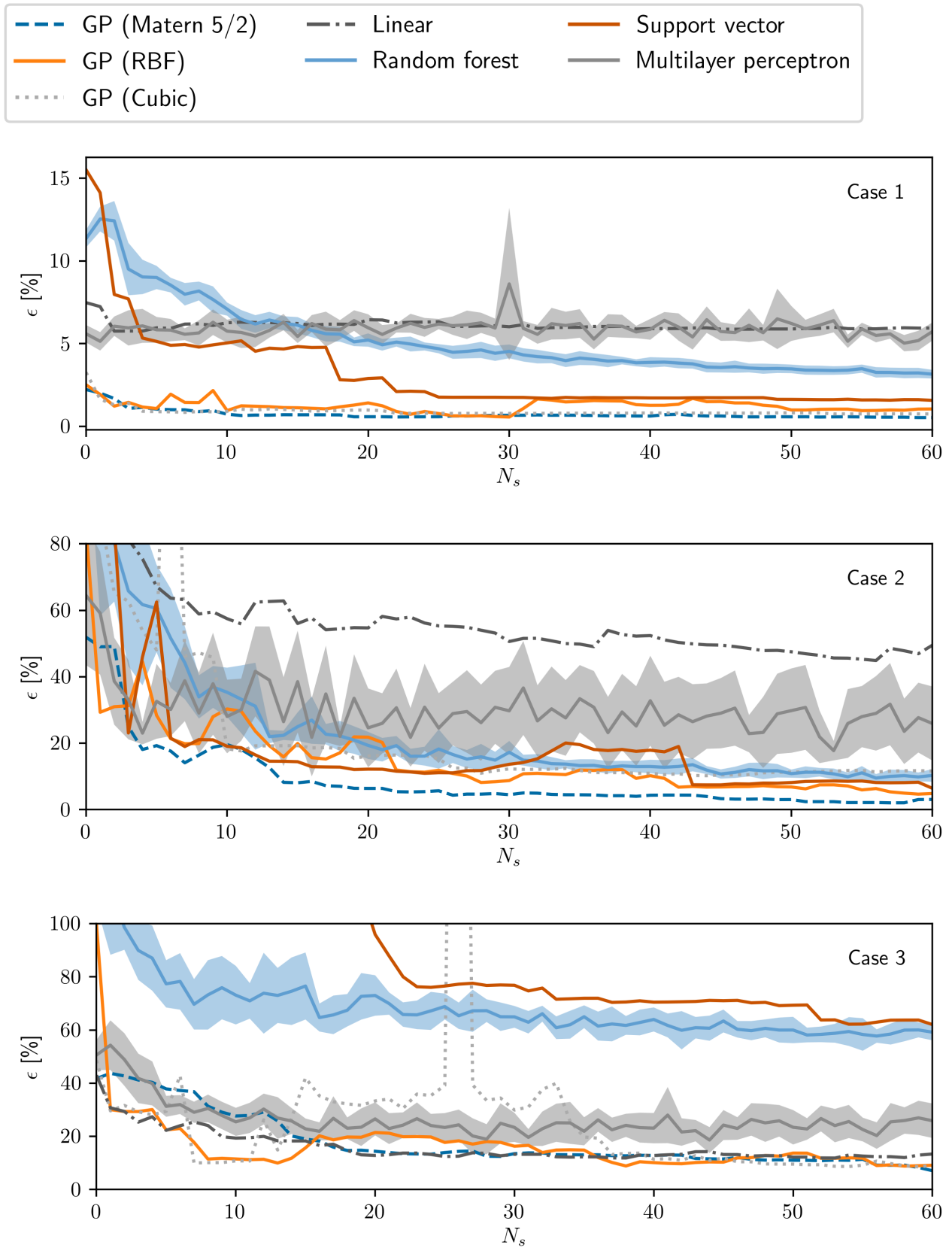


Figure 6.12: Error as a function of number of samples beyond the ones used for the initialization for different regression strategies, for case 1 (top), case 2 (middle) and case 3 (bottom)

mance comparable or slightly better than the random baseline. For the latter, in particular, the errors obtained with the variational, greedy I and greedy I/O strategies were lower than half of the baseline values, with more than approximately 5 samples. For case 3, the variational and greedy I significantly outperformed random sampling in the range of 5 to 30 samples. Despite the relatively low dimensionality of the cases that were examined, some positive effect may be observed already with the use of the passive or active strategies, especially at low numbers of samples.

The scalability of the techniques to more complex systems can be evaluated by analyzing Fig. 6.14, which presents the performance of the regression and sampling techniques as a function of the number of simulations performed on case 4. The general trend is somewhat similar to the one observed for case 3, a similar mixer setup. However, due to the limited samples and larger parameter space, instances of severe overfitting are observed in some situations, leading to predictions outside of the training data to be completely erroneous. In fact, the only sampling technique that seems to be able to provide reasonable predictions for the GP model is the GIO algorithm.

The overfitting problem is illustrated explicitly in Fig. 6.15, which compares the predictions for training and test data, for two different sampling methodologies. The GP fit is quite flexible and able to reproduce the set of training data very well. In complex cases, however, the hyperparameter optimization may lead to length scales which are too small, such that the regression function collapses into a combination of singularities around the training data. This results in meaningless values for any new data outside the immediate neighbourhood of the training set. Although this could be addressed through fine tuning of the algorithm, it would require a case-by-case analysis. In this case, the GIO strategy seems to achieve a balance between density and coverage of the sampling space, leading to a smoother convergence of the length scale to an adequate value.

Similar comparisons of predictions and reference values are shown for the other cases on Fig. 6.16. Systematic deviations may be observed in some situations for variational, GI, and GO sampling. Using a more balanced sampling approach such as GIO, which does not focus on one

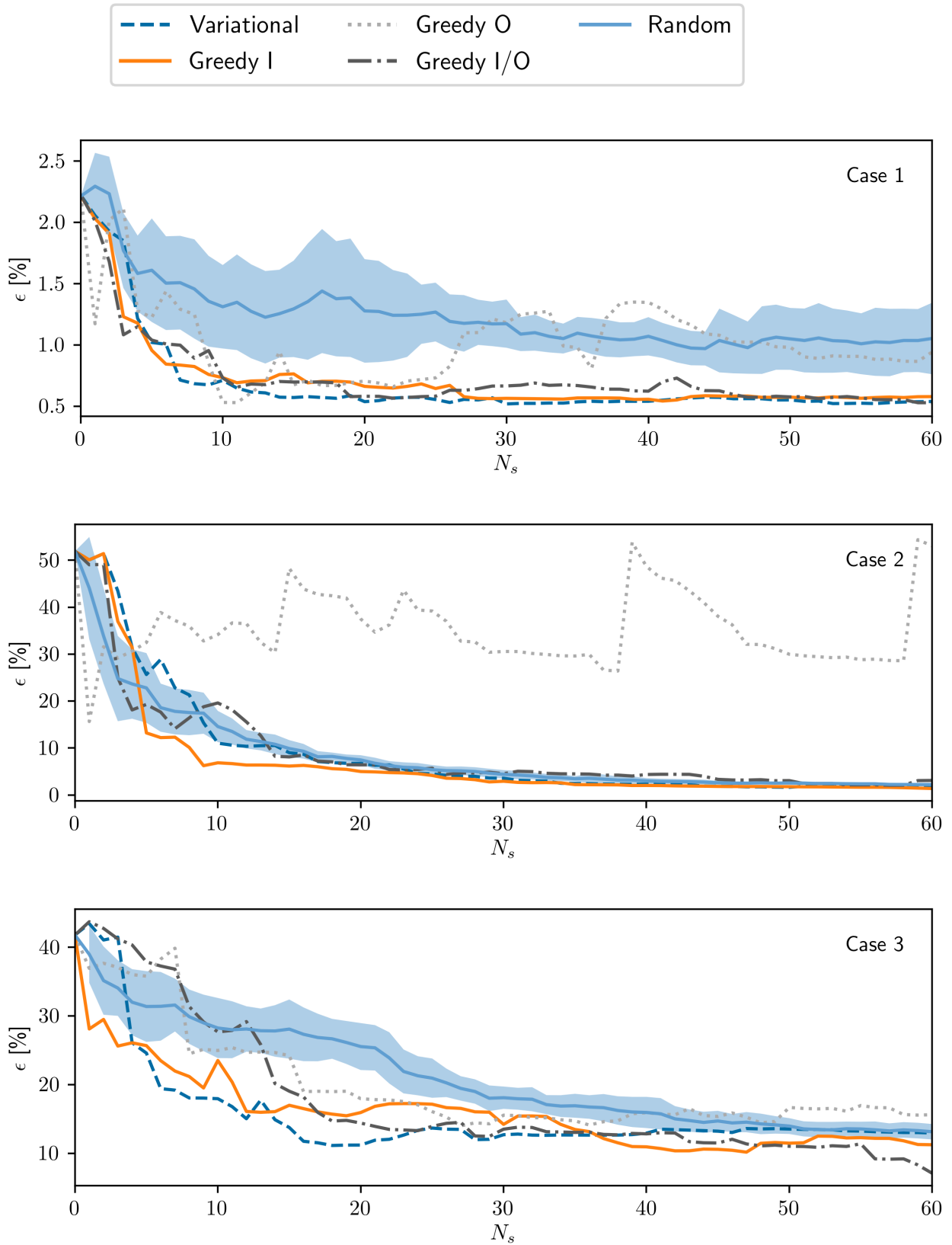


Figure 6.13: Error as a function of number of samples beyond the ones used for the initialization for different sampling strategies, for case 1 (top), case 2 (middle) and case 3 (bottom)

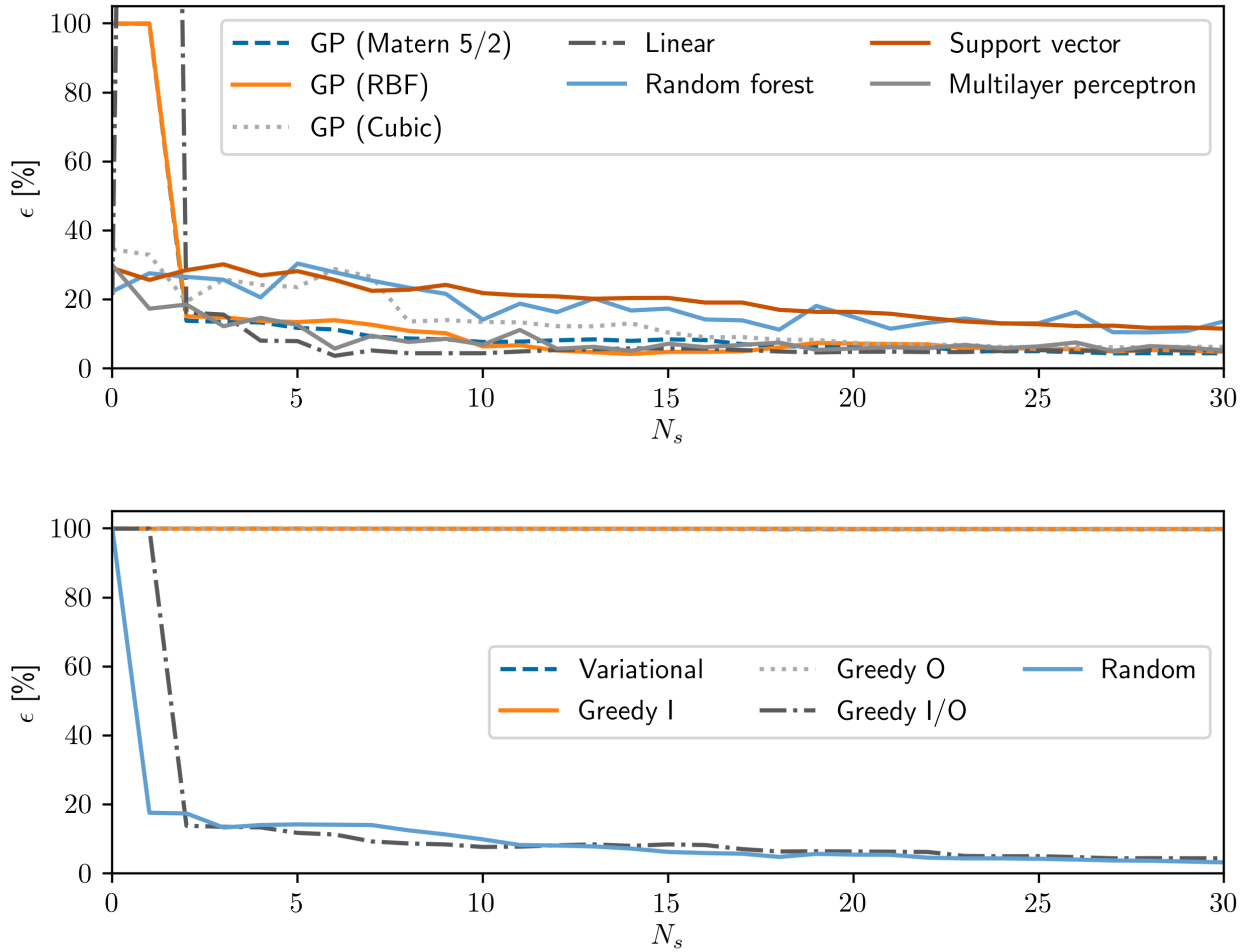


Figure 6.14: Error of the regressions developed for Case 4 as a function of number of samples beyond the ones used for the initialization, for different regression strategies (top), and different sampling strategies (bottom)

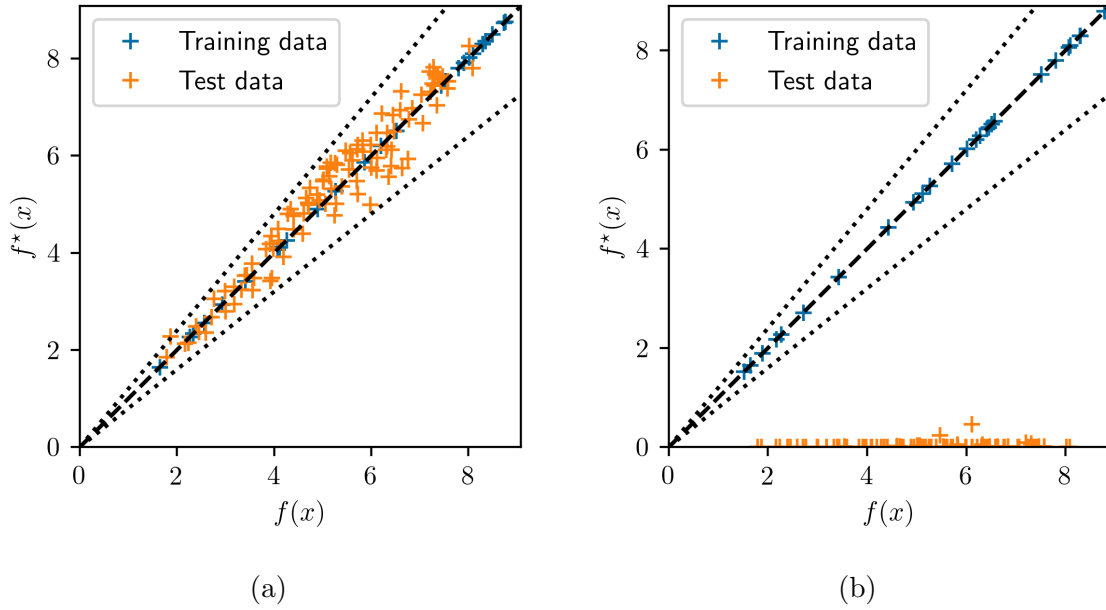


Figure 6.15: Comparison between predicted and reference values for the GP52 regression with GIO, (a), and variational sampling, (b), generated with 20 samples, for Case 4

specific area of the parameter space seems to aid the most stable result outcome without the need of additional fitting procedures.

A summary of the error values obtained with each sampling strategy, for selected numbers of samples (5, 10 or 20), is shown in Table 6.5. The active learning strategies managed to outperform random sampling in most of the chosen configurations. The variational method, based on estimates of standard deviation provided by the GP, presented the best performance on cases 1 and 3, followed closely by the greedy input passive sampling. On case 2, the latter performed particularly well, although the variational approach also presented satisfactory results in the case of 10 and 20 samples. Greedy sampling on the outputs strategy proved inconsistent across the three two-dimensional cases, where it performed particularly bad for case 2. Once more the last remaining greedy strategy (GIO) proved to work persistently across the first three cases, whereas for case 4 it was the only algorithm that provided satisfactory results. In the three-dimensional case GIO outperformed random sampling for low query numbers, whereas the latter began to be increasingly competitive as the number of samples was increased.

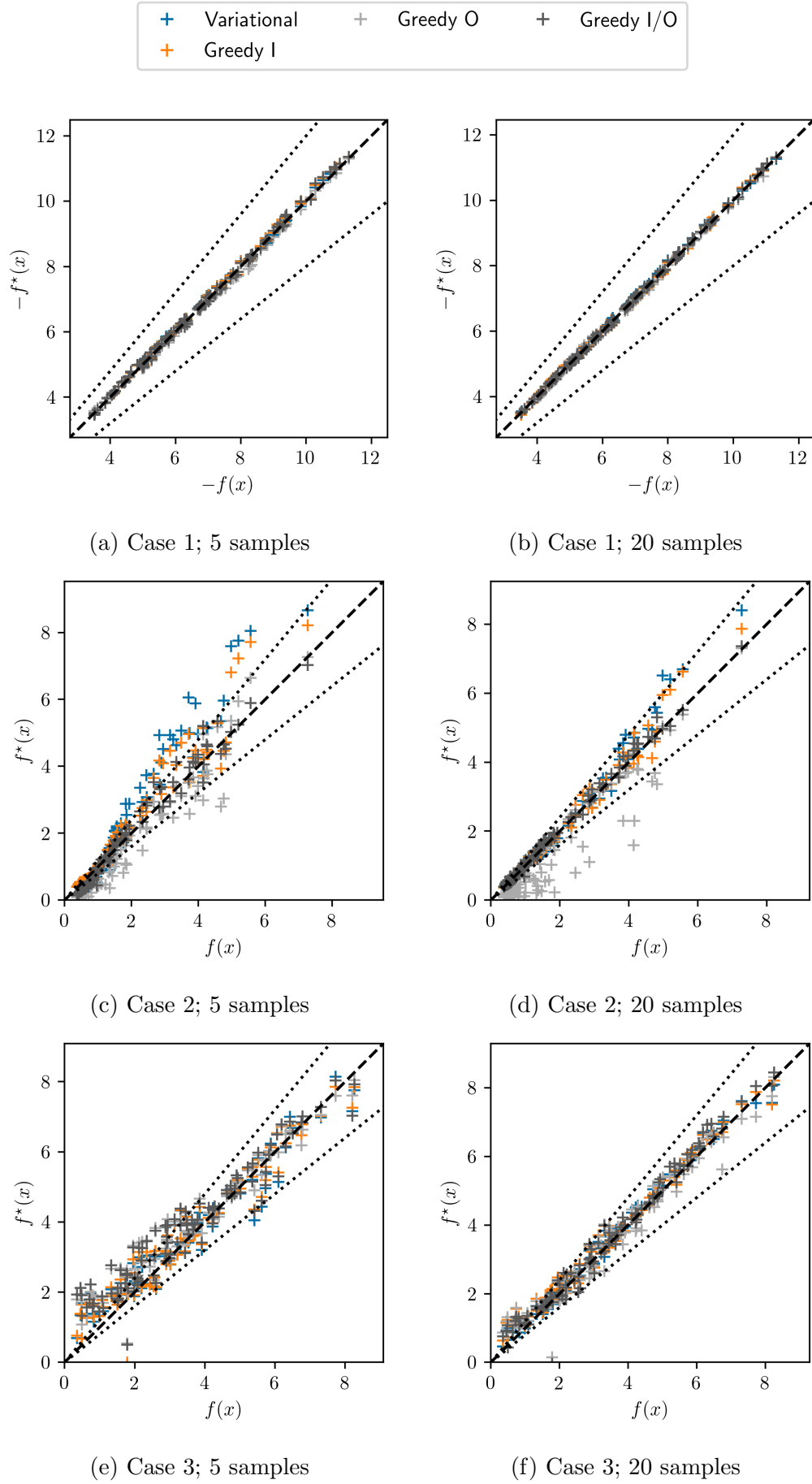


Figure 6.16: Comparison between predicted and reference values for each Cases 1 to 3, with 5 (left) or 20 samples (right). Dashed lines represent a 20% error.

Table 6.5: Error for different sampling strategies, for 5, 10 or 20 queries (V: variational, GI: Greedy sampling on the inputs, GO: Greedy sampling on the output, GIO: Greedy sampling on both inputs and output, R: random). Bold values represented the best performance in each configuration.

Case	Queries	Strategy				
		V	GI	GO	GIO	R
1	5	1	0.96	1.2	1	1.6 [1.2-2.0]
	10	0.71	0.73	0.53	0.73	1.3 [0.97-1.7]
	20	0.54	0.66	0.7	0.58	1.3 [0.85-1.7]
2	5	26	13	32	19	23 [15-30]
	10	11	6.8	34	20	15 [11-18]
	20	6.7	5	37	6.4	7.5 [6.5-8.5]
3	5	25	26	36	38	31 [26-37]
	10	18	24	25	28	28 [24-33]
	20	11	16	18	14	26 [22-29]
4	5	100	100	100	12	14
	10	100	100	100	7.7	9.9
	20	100	100	100	6.4	5.5

6.5.3 Surrogate model for wax deposition simulator

The results of the surrogate model for wax deposition, obtained with a random forest regression, are exhibited in Fig. 6.17, where sampling locations are shown with black dots – 9 simulations were used for initialization of the surrogate, followed by 240 samples obtained with the active-learning procedure (GIO). The model predicts a significant enhancement of the deposition as the superficial velocity of gas increases and the flow pattern transitions from stratified to intermittent flow. Under slug flow, the increase in the flowrate of liquid or gas magnifies the shear effect, leading to lower deposit thickness. As expected, the deposition is a strong function of the temperature, and it becomes negligible at temperatures above approximately 25 °C. In the present model, a discontinuity is observed at the transition between flow regimes, due to the fitting procedure of the shear model constants. Characterization of the transition region with experimental campaigns would allow for a better description of these conditions.

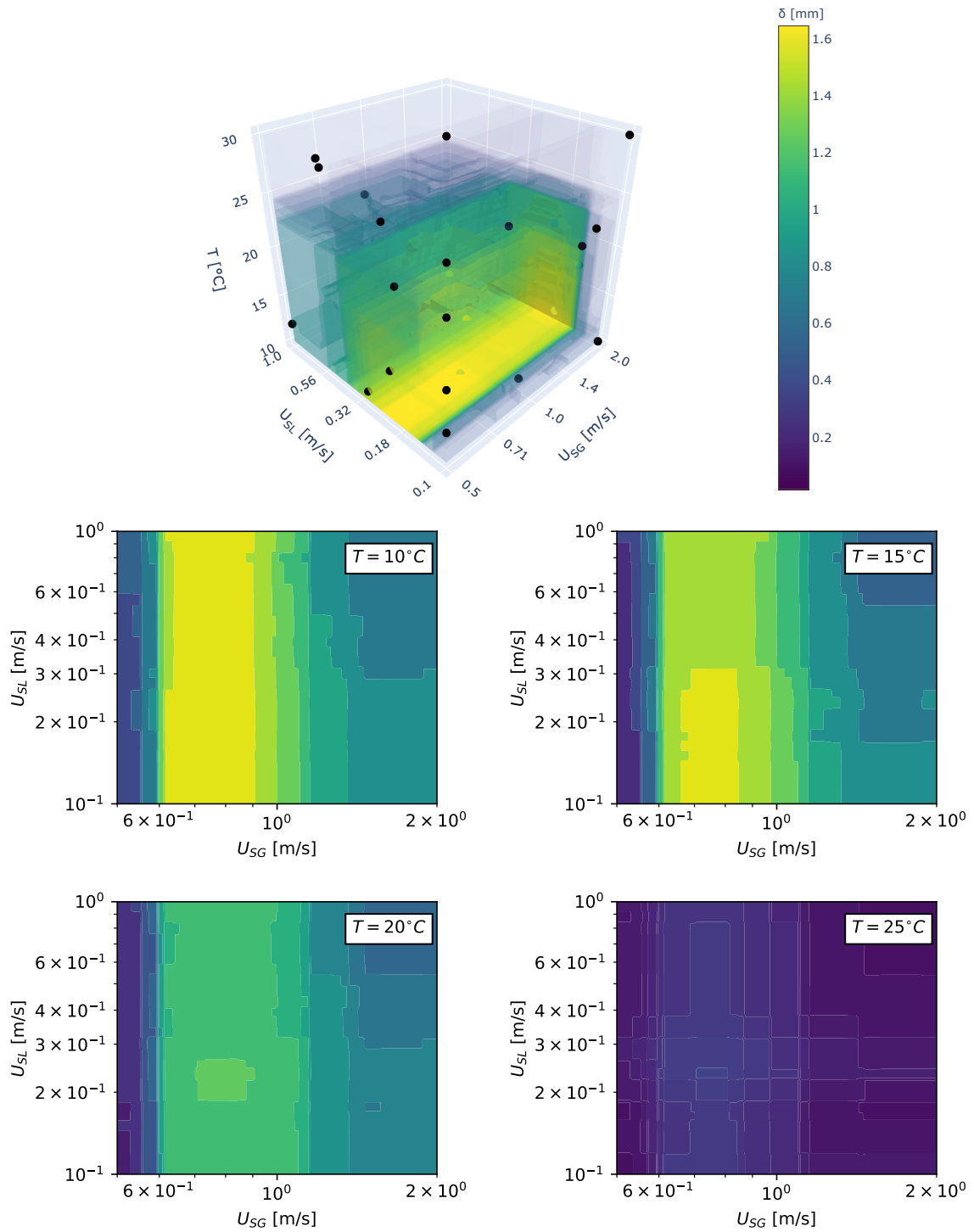


Figure 6.17: Surrogate model for deposit thickness after 24 h, as a function of temperature and gas and liquid superficial velocities.

6.6 Final remarks and future directions

We have evaluated different active-learning strategies for the development of surrogate models based on CFD simulations. The procedure was applied to a selection of industrially-relevant flow cases, and an extensive comparison between different regression and sampling algorithms was performed. In general, one active learning strategy (GIO) proved to work consistently across all cases, outperforming random sampling in most instances. This strategy proved superior to other active learning strategies particularly for Case 4, where it provided meaningful results without the need for additional fine tuning of the fitting algorithm. For the lower dimensional (Cases 1 to 3), two active-learning strategies (Variational and Greedy Sampling on inputs) outperformed random sampling for all cases considered.

The very small sample sizes, in this study, due to the restriction on the number of queries ensures that only a limited part of the parameter space for low dimensional cases is explored, which is also the case in high-dimensional problems even with increased samples. Hence potentially similar results could hold for higher-dimensional problems but this needs to be quantified in future studies. Using the methodology presented here, further benchmarks need to be developed for other classes of flow problems, involving, for example, discontinuous parameter spaces and/or noisy or stochastic results. The algorithms could also take into account the non-uniform computational cost of the simulations using an approach similar to that followed by Snoek et al. (2012). To improve upon the present results in future work, the CFD-agnostic active-learning schemes employed in the present paper might need to incorporate physical insights and case-specific knowledge.

The methods studied here were also applied to a mechanistic simulator with a lower computational cost but a large number of possible parameters, where active learning could be used to facilitate tasks such as optimization and uncertainty quantification.

Chapter 7

Conclusions & Future Work

7.1 Conclusions

The problem of wax deposition is very complex, and it is unlikely that universal models can be developed to handle any situations. Having a number of different models available is important in order to be able to execute varying workflows and evaluate the robustness of the methodologies. Here, an extensive analysis of different possibilities for modelling flows with solid deposition was performed, which included physics-based and data-driven based approaches. These methods offer trade-offs in complexity/computational cost, necessity of external closure relations, robustness to changes in conditions, and accuracy.

In the literature review, it was highlighted that despite four decades of intense research, many lines of enquiry remain open in the study of flows with deposition. A critical overview of the evolution and the state of the art in wax modelling approaches was presented. Other techniques used in the thesis, such as thin film modelling, volume of fluid simulations, graph neural networks, and active learning were introduced. Following that, the different modelling approaches were explored systematically, going from more detailed, fully resolving techniques, to global modelling alternatives.

Firstly, the existing state of the art methodology for modelling flows with wax deposition

with interface capturing approaches was reproduced in an open-source platform. Some key implementation details were discussed and contrasted, including a comparison between the original results and the open-source version. In order to overcome the high computational cost and the strict constraints induced by the time and length-scales, an approach for emulating the physical solution with a data-driven technique was explored. For that purpose, a library of functions for manipulating CFD data with graph techniques was developed. The viability of this technique was demonstrated with two test cases, one of which being a complex model of wax deposition.

Another modelling approach that was examined was the possibility of simplifying the solution procedure with the assumption of a thin deposit. This model was tested and validated with single- and two-phase flows, as well as a more complex geometry (e.g, elbows). With calibration of rheological properties of the deposit, both qualitative and quantitative observations of the deposition behaviour could be reproduced accurately. In particular, the model could explain local variations in deposit thickness, due to low shear zones and levels of turbulence. This approach can be a useful alternative to the full interface resolution since it provides important local deposit information while keeping the computational costs low.

The next technique analyzed was the mechanistic modelling of the flow with a low-dimensional formulation. A one-dimensional approach was described in detail, along with all the necessary closure relations. A large database of two-phase flow data was assembled, and the model was shown to predict flow quantities such as pressure drop and holdup very accurately, usually within a 20% error band, in a large range of operating conditions. Following that, the model was also successfully validated with wax deposition data for single-phase, stratified, and slug flows. Notably, the model includes the effects of shear removal due to turbulence, as well as the thin film created in the bubble region of a slug unit cell, which have been observed to be significant in a number of situations.

Finally, a comparison of regression and active-learning techniques for computationally intensive simulations was performed. The framework analyzed here aimed to generate surrogate models for any quantities of interest in an engineering problem, based on a limited number of physical

simulations. The use of active-learning was shown to be clearly helpful in decreasing the number of evaluations required to achieve a required accuracy, in comparison to a naive random sampling. This methodology was demonstrated in a case study of mechanistic simulations of wax deposition. The insights provided here will be useful for industrial applications, where data are often plentiful but the parameter space can be very large.

7.2 Future Work

This work has contributed to identifying and extending the state of the art in several modelling techniques. With that said, the base concepts introduced here have a large potential for future improvement and extension. In particular, the different methods could be combined into a unified multi-fidelity approach, which automatically transitions from high to low levels of details, as needed. This type of approach was used in a preliminary way in the integration of VoF simulations and graph network extrapolation, in Chap. 3, and in the combination of mechanistic model and data regression, in Chap. 6, but could be further explored, validated, and refined.

Along the same lines, as noted in Chap. 3, the graph-based approach itself has several possible avenues of exploration. One promising line would be the use of physics-informed neural networks, which would include in their architecture knowledge about the governing physical phenomena. Alternatively, work could be performed in generating extensive training data, or in improving the criteria for switching or combining simulation and surrogates. All of these approaches could contribute significantly to improving the robustness of the methodology.

With regard to the fundamental wax dynamics, extending the applicability of closure relations should be one of the priorities in the development of the models. The mechanisms for removal of material from the wall, in particular, have been shown many times to be a critical element of the problem, and existing models have struggled to describe them in a robust way.

The effect of thermodynamic models is also significant for wax deposition, and in some cases a simple model had to be adopted due to computational constraints. Mathematical approxima-

tions or data-driven models could be used instead to make a more complete description possible at reasonable computational costs.

The methodology based on the CFD simulations and thin film models proposed here is very novel and could be extended in numerous ways. The effect of the different sub-models on deposit formation and dynamics should be analyzed, and other complex geometries, such as valves or heat exchangers, could be simulated.

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