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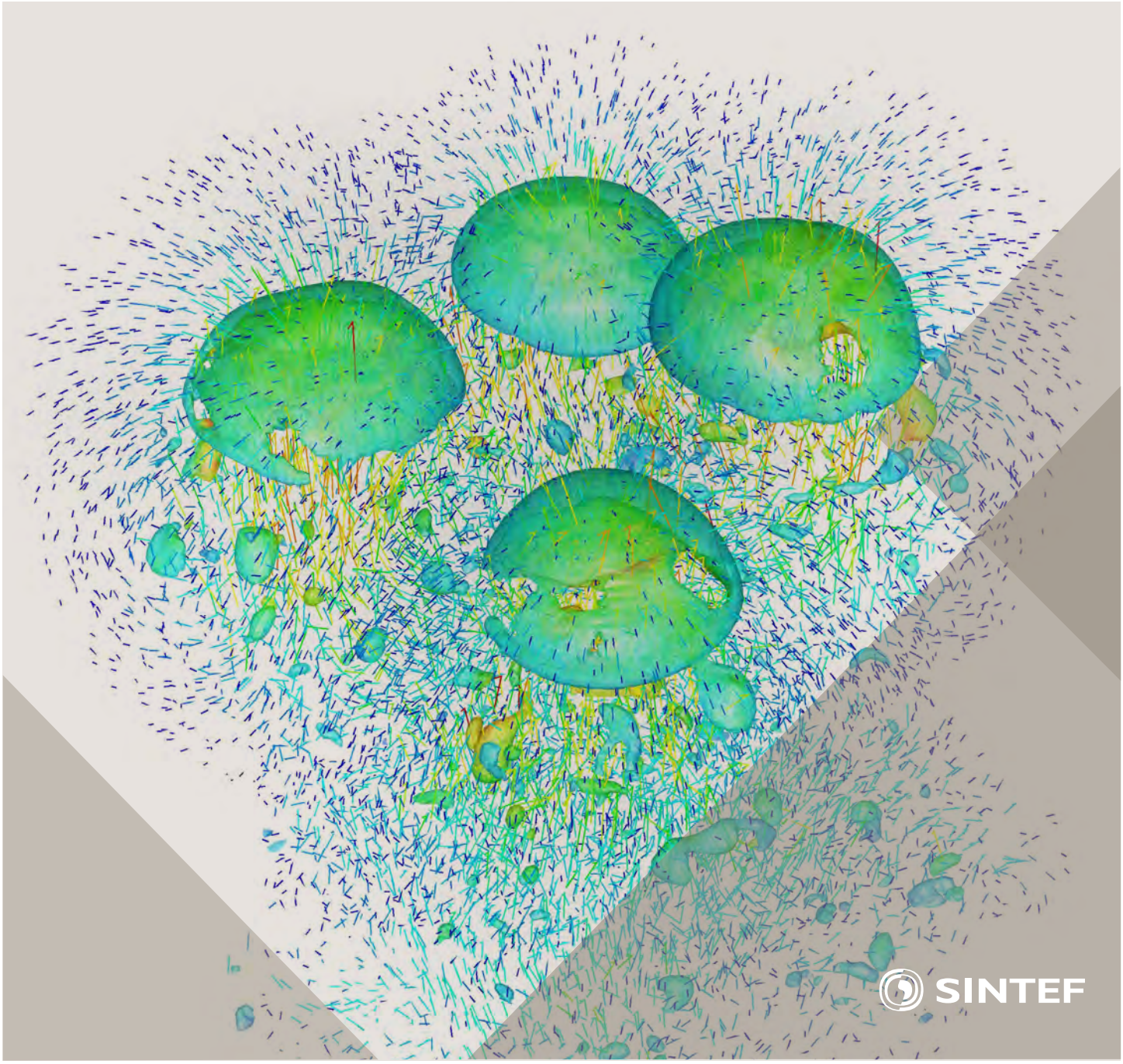
Selected papers from 10th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries

Progress in Applied CFD



SINTEF Proceedings

Editors:
Jan Erik Olsen and Stein Tore Johansen

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SINTEF Academic Press

SINTEF Proceedings no 1
Editors: Jan Erik Olsen and Stein Tore Johansen
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Key words:
CFD, Flow, Modelling

Cover, illustration: Rising bubbles by Schalk Cloete

ISSN 2387-4287 (printed)
ISSN 2387-4295 (online)
ISBN 978-82-536-1432-8 (printed)
ISBN 978-82-536-1433-5 (pdf)

60 copies printed by AIT AS e-dit
Content: 100 g munken polar
Cover: 240 g trucard

SINTEF Academic Press
Address: Forskningsveien 3 B
PO Box 124 Blindern
N-0314 OSLO
Tel: +47 22 96 55 55
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PREFACE

This book contains selected papers from the 10th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in June 2014 and is also known as CFD2014 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focus on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. The papers in the conference proceedings and this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are presented in the conference proceedings. More than 100 papers were presented at the conference. Of these papers, 27 were chosen for this book and reviewed once more before being approved. These are well received papers fitting the scope of the book which has a slightly more focused scope than the conference. As many other good papers were presented at the conference, the interested reader is also encouraged to study the proceedings of the conference.

The organizing committee would like to thank everyone who has helped with paper review, those who promoted the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: FACE (the multiphase flow assurance centre), Total, ANSYS, CD-Adapco, Ascomp, Statoil and Elkem.

Stein Tore Johansen & Jan Erik Olsen

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CONTENTS

PRAGMATIC CFD MODELLING APPROACHES TO COMPLEX MULTIPHASE PROCESSES

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ABSTRACT

Modelling of complex multiphase processes in the minerals and energy resources industries requires a balance between the pursuit for detail and recognition of computational resource limitations, if it is to lead to effective and productive outcomes. Computational fluid dynamics (CFD) modelling can be a powerful tool to assist in improving these processes or designing new processes and equipment, since flow-related operations such as mixing, reaction or separation very often limit effectiveness. However, highly detailed CFD models for such complex and large-scale processes generally require such enormous amounts of computer resources that their effectiveness for actual process improvement can be limited. High level expertise is required to ensure that proper account is taken for multi-phase interactions, multi-scale effects, and additional non-flow physics and chemistry critical to the process while allowing outcomes to be obtained on industrially useful timescales. This may be termed the pragmatic approach.

Keywords: CFD, multiphase flow, chemical reactors, flow modelling, multi-scale, pragmatic modelling.

NOMENCLATURE

Greek Symbols

α Volume fraction, [-].
ρ Mass density, [kg/m^3].
μ Dynamic viscosity, [kg/m.s].

Latin Symbols

$\mathbf{M}$ Source term (interphase interactions), [kg/m^2.s^2].
p Pressure, [Pa].
$\mathbf{S}$ Source term (body forces), [kg/m^2.s^2].
t Time, [s].
$\mathbf{u}$ Velocity, [m/s].

Sub/superscripts

i Phase.

INTRODUCTION

Processing in the resources industries generally involves large flow rates and reactor volumes, and must be performed at minimal cost given the products are bulk commodities. Small improvements in energy efficiency or product recovery efficiency can thus make a significant difference to economics of the overall operation. Such improvements can be difficult to identify and risky to realize through trial-and-error at the plant. Similarly, radical improvements are hard to test at full-scale and involve substantial risk to the operating company during implementation. Computer simulation is the obvious tool to assist process optimisation while minimising risk (Schwarz, 1994).

Processing of mineral resources to extract valuable metals or chemicals involves unit operations that are designed to achieve mixing, reaction or separation, or a combination of these, often in the same unit (Schwarz, 1991). To achieve these ends in the most efficient way, achieving the greatest product yield, requires careful design of the flow field within the reactor.

A critically important characteristic of the flow field is the intensity of turbulence. Mixing and reaction are usually achieved most rapidly and with minimum energy requirement in a highly turbulent field. On the other hand, separation requires either careful control of the turbulence field, or ideally a laminar flow. These principles are further complicated for multi-phase situations. For example the desirability of high turbulence for mixing and reaction can sometimes be tempered by the need to avoid breakage of droplets into a fine dispersion (this can reduce the efficiency of subsequent separation steps) or the breakage of particles such as catalysts. On the other hand, separation of droplets may be improved by moderate turbulence to enhance coalescence, and hence settling speeds. Clearly the design of reactors, particularly multiphase reactors, requires nuanced consideration of the optimal conditions - all the more so if two or three functions (such as reaction and separation) are being carried out in the same vessel, in which case different flow zones may be desirable.

To achieve such particular and specific conditions in a vessel which must be large to accommodate bulk flows is a demanding task unlikely to be accomplished by a

trial-and-error approach. In the past, room temperature physical modelling has been used to attempt this task, but only general information can normally be obtained because of the impossibility of exact similitude in situations with complex multiphase effects, reactions, high temperatures, etc. As an alternative, computational fluid dynamics (CFD) modelling provides a powerful tool to assist in improving these processes or designing new processes and equipment by simulating actual reactor conditions.

While there has been welcome development of powerful and versatile commercial CFD solvers (eg ANSYS CFX, 2002), the degree of difficulty in obtaining realistic yet practical models of processes in the minerals and energy domains should not be underestimated. The challenge is to represent the critical multi-phase flow physics and chemistry sufficiently realistically that factors limiting performance can be analysed, yet at the same time design the model so that it can be run in industrially-useful timescales. This may be called the pragmatic modelling approach. It requires the highest level of expertise in fluid dynamics modelling and numerical analysis, as well as the ability to interface effectively at all stages of the modelling process with process expertise, engineering requirements and experimental programs.

Pragmatic modelling generally seeks to answer a limited range of specific questions about a system to assist in design or process improvement, rather than seeking to build a “virtual reality” that would mimic every aspect of a system exactly. While this latter type of model is the ultimate aspiration, industrial-scale multiphase systems are too complex to achieve anything of this sort at present. This means that some aspects of such systems must be modelled, rather than relying on brute-force simulation to produce a virtual reality. (Modelling here means invoking physical and chemical laws to approximate a system by equations of lower order; as opposed to simulation, which implies computing the behaviour of a complex system simply by performing a huge number of basic calculations at an element level. Pragmatic CFD inevitably involves a mix of modelling, in this sense, and simulation.) Though perhaps counter-intuitive, well-designed pragmatic modelling of this kind requires far greater expertise than brute-force simulation.

Staging can be a valuable aspect of modelling. A pragmatic staged approach is schematically represented in Figure 1. Staging of CFD model development is advisable to ensure that model results are reliable as each new degree of complexity is introduced. The approach shown above integrates this procedure into a feedback loop where the results at each stage are interrogated to determine implications for process improvement. In this regard, the modeller should heed the maxim expressed by Glasscock and Hale (1994), that 80% of the benefit comes with the first 20% of model complexity! Such staging can lead to a productive cycle of innovation, whereby both process productivity and modelling development benefit.

In this paper we will consider several of the complexities involved in reacting multi-phase processes, and how to pragmatically deal with these, using examples from the resources industries as illustrations of the approach.

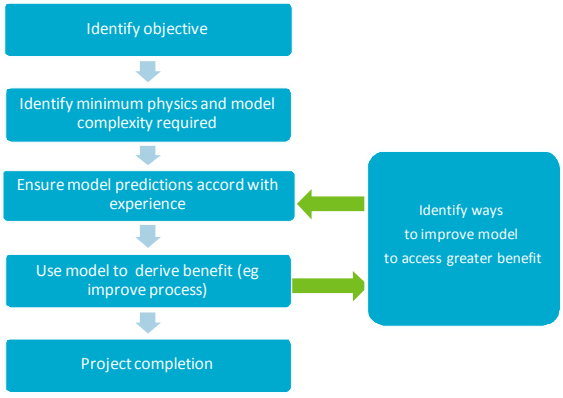


Figure 1: Flow diagram representation of a pragmatic staged approach to CFD modelling.

MULTIPHASE INTERACTIONS

Modelling Techniques

There is a vast literature on modelling techniques for multiphase flows which can be classified as dispersed or separated. The focus here is on dispersed flows, that is, flows in which an ensemble of many bubbles, droplets or particles moves within a bulk, continuum fluid; techniques for separated flow, while certainly non-trivial, tend to be more straightforward to develop and implement.

The continuum is almost always modelled by Eulerian flow equations solved using finite volume or finite element techniques over a discretised mesh (one exception being Smoothed Particle Hydrodynamics, see Monaghan, 2012).

Techniques for the dispersed phase could be conveniently categorised into three types:

- Particle tracking (Lagrangian)
- Multi-fluid (Eulerian)
- Direct simulation

Particle tracking is in principle straightforward, and is ideal for low dispersed phase loadings: most techniques of this kind do not account for the volume of the phase, nor intra-phase interactions, though particle-particle collisions are now being allowed for in coupled CFD-DEM models (Feng and Yu, 2007) and versions of the Particle-in-Cell method such as Barracuda (Snider, 2001). These limitations mean that most practical industrial modelling of large-scale dispersed systems uses the multi-fluid method as the pragmatic approach.

Multi-fluid techniques are however substantially more complex, both conceptually and in practice. The equations can be derived rigorously by averaging the

exact equations for multiple phases (by ensemble-, time- or space- averaging; see the work by Drew and co-authors, Drew, 1983, Arnold et al., 1988, Kashiwa and VanDerHeyden, 2000), giving:

Continuity equation

$$\frac{\partial \alpha_i \rho_i}{\partial t} + \nabla \cdot \left(\alpha_i \rho_i \mathbf{u}_i \right) = 0 \qquad (1)$$

Momentum equation

$$\frac{\partial \alpha_i \rho_i \mathbf{u}_i}{\partial t} + \nabla \cdot \left(\alpha_i \rho_i \mathbf{u}_i \mathbf{u}_i \right) = -\alpha_i \nabla p + \nabla . \alpha_i \mu_i \nabla \mathbf{u}_i + \mathbf{S}_i + \mathbf{M}_i \qquad (2)$$

However, terms appear in the averaged equations that cannot be evaluated and must be modelled, and the usual way of proceeding is to heuristically relate these terms to physical forces (eg drag, lift, virtual mass, etc.) and then replace them by expressions obtained from experiment or a combination of experiment and theory (e.g. Ishii and Zuber, 1979). The rigorous averaging step is important because the form of some of these terms can be non-intuitive (e.g. the terms to account for turbulent diffusion when using Favre averaging, Burns et al., 2004). In general, terms other than drag are often poorly known, particularly when turbulence is involved. For example, the classical Saffman and Magnus lift forces are known for isolated rigid particles under limiting Reynolds number conditions, but bubbly flows allow no accurate theoretical description (Sokolichin et al., 2004).

The pragmatic approach is to determine constants in expressions for interphase interaction terms from experiment: simple experiments that seek to isolate the specific interaction and/or simplified archetypes of the process conditions involved. The important aspect of the approach is that the form of the expressions used should be based on sound multiphase physics (and chemistry where appropriate). This then maximises the range of applicability of the fitted expressions.

The third category of multi-phase model, direct simulation, attempts to solve the exact equations at the particle/bubble/drop scale for a large ensemble. DEM methods are used for particles (though even here modelling must be invoked for the inter-particle forces), moving embedded grid and immersed body grid techniques can be used for particles or non-deformable drops or bubbles, while free-surface methods must be employed for deformable drops or bubbles. In general direct simulation is still not possible for most industrial scale systems, but it can be valuable for sub-domains, (see the discussion in the Multi-scale Interactions section of this paper). This approach is only now beginning to be used to determine more reliable expressions for multi-scale interactions for use in multi-fluid simulations.

Turbulence

Derivation of the multi-fluid equations for turbulent multi-phase equations involves double averaging (either explicitly or implicitly) – over turbulence (Reynolds averaging) and over phase structure (Elghobashi and AbouArab, 1983, Kataoka and Serizawa, 1989). This results in terms that contain correlations between turbulence fluctuations and phase fluctuations, evaluation of which cannot be done heuristically. Resolution of this complexity requires more detailed modelling (e.g. Large Eddy Simulation, LES, or Direct Simulation) backed by careful and detailed experimental measurements. An example is the work on stirred tanks by Tabib and Schwarz (2011) and Tabib et al. (2012). A thorough analysis of LES techniques for multi-phase flows has been given by Fox (2012). As he has pointed out, the probability density function formalism for deriving the multi-fluid equations (Pai and Subramanian, 2009) may be more suitable than averaging for determining closures, particularly for determinations based on meso- and micro- scale simulation "experiments".

Of most importance is the effect of particles and bubbles on turbulence. It is found from experimental studies that large particles and bubbles generate additional turbulence whereas small particles have the effect of damping turbulence (Crowe, 2000). Turbulence is generated in the wakes of large particles and bubbles, and various expressions have been proposed to account for this effect, with parameters that need to be derived from experiment. Unfortunately, there is no general agreement on a definitive expression at this stage. The damping effect caused by small particles results from the lag in response of a particle to random eddy movements. Expressions have been derived for this effect dependent on the ratio of particle size to turbulence length scale (Crowe, 2000), Stokes number, or force considerations (Kataoka and Serizawa, 1989).

Diffusion (dispersion) of a particulate or bubble phase can be problematic to model. Diffusion of a bubble plume in an industrial application was first introduced by Boysan and Johansen (1985) and Johansen et al. (1987) in Euler-Lagrangian simulation, and by Schwarz and Turner (1988) in Euler-Euler simulation; they showed it could have a substantial effect on predicted plume velocity. In the case of bubble plume, diffusion is caused both by turbulent dispersion and bubble-wake interactions, which in the simplest case of a single spherical bubble is described as the "lift force", but in the case of a swarm of bubbles, some of which are highly distorted and wobbling, is rather more complex. Moraga et al. (2003) discuss some of these complexities in more detail.

Unexpected particle-turbulence interaction effects also occur. Brucato et al. (1998) found that the slip velocity of particles/bubbles decreases as the particle size increases relative to the turbulence scale, and Lane et al. (2005) showed that local voidage values could not be correctly predicted for a stirred tank with air sparging,

unless this effect is taken into account in the multi-phase CFD model. Further data was obtained by Doroodchi et al. (2009), but the effect is still not well understood. It may be that it reflects varying degrees of centrifuging of particles/bubbles to the edges/centres of turbulent eddies.

As with the multi-phase closures discussed in the previous section, the pragmatic approach seeks to use the best physics knowledge available together with empirical constants obtained from available experimental data to develop expressions for the turbulent multi-phase closures. Pragmatism demands a high level of understanding of the flow physics involved, together with the ability to design and interrogate experiments to develop the sub-models required for the CFD simulations.

Transient Flows

Turbulent flows are of course time-dependent, but this dependence is generally removed by Reynolds averaging, resulting in effectively steady-state equations. When unsteadiness is forced by impellers or pulsing, it is found that U-RANS (Unsteady Reynolds Averaged Navier-Stokes) models such as k-ε perform well: good agreement has been found for stirred tanks (Lane et al., 2000) and for periodic variation in a pulsed column (Bujalski et al., 2006).

However flows can also be subject to internally generated large-scale instabilities that are not properly described as turbulence, and this is particularly so for multi-phase flows. Straightforward application of U-RANS can result in damping of the large-scale unsteadiness that one wishes to capture, and one approach to overcome this is to use LES.

An important example of an industrial reactor in which such phase-driven unsteadiness is a major characteristic of the flow is the fluidised bed, models of which were pioneered by Gidaspow (1994) and implemented first in CFX by Witt et al. (1998). In bubbling beds, it is believed that damping due to the high solids loading prevents any shear-related turbulence, so the continuum is modelled with a laminar assumption. The same assumption is used to model fast fluidisation and circulating fluidised beds, although its validity is likely to be questionable in the lean regions.

A pragmatic compromise between U-RANS and LES, (dubbed Very Large Scale Eddy Simulation, VLES) was used by Schwarz (2001) and Davis et al., (1998) to simulate gas-agitated baths. This technique has been placed on a firmer footing for certain single phase flows by Labois and Lakehal (2011) (see also Johansen et al., 2004).

In some cases capturing the transient behaviour fully in a CFD simulation may be beyond what can be achieved in an industrially-relevant time-frame. Other modelling techniques can then be called upon to complement the steady-state CFD simulations. An example is the coupling between bubble plume dynamics and surface wave motion in a system such as ladle refining. Schwarz (1990, 1995) developed a mathematical model for the coupling that could be used in a pragmatic way together with a steady-state multi-fluid model of the bubble plume to provide a more complete picture of the flow dynamics in the system.

Example of a Gravity Thickener

Gravity thickeners are large tanks used to separate fine solids from slurries by flocculating them into aggregates. The solids then settle more readily to a bed which can be readily removed via an underflow. Modelling of thickeners was conventionally confined to one-dimensional modelling of bed consolidation until CSIRO researchers recognized that upstream conditions and flocculation performance would substantially control the effectiveness and extent of bed consolidation. This together with the introduction of three-dimensional multiphase CFD modelling revolutionized the understanding of thickeners. This research has been conducted at CSIRO through a long-running series of projects (labeled P266), substantially funded by the mining industry through its research broking organization, AMIRA International.

One of the first important findings was that density currents, flows generated by differences in effective slurry density from one part of the tank to another, can be remarkably strong. The density differences arise from differences in solids concentration, and are most pronounced when the feed has a reasonably high solids concentration, say more than 5%. In such situations, the feed stream can sink quite rapidly out of the feedwell, without mixing into the dilution streams being entrained into the well, as illustrated in Figure 2 (Johnston et al., 1996). The most serious situation arises when the feed-stream leaves before mixing with flocculant, as this results in both poor flocculation and waste of expensive flocculant. Kahane et al. (1997) showed that use of CFD could ensure that flocculant sparges were optimally placed for mixing into the feed, and that shelves could be used to reduce the short-circuiting induced by density currents. In fact, in one case (at Worsley Alumina) such design changes were so successful that the throughput could be doubled with no degradation in performance, saving the company millions of dollars in capital and operating costs (Kahane et al., 2002).

Perhaps the most remarkable aspect of the CFD modeling behind this initial research is that it incorporated very little of the flocculation mechanisms themselves, and did not include the presence of the bed. This highlights an aspect of pragmatic modeling – that a model does not need to incorporate all the detail of a process to be valuable.

To guide more refined design changes, the CSIRO model has been extended in stages to include aspects of the flocculation process. Schwarz and Johnston devised a model for flocculant mixing and adsorption onto particles (Kahane et al., 1997) which has been used

extensively to assist many sponsor companies improve their thickener design and performance (Kahane et al., 2002). More recently, Heath and Koh (2003) have incorporated a full population balance model for aggregate size within the CFD model, and the model has been extended to further enhance the diagnostic capability (Nguyen et al., 2006).

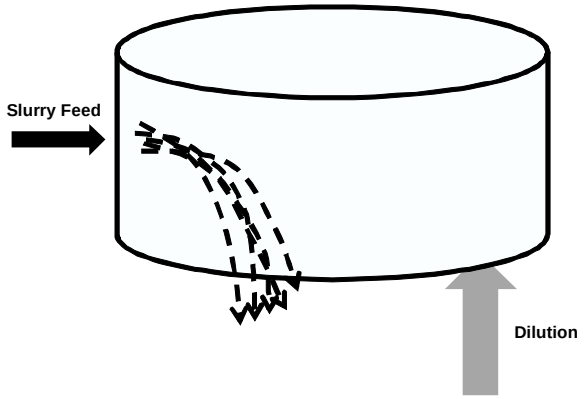


Figure 2: General behaviour of slurry feed in thickener feedwells found from CFD modelling (after Kahane et al., 1997).

COMPLEX PHYSICS AND CHEMISTRY

Additional variables that must commonly be solved for in CFD simulations are temperature and species concentration, as expected for applications involving heat and mass transfer. In the simplest situation, this is done by solving the standard advection-diffusion equation. However the situation quickly becomes more complex when reactions, solidification, melting, etc., are involved. Techniques are well established for homogeneous turbulent reacting systems (e.g. gas phase reactions), but when reactions involve particles, drops or bubbles, care must be taken to properly account for boundary layer diffusion, chemical kinetics and surface effects. These are all very situation dependent.

One of the most prevalent reaction systems in industry is combustion, and coal combustion is a multi-phase system for which there has been some effort developing CFD modelling techniques (Stopford, 2002), but the wide variety of properties of coal used and the complex fluid dynamics of multiple interacting industrial-scale jets mean that these are still challenging systems (see, e.g., Tian et al., 2010).

Other physical effects that can be important include particle attrition, surface erosion, droplet and bubble coalescence and breakup, effects due to magnetic and electric fields, Marangoni effects, and so on.

Bath Smelting Model

The HIsmelt Process is an iron-making process based on molten iron bath smelt-reduction (Davis et al., 1998). Iron ore fines and coal are injected into the iron bath through submerged inclined lances. Coal is devolatilised and carbonises the iron bath; iron ore reacts with the carbon to generate large volumes of CO gas, which, together with the volatiles, throw iron and slag drops and streamers into the topspace of the smelting vessel. The CO and H_2 gases are burnt in the topspace in a swirled flame, and the heat returned to the bath by slag droplets. It is important that iron drops are not oxidised in the oxidising atmosphere of the topspace. Designing and scaling-up the process thus involved many challenges, and CFD modelling was applied extensively to assist using a staged pragmatic process, as suggested in the Introduction.

Development of a CFD model of the smelting bath (Schwarz, 2001, Schwarz and Davis, 2011, Stephens et al., 2012) required linking together multi-phase techniques with considerable physics and chemistry that required experimental inputs. The two liquid phases (slag and metal) are agitated extremely vigorously by very large rates of submerged gas generation. The first pragmatic decision made was to split the problem into a "bath model", which involves considerable transient multi-phase complexity, and a "topspace model", which focuses on gas-phase combustion with heat and mass transfer to droplets. The splitting allowed faster development of each model, and, since the latter is steady-state, more rapid evaluation of design options.

The two models are coupled primarily by means of the fountain of droplets generated by the bath – fountain characteristics (mass, height, etc) determined by the bath model were fed into the topspace model. Because of the long run-times for the bath model, a "correlation", based on semi-theoretical derivation and fitted to "data" from a limited number of CFD simulations, was used to interpolate fountain characteristics for design investigations. Surrogate modelling of this sort can be a successful feature of a pragmatic approach.

The bath was initially modelled using a two-phase model of gas injection into a molten iron bath (Schwarz et al., 1987, Schwarz, 1995), with an "instantaneous-reaction rate" model i.e. gasses generated instantly from coal devolatilisation and ore reduction. Data from water, molten tin and molten iron baths were used for validation.

A slag phase was later added, with the three phases treated by the multi-fluid (Eulerian) technique, and the interaction between the two liquids was treated with the algebraic slip (or mixture) model. Coal and ore particle tracking was also added using the Lagrangian technique, with the particles able to penetrate into the liquid phases, where they then react, generating gases. Simplified reaction kinetics were designed to capture important timescales of both coal devolatilisation and ore reduction, without attempting to simulate all the details of what are extremely complex interaction phenomena at the particle scale.

A considerable amount of experimental work, both in the laboratory and from pilot plant, was done to assist

the development and validation of the model at various stages of its advance (Schwarz, 2001, Schwarz et al., 2011).

Keys to the success of the pragmatic approach were: staging of the development, with the model assisting design and scale-up along the way; close-coupling of modelling with plant trials and experimental work, with modelling suggesting further experimental work and engineering considerations driving modelling developments; and an objective-driven team approach.

An example of the computed liquid distribution on one plane through the reactor at one instant of time is shown in Figure 3. Gas (red) generated near the tips of the lances throws splash in the form of drops and streamers up into the topspace of the vessel. The positioning of the lances is critical to ensuring that gas is generated in appropriate locations to drive the required amount of splash to the required height in the vessel. The fountain of slag splash must be positioned so as to enable transfer of heat back to the iron bath, but also to ensure that iron is not re-oxidised by the topspace atmosphere.

Figure 4 shows typical computed trajectories of ore particles in the CFD model of HIsmelt reactor. The red tracks show the jets from the lances, while the orange tracks show particles at various degrees of reaction. Results of such models were used to determine fountain characteristics such as height, mass, and position relative to the top jet flame, and hence assist design of injection configuration and lance positioning. CFD modelling was a critical component of the process development which resulted in successful operation of a demonstration-scale plant (nominally 0.75 Mt/yr).

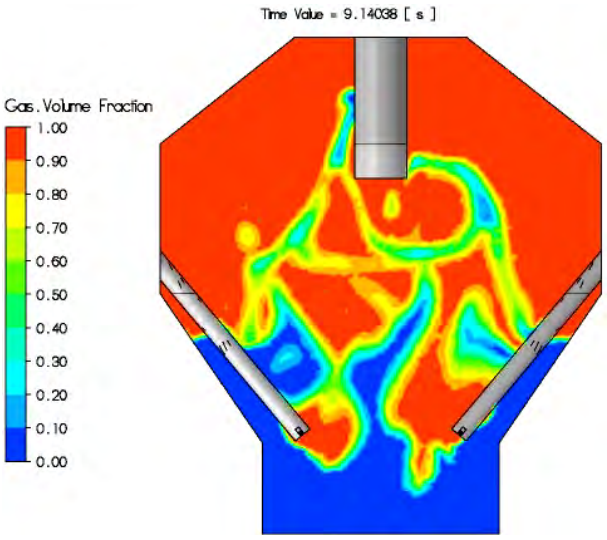


Figure 3: Gas volume fraction contours and splashing of liquid at one instant of time in CFD model of HIsmelt reactor. From Stephens et al. (2012).

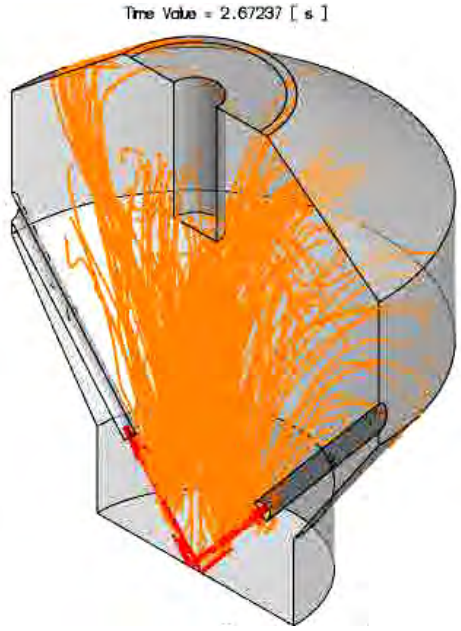


Figure 4: Typical computed trajectories of ore particles in CFD model of HIsmelt reactor. From Stephens et al. (2012).

FCC Regenerator Model

The FCC (Fluidised Catalytic Cracker) regenerator is a turbulent fluidised bed in which catalyst is regenerated by burning off the coke deposited during cracking. In the facility at the BP Bulwer Island refinery, air and oxygen enriched air is injected through distributor rings near the base of the bed and as carrier gas for catalyst being returned from a cooler (Schwarz and Lee, 2007). Prior to 2006, there had been some indications that the regenerator performance could be improved, for example, measurements showed temperature differences from one side of the vessel to the other. Catalyst performance is sensitive to overheating, so optimum performance of the regenerator would be obtained with a uniform internal temperature.

As mentioned previously, fluidised beds can be modelled using the two-fluid approach in which the solids phase is treated as a quasi-fluid. This is a sensible pragmatic approach, but it must be remembered that interaction terms such as drag, solids pressure and solids viscosity can be quite complicated. Particles tend to cluster in turbulent (and fast) fluidisation, but the small-scale structures (i.e. clusters) are too small to be captured in industrial simulations. As a result, drag is far too high if the single-particle drag formulation is used. While techniques are being developed to overcome this problem (e.g. Li et al., 2010), no entirely satisfactory solution exists. In this work, a pragmatic approach was adopted, in which effective cluster size was determined from experimental pressure drop.

A pragmatic approach was also applied to modelling combustion, with reactions limited to four species, and kinetics determined from experimental work. One additional element needed to be added to the modelling strategy: the fluidised bed model requires a very short

timestep (of order ms) for stability, yet the thermal timescale is of order many hours. To address this issue, a specialised averaging technique was developed (Schwarz and Lee, 2007): a smart pragmatic approach as opposed to brute-force integration which would not have been possible in a realistic time-frame.

A relatively sophisticated multi-phase reacting model of the regenerator could then be developed: analysis using the model together with plant experience identified likely by-passing by some oxygen through the bed. The model was then used to trial possible modifications to the catalyst return distributor, identifying one which was likely to improve the situation. When implemented in the plant, the modified distributor resulted in improved oxygen utilisation and increased temperature uniformity (Schwarz and Lee, 2007).

Figures 5 and 6 illustrate the computed gas distribution and catalyst flow field on one plane through the regenerator before the modifications were made.

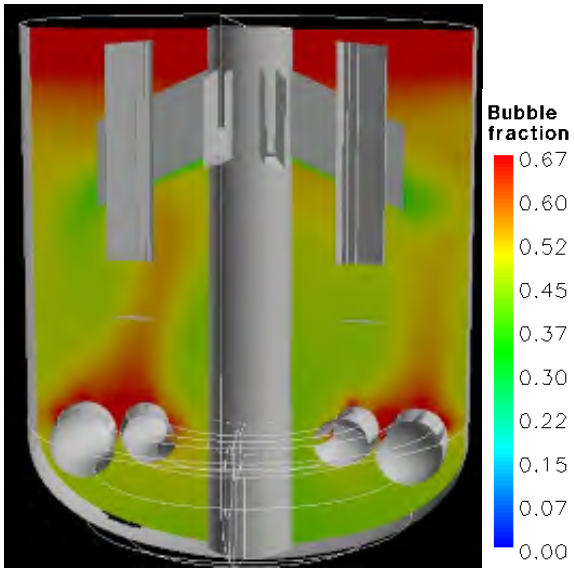


Figure 5. Computed time-averaged bubble fraction plotted on a vertical plane bisecting the regenerator for the original configuration. From Schwarz and Lee (2007).

MULTI-SCALE INTERACTIONS

Techniques

Techniques for multi-scale modelling have been pursued with enthusiasm and some success in the field of materials science. However, attempts to develop a methodology for CFD simulations of complex process applications have not progressed far, though some mathematical methodologies have been formulated for single phase flows and for porous media applications in the oil and gas industries where the technique is known as up-scaling.

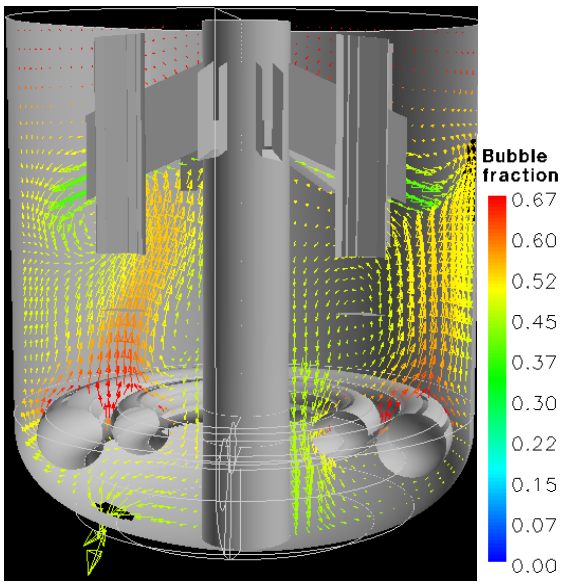


Figure 6. Computed time-averaged vector velocities plotted on a vertical plane bisecting the regenerator for the original configuration. Vectors are coloured by bubble fraction. From Schwarz and Lee (2007).

Multi-phase processing-related flows are often rich in phenomena occurring at a wide range of length and time scales. Of course turbulence itself is a multi-scale phenomenon, where the length scales are widely separated in the case of high Reynolds number, and well developed techniques exist, supported by a huge experimental data base.

Many of the characteristic scales in processing applications are defined by the length-scales of phase structures, e.g., bubbles, particles, drops, etc., and although multi-phase modelling techniques can be used to simulate a wide range of related effects, many of the terms remain uncertain, and more complex interactions are simply beyond standard methods.

E (2011) has summarised and categorised multi-scale modelling methodologies. Some researchers define multiscale modelling narrowly as simulation at various scales simultaneously (termed concurrent by E): the quantities needed in the macroscale model are computed *on-the-fly* from the microscale models as the computation proceeds. Development of computer algorithms and programming necessarily plays a large part in this approach. On the other hand for complex processing applications, sequential multiscale modelling has been found to a more fruitful approach at CSIRO. E defines this method to be one in which some details of the constitutive relations in a macroscale model are precomputed using microscale models. This is a more efficient approach when the microscale simulations are time-consuming, and the macro-scale simulations require results from many points of the micro-scale parameter space (in the case of CFD models, results are typically required at many spatial points, at many times, and at many stages during the convergence procedure).

Such multi-scale modelling has the characteristics of pragmatic modelling, since it aims to use smart techniques to avoid the pit-falls of a straightforward brute-force approach.

An intrinsically multi-scale system of importance in process engineering is the fluidised bed. As mentioned, hydrodynamic instability leads to the formation of particle clusters, particularly in turbulent and fast fluidisation, and these cannot normally be fully resolved in simulations of very large systems such as industrial-scale circulating fluidised beds (CFB). Multi-fluid models of CFB risers in which gas-solids drag is given by the single particle value predict incorrect solids velocity. One approach to solve this issue is the EMMS (energy minimization multi-scale) model (Li et al., 2010), in which an equation based on energy minimisation is effectively solved for cluster size as a function of position in the riser; this diameter is then used in a multi-fluid simulation.

On the other hand, Igci and Sundaresan (2011) have used the sequential multiscale modelling approach as defined by E (2011): they present a methodology where computational results, obtained through highly resolved micro-scale simulations of gas-particle flows, are used to improve macro-scale models. Results from microscopic models are filtered to deduce models for the residual correlations (or closures) appearing in the corresponding filtered two-fluid model (TFM) equations that are appropriate for coarse grid simulations (their so-called coarse grained equations). Using the kinetic theory-based TFM, they obtained computational data on the filtered drag coefficient, the filtered particle phase pressure, and the filtered particle phase viscosity, which they reduce to the form of correlations that can readily be employed in coarse-grid simulations.

This sequential approach has been taken at CSIRO for the complex multi-phase system involved in mineral flotation. Detailed models of particles in a turbulent stream flowing past a single rising bubble (Liu and Schwarz, 2009) have led to improved expressions for collision rates and hence particle-bubble attachment rates. These can be used to improve macro-scale models of the entire flotation cell (Koh and Schwarz, 2008) in which statistical techniques must be used to quantify attachment rates. With such a complex process with length scales of importance ranging from metres down to the nano-scale, experiment inevitably plays an important role. Verrelli et al. (2014) have designed a well-controlled experiment to study the attachment process with interactions occurring in a realistic way, as in industrial flotation. In the following sub-section, we summarise a similar approach being taken for a smelting process.

Aluminium reduction cell modelling

Aluminium is produced industrially by electrolysis in the Hall-Heroult process: an electrical current is passed between carbon anodes partially submerged in a bath of molten cryolite electrolyte and a cathode on which a pool of molten aluminium forms. Alumina is dissolved in the cryolite and CO_2 bubbles are evolved on the bottom surface of the anodes as a result of the reduction. The bubbles slide along the anode until they reach channels in which they can rise to the electrolyte surface. As they rise, they drive recirculating flows in the cryolite that are critical to the process: the flows assist in the dissolution and mixing of alumina normally fed at a small number of discrete points in the cell, and they are critical to the maintenance of a stable frozen cryolite layer (or “ledge”) on the side walls of the cell which protects the walls from chemical attack by the molten cryolite.

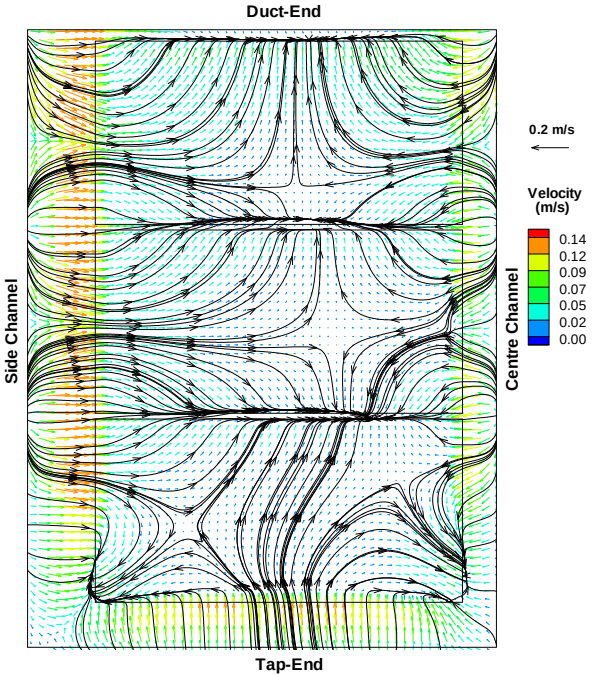
Feng et al. (2010) have developed a two-fluid model of bubble driven flow in the cell to investigate issues such as alumina dissolution, heat transfer to the ledge, and minimisation of the bubble-related component of electrical resistance by reducing the hold-up of bubbles under anodes. The model was validated using PIV (Particle Image Velocimetry) measurements of velocity in an air-water physical model of a cell built at industrial scale and comprising three anodes. Figure 7 compares the water velocity distribution over a horizontal plane just below the anodes obtained with a two-fluid CFD simulation with that measured by PIV. The measurement plane is halfway between the base of the anodes and the bottom of the water bath; since water is used to simulate the electrolyte, the bottom of the water bath represents the boundary between cryolite and molten aluminium.

The agreement between model and measured flows found in Figure 7 is remarkable given the complexity of the pattern, and the sensitivity of the flow to minor perturbations – the lower faces of the anodes are all flat and horizontal, so bubbles do not *a priori* have any preferred direction of travel along the faces. In reality the bottoms of the anodes wear to a somewhat rounded shape, which then biases the movement of bubbles in the direction dictated by buoyancy.

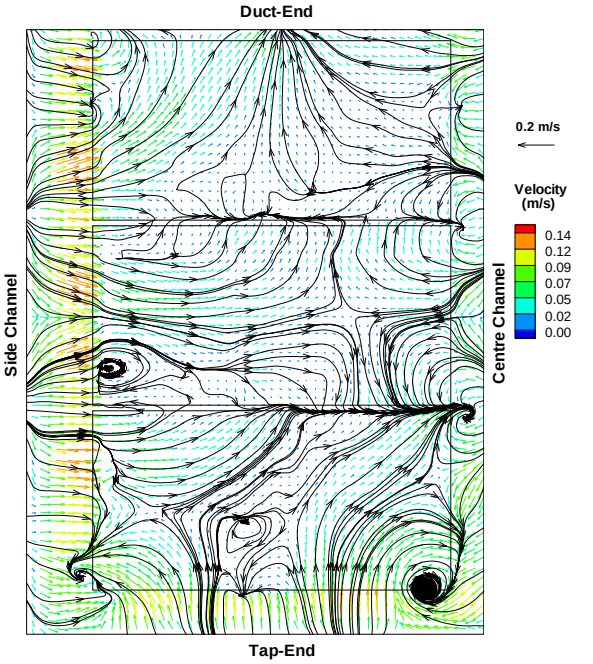
It is believed that bubbles initially form in the fine sub-millimeter size range and coalesce as they move under the anodes. The complexity of bubble shape, contact angle issues at the surface of anode, bubble coalescence (and breakage in the vertical channels), and other such phenomena cannot be accounted for in the two-fluid model with standard sub-models. The approach being pursued is to use a VOF (Volume of Fluid) approach to simulate individual bubbles to determine constitutive relationships for the multi-fluid macro-model (Zhang et al., 2013).

Figure 8 illustrates bubble shapes calculated with such a VOF model by Zhang et al. (2013). Three different bubble sizes are shown sliding under an anode base inclined at 1.5° to the horizontal. The shapes and thicknesses calculated for an air-water system (Figure 8(a)) are in good agreement with experimental observations in such physical models. Figure 8(b) shows the corresponding computed bubble shapes for a

CO_2-cryolite system. The shapes are very similar, lending support to the use of air-water models to study electrolyte dynamics, though the thickness of the bubbles is less for the real CO_2-cryolite system.



(a) CFD



(b) PIV

Figure 7: Water velocity distribution over a horizontal plane in the middle of anode-cathode gap: (a) CFD simulation; (b) PIV measurement. From Feng et al. (2010).

Standard closure relationships for drag and other interphase interactions do not exist for the unusual bubble shapes shown in Figure 8, and indeed the motion of those bubbles along the bottom surface of the anodes also invalidates the use of standard closures. The multi-scale approach adopted here aims to determine the closures from such micro-scale simulations by treating them as numerical "experiments". Examples of quantities that can be readily determined are bubble size, shape and drag coefficient, and the results can also be interrogated for more complex characteristics such as bubble-turbulence interactions.

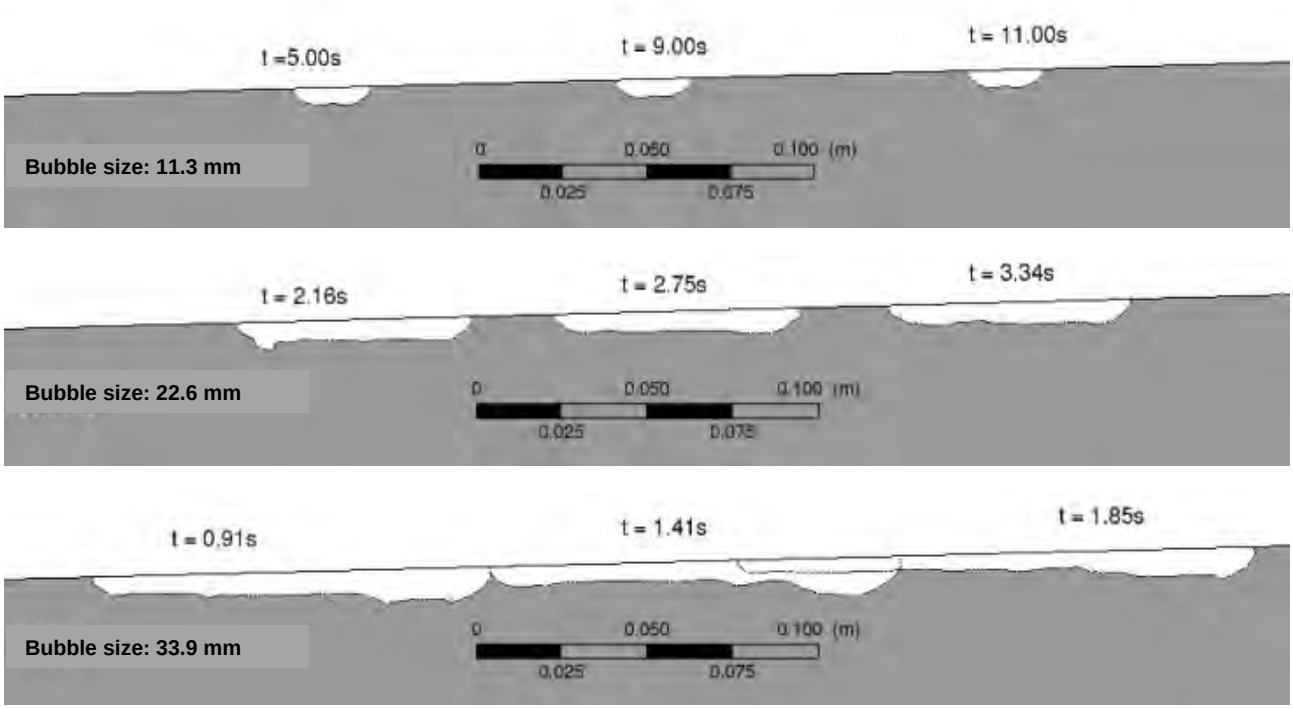
VALIDATION AND UNCERTAINTY

It is important that CFD models are validated so that they can be applied with confidence. There are two quite different processes involved in ensuring that a CFD model is reliable. The first entails ensuring that the intended algorithm for solving the discretised equations has been properly coded, that the solution converges to the actual solution as the mesh and time-step are refined. When using a commercial code, much of this process has already been done, but given the necessity to incorporate process specific physics and chemistry, it is important that additional checks are done by the user. For multi-phase flows, this checking process should be conducted against behaviour expected by analysis of the equations (usually for simplified cases), not against experimental data, which is always subject to uncertainties.

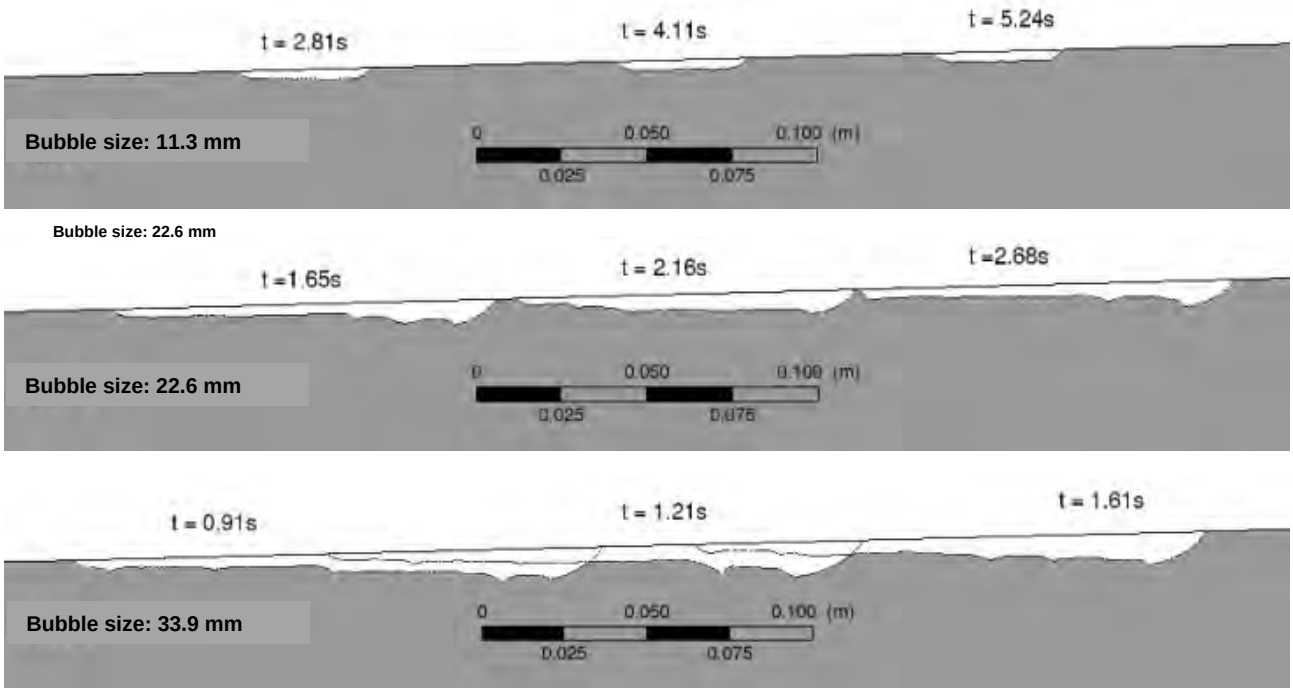
The second process of model validation entails ensuring that the equations, and especially the terms for complex physics and chemistry, correctly represent the actual physics and chemistry. This is a much more complex process because, as mentioned, constitutive closures for complex multiphase situations are generally poorly known. Development and validation of a CFD model is often undertaken in a stage-wise fashion, with targeted laboratory experiments designed to assist specific aspects of the physics and chemistry implementation. Finally, the model is preferably checked against some measurements taken from the actual plant: often these will be more integral in nature (e.g. pressure drop or overall reaction rate), or a limited number of point measurements of quantities such as velocity, temperature, and concentration. By their nature, these data are intrinsically less useful for model development or improvement than for assessment of model reliability.

Detailed flow measurements are always difficult to make in complex multi-phase flows because of issues such as lack of transparency to visible light, high levels of turbulence, other sources of variability, and biasing effects whereby average measurements are often weighted to either high or low levels of dispersed phase volume fraction. Additionally, detailed measurements are usually constrained to room temperature non-reactive physical models of the actual system, whereas reaction and temperature effects can interact in a significant way with flow behaviour. To overcome this limitation, one can use a multi-scale modelling approach, whereby constitutive relationships are derived on the basis of micro-scale computational models which can capture the actual physics and chemistry more exactly than a macro-scale model of the entire process. This approach has been described in the section Multi-scale Interactions, with an example of the aluminium reduction cell: micro-scale models can capture the movement of CO_2 bubbles in molten

cryolite under an anode with more reliability than air-water physical models.



(a) Air-water system



(b) CO_2-cryolite system

Figure 8: Computed bubble shapes for bubbles of three sizes sliding along the bottom surface of an anode in (a) an air-water system, and (b) a CO_2-cryolite system.

The reality of financial pressure in industry means that CFD modelling will often be carried out using standard constitutive relationships together with minimal checking of model behaviour against plant experience. While this is less than ideal for complex processes, modelling results using this approach can still indicate likely paths for process improvement.

As CFD modelling becomes more mainstream, there are increasing demands for uncertainty (or error bounds) to be provided with results. While this is possible for simpler single phase flow situations where uncertainties are dominated by numerical considerations (Karimi et al., 2012), it is much more challenging for multi-phase process applications, where uncertainties are typically dominated by uncertainties in constitutive closures and the representation of the multi-phase physical and chemical interactions. No general procedure exists for assessing uncertainty in such situations, though parameter sensitivity tests can certainly be valuable.

Such an assessment carried out thoroughly is expensive and requires some knowledge of possible ranges in values for parameters from correlations used to describe physics and chemistry. Drzewiecki et al. (2012) were able to carry out such an assessment for a well defined benchmark case because of the limited run times needed for the two-dimensional model used. Gel et al. (2013) avoid the high cost by utilising a surrogate model to propagate uncertainties in inputs through to the end results. Another approach involves comparison of predictions with measurements from plant if available. Care must be taken here however, since experimental uncertainty is rarely properly assessed for plant measurements, plagued as they are by factors such as variability and uncertainty in feed rates and characteristics: measurement error is often not the major source of uncertainty.

Though it will be far from straightforward, research should be conducted on methods of uncertainty assessment for complex multi-phase flows. Furthermore, canonical flows involving reasonably complex but well-defined multi-phase situations should be identified and characterised with a high degree of accuracy as a platform for model validation and uncertainty.

CONCLUSION

Resource processing operations are complex, involving multi-phase and multi-scale effects as well as other physical and chemical phenomena. Detailed flow-based computer models incorporating these effects are the obvious design and optimisation tool, but must be developed with care to ensure they are realistic, predictive and applicable on industrially-relevant time-frames. Expert pragmatic modelling employs suitable approximations to achieve this aim.

Multi-fluid techniques are presently the most versatile and well-developed methods for modelling complex industrial-scale multi-phase processes, and have been shown to be valuable in improving the efficiency of existing processes and equipment such as gravity thickeners and in assisting the development of new processes such as the HIsmelt Process. This approach does not seek to simulate every individual bubble, particle, or droplet, but uses physical, chemical and engineering expertise to model their interactions.

The following guidelines should be followed to ensure optimal outcomes:

1. Staging of model development, with process implications being sought at each stage and feedback from plant to model, results in faster industrial application, and can lead to a productive innovation cycle.
2. Close coupling with process engineers during staged development ensures that the model is designed to address critical issues, and that it reflects observed plant trends.
3. Constitutive closures for interphase interactions necessarily involve empirical input for moderate-to-high dispersed phase loadings in turbulent flow regimes. Expressions for interphase interactions should however be based on sound physical and chemical principles, albeit with fitting parameters.
4. RANS methods appear to be satisfactory for transient flows resulting from imposed forcing, but processes with internally generated flow instabilities may be better tackled with multi-fluid large eddy simulation (LES) methods.
5. Sequential multi-scale modelling using meso- and micro-scale models is a powerful tool for determining constitutive closures and improving macro-scale models of micro-scale physical and chemical processes.
6. Effort needs to be undertaken to refine validation methodologies and to identify ways to assess prediction uncertainty.
7. Teamwork is often a hallmark of successful process design and optimisation using CFD, since sophisticated interfacing with experimental, plant, process engineering and chemistry expertise may be needed.

ACKNOWLEDGEMENTS

The authors wish to thank CSIRO for permission to publish this paper, and all our colleagues and collaborators for their contributions.

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