Computational Fluid Dynamics

Applications in Environmental Hydraulics

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1

Computational Fluid Dynamics modelling for environmental hydraulics

P.D. Bates, S.N. Lane and R.I. Ferguson

1.1 Introduction

Computational Fluid Dynamics (CFD) was developed over 40 years ago by engineers and mathematicians to solve heat and mass transfer problems in aeronautics, vehicle aerodynamics, chemical engineering, nuclear design and safety, ventilation and industrial design. Whilst the fundamental equations of fluid motion that formed the basis of such codes had been well known since the 19th century, their solution for problems with complex geometry and boundary conditions required the development of efficient numerical solution techniques and the ability to implement these on digital computers. The development of this technology in the 1950s and 1960s made such research possible, and CFD was one of the first areas to take advantage of the newly emergent field of scientific computing. In the process, it was soon realized that CFD could be an alternative to physical modelling in many areas of fluid dynamics, with its advantages of lower cost and greater flexibility.

Computational fluid dynamics is therefore an area of science made possible by, and intrinsically linked to, computing. Its development has paralleled that of computer power and availability, and as we move into an age of cheap, powerful desktop computing it is now possible, with a little knowledge, to run large and complex 3D simulations on an average personal computer. However, most research advances in CFD continue to originate in the aeronautics and industrial design communities as a

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result of the significant investment levels available in these areas. In such applications the boundary conditions, problem geometry and material properties of any solid surfaces (e.g. drag coefficients) are typically known very precisely and the code is applied to a closed system. In such cases it may be possible to characterize the complete set of process mechanisms that exist and also obtain good experimental data for model validation. Major research questions, therefore, concern improvements to the quality of the numerical solution, the scales of flow resolved by the model for fixed computational costs and the representation of sub-grid-scale processes such as turbulence. Considerable effort is expended on topics such as numerical analysis, turbulence modelling, grid generation and adaptive meshing. Tolerance of solution errors is also low, and such codes are predominantly used in a deterministic fashion as alternatives to laboratory experimentation. This reductionist epistemology serves industrial engineering applications well, and the techniques thus developed have considerable spin-off benefit in other disciplines such as environmental hydraulics.

Early on in the development of CFD it was realized that the technique could also be applied to environmental problems to simulate heat and mass transfer in rivers, lakes, oceans, atmospheres and porous media such as soil and rock (e.g. Freeze and Harlan, 1969; King and Norton, 1978; Fischer *et al.*, 1979). The potential for using computer models to simulate environmental flows was obvious; however, these early applications adopted the same deterministic methodology used in industrial applications which often proved inappropriate, given the data then available. In reality, the application of CFD to environmental flows leads to a series of problems not encountered in industrial applications: geometry and boundary conditions are rarely known with any precision; drag coefficients vary in time and space as result of complex interactions between the material properties of the surface and the flow itself; the driving forces are highly variable, often at scales smaller than the model grid; and the geometry of the problem rarely approximates to a simple, easily meshable surface. Moreover, environmental systems are open and should be conceived as complex assemblages of many different processes and inputs, not all of which will be well characterized in any given application. Model validation data may not be available which tests all relevant aspects of model performance to a sufficient level of detail. In fact, given that CFD models adopt finite representations of time and space that may be very different to the time and space scales over which observations are obtained, it may actually be very difficult to measure those quantities predicted by a given code. In contrast to industrial applications of CFD, environmental applications are characterized by considerable uncertainty over almost every aspect of the modelling process and it may therefore become very difficult to diagnose why a model is going wrong. For example, a mismatch between a model and available validation data may be the result of a poor choice of conceptual model given the problem in hand, lack of data to characterize the problem geometry and boundary conditions, an incorrect parameterization or just insufficient or inappropriate validation data. Most likely all these factors will apply! Whilst this does not mean that CFD models cannot be used to perform numerical experiments in environmental hydraulics, it does suggest that care is required in interpreting model studies which purport to mimic real flow events and which include comparisons with real data.

Environmental applications of CFD thus have some fundamentally different characteristics from other applications of this technology, and as a consequence such applications may have very different research priorities. This is not to say that environmental CFD modellers should be unconcerned about the numerical techniques they use or about the quality of the numerical solutions they produce. Neither does it imply that more highly resolved model grids and greater levels of process inclusion will not lead to more physically realistic models (even if the utility of this reductionist approach may be difficult to prove in our case). Rather, it suggests that the greatest uncertainties in environmental CFD modelling lie elsewhere, and that the key research challenges relate to the identification, quantification and reduction of these. This new research agenda focuses on such questions as: coupling CFD with complex natural terrain; extending process representation to consideration of coupled sediment-flow, water quality-flow and biotic–abiotic problems; scale and resolution effects, including upscaling; issues over what makes sufficient process representation in terms of model simplification; model validation; complex sensitivity and uncertainty analysis; and possible model equifinality. Uncertainty is a particular challenge as uncertainties may be compensating, interacting and non-linear. Further, the data sets available to understand them may be sparse and contain significant but poorly known errors that vary strongly in time and space. The result is that there may be many combinations of models and parameters that fit the available data equally well.

In proposing solutions to these problems, environmental CFD modellers have a distinctive contribution to make to the overall discipline and there is the potential to contribute significant innovative science that may find application in many fields. Whilst much research in 'mainstream' CFD requires very high level mathematical ability that is typically the preserve of a select group of specialists, solution to the problems outlined above requires a different skill set for which environmental scientists may be well suited. The ability to deal with problems characterized by sparse and uncertain data where there may even be debate over the fundamental process mechanisms at work is a key part of scientific training in environmental engineering and the geosciences. Hence, in environmental applications of CFD there are scientific problems of model development and analysis that are not well anticipated or solved by standard CFD research and to which civil engineers, environmental scientists and geographers can contribute significant insight.

Application of CFD techniques to real-world environmental problems has increased sharply in the last decade due to an improving ability to deal with the uncertainties noted above. In part this has been due to improvements in computer power and storage, which have allowed flows over complex natural topographies to be simulated for the first time, and to wider availability of user-friendly code. However, this alone does not explain the rise of environmental applications of CFD. A further major factor is the increased availability of the necessary digital data sets to set up and to test such models. Instrumentation development in a variety of fields has yielded new technologies for topographic surveying (including airborne laser altimetry, stereo-photogrammetry and the Global Positioning System), bathymetric survey (including sidescan sonar and wide swath sonar) and velocity measurement (including acoustic Doppler current profilers and large-scale particle image velocimetry). Such instruments yield data that are critical for environmental applications of CFD and allow users to at least begin the process of uncertainty characterization and reduction. As a consequence, the extent and scope of environmental research now carried out with CFD models is considerable (Hodskinson and Ferguson, 1998; Lane and Richards, 1998; Meselhe and Odgaard, 1998; Sofialidis and Prinos, 1998; Sinha *et al.*, 1998; Bijvelds *et al.*, 1999; Lane *et al.*, 1999, 2000; Nicholas and Smith, 1999; Bradbrook *et al.*, 2000a,b, 2001; Nicholas, 2001), and likely to rise as a result of the continuance of the trends identified above.

In effect, we are beginning to see the development of a coherent body of research that attempts to address the research challenges identified above, but which also acknowledges the more fundamental aspects of CFD modelling that are long-established within the engineering community (e.g. control of numerical accuracy). The purpose of this book is to document this newly emergent science and to provide an accessible 'primer' to CFD modelling for environmental engineers and geoscientists. Accordingly, the book is split into two parts. In Part One, basic topics in CFD modelling are addressed in a thematic manner to provide the necessary theoretical background for students and researchers in the environmental sciences with material specifically tailored to CFD applications to complex natural systems. In Part Two, reviews of leading-edge research applications are presented that exemplify and add understanding to the themes raised in Part One. Central to these reviews is the demonstration of how good practice in CFD modelling can be achieved, with reference to both established and new applications. The remainder of this introduction provides a brief overview of the structure of the book and tries to identify directions for future research in this area.

1.2 Part One: An overview of computational fluid dynamics schemes

At the heart of any CFD model is a set of governing rules, usually written in the form of simultaneous partial differential equations derived from principles of mass and momentum conservation, which define in mathematical form the physical processes to be represented by the model. This representation may not, and likely will not, encapsulate all the physical mechanisms known to occur in a given application, but rather is a statement of the modeller's assumptions about those processes that are critical to the problem in hand. In Keith Beven's terminology (Beven, 2002), the first stage in model building is therefore to move from a *perceptual* model, representing everything we perceive or know about a given flow problem (and which may still be incomplete), to a *conceptual* model that represents our best estimate of the processes, parameters and forcing functions that control the development of a flow field at a particular scale. This conceptual model may be as simple as a series of logical statements, but at some point this needs to be translated into mathematical notation if it is to be turned into computer code and solved for the problem of interest. This volume begins, therefore, with five chapters that outline the fundamental equations used to build computational fluid dynamics models for flow (Ingham and Ma), solute transport (Guymer *et al.*), sediment transport (Mosselman), turbulence (Sotiropoulos) and moving boundaries (Bates and Horritt). Readers should note that these distinctions are somewhat artificial, but are a convenient way to organize the book. In reality, flow calculations need to consider turbulence closure, solute and sediment transport are driven by advective (flow) and dispersive (turbulent) processes and so on.

Derek Ingham and Lin Ma (Chapter 2) consider the variety of equations available for the simulation of flow processes in fluvial applications. These are all derived from the well known 3D Navier–Stokes equations (Batchelor, 1967), which are typically simplified for environmental applications by averaging in time, to yield the Reynolds-averaged Navier–Stokes equations, and/or in space, to yield 1D or 2D models. None of the resulting equation sets have general analytic solutions for non-trivial problems, and can only be solved using numerical approximation. As Ingham and Ma point out, neither is the process of simplifying the Navier–Stokes equations straightforward. In fact, averaging in time and space invariably introduces new terms into the controlling equations to represent dispersion processes at scales below the model grid or time step over which the averaging occurs. In the case of time averaging these dispersion terms are dominated by the effect of turbulence and require the introduction of some additional model to represent these effects. In a similar fashion, averaging in space also leads to additional dispersion terms because of velocity gradient variations in the flow field. Ingham and Ma discuss briefly the treatment of these effects using turbulence models, with a fuller treatment being given by Sotiropoulos (Chapter 5). The chapter concludes with a discussion of methods to treat the model boundaries in CFD codes, and in particular covers free surface, open flow and wall boundaries. Unlike in standard CFD application areas, free surface flows are common in the environment and require careful treatment, particularly for dynamic problems. Similar consideration needs to be given to inlet and outlet boundaries of the model and to the treatment of flows in the boundary layer below the scale of the model grid. The latter is particularly important because of the significance of bed roughness to the development of fluvial flows.

Ian Guymer *et al.* (Chapter 3) discuss the modelling of solute transport processes in CFD schemes using numerical solutions of the advection–dispersion equation. Combined environmental flow and transport problems are increasingly being treated with a CFD approach as a result of legislation to regulate point and non-point source pollutant discharges and maintain river ecology. Guymer *et al.* demonstrate the importance of turbulence, dispersion and dead zones to the mixing process in real rivers and outline ways in which these can be treated in CFD codes. The transport theme is continued by Erik Mosselman (Chapter 4) who considers ways to model the transport of bed material by rivers to yield simulations of fluvial morphodynamics over various space and timescales. Again, this is based on consideration of the principles of mass and momentum conservation, but is complicated by the number of possible transport modes (suspended load, bedload, etc.) and by the need to employ empirical closure relationships for many of the key terms, particularly in the momentum equations for sediment transport, to facilitate simulations at scales of practical interest. As a result, Mosselman notes that the sediment transport momentum equation becomes, to a large extent, empirical. To counter this, Mosselman argues that sediment transport formulae should not be derived from sediment transport measurements alone, but also from bed level measurements, and that further research into the effect of bed slope and vegetation on sediment transport should be conducted.

In Chapter 5, Fotis Sotiropoulos provides an in-depth review of the treatment of turbulence in CFD schemes. In principle, with a model grid and time step sufficiently fine to resolve turbulent eddies down to the Kolmogorov scale, all turbulent motions can be simulated directly. However, for problems of practical interest, and particularly for environmental problems with complex topography and roughness, methods for parameterizing the impact of turbulent eddies on the large-scale flow development will continue to be required for the foreseeable future. Sotiropoulos discusses Direct Numerical Simulation (DNS), Large Eddy Simulation (LES) and Reynolds Averaging as solutions to these problems, and reviews the entire hierarchy of turbulence models with emphasis on modelling issues that are relevant to environmental engineering applications.

As the final contribution to this introduction to governing equations for CFD schemes, Paul Bates and Matthew Horritt (Chapter 6) consider methods to treat the dynamic extension and retreat of the flow. Moving boundary problems are common in environmental hydraulics, and include overbank flooding, coastal, estuarine and dam-break flows. Methods to treat such problems can be broadly classified into those that adapt the model grid to track the moving shoreline, and simpler methods which retain a fixed numerical grid, but implement additional algorithms to deal with potential discrepancies in mass and momentum conservation in partially wet cells. In each method the topography can be defined as a continuous function (albeit as discretized on the model grid) or a discontinuous staircase. Different treatments apply in each case and are reviewed in this chapter. The chapter deals predominately with treatments for the flow equations, but concludes with a brief discussion of methods to treat combined flow and transport in the presence of a moving boundary.

Having defined the equation set to be solved to represent a given application, the next task is to formulate a way to solve the resulting system in time and space that can be implemented on a digital computer. This problem is considered by Nigel Wright in Chapter 7. As the resulting equation sets used in CFD codes have no general analytical solution, recourse must be made to approximate numerical methods. The first stage in any of these methods of numerical analysis is to convert the differential equations, which are continuous functions, into a set of algebraic equations that connect values at discrete points. There are various techniques for achieving this, and the main ones encountered in CFD modelling are the Finite Difference (FD), Finite Element (FE) and Finite Volume (FV) methods. Wright provides an introduction to each of these methods, using simple examples, before going on to discuss related issues of grid generation and numerical error. Once a discrete form of the governing equations has been defined over a grid, the resulting non-linear algebraic system of equations can be solved with a technique appropriate to the discretization method. Wright emphasizes that the numerical solution should not be treated as a black box by modellers, and that correct interpretation of CFD code output requires a thorough understanding of the numerical method being used.

This theme of good practice is continued in the final two chapters of Part One by Stuart Lane *et al.* (Chapter 8) and Matthew Horritt (Chapter 9). Chapter 8 by Lane *et al.* proposes a framework for the verification and validation of CFD schemes. This is derived from the guidelines for publication of CFD research proposed by the American Society of Mechanical Engineers (ASME), but extended here for the specific case of open channel flows. These guidelines cover such areas as reporting standards, solution accuracy in space and time, mesh independence testing, convergence testing and comparison with experimental results. Lane *et al.* demonstrate how these guidelines may not be sufficient for many practical fluvial applications, but can provide a minimum framework. In particular, ASME criterion 10 requires that 'reasonable agreement' between the model and experimental results be shown. However, Lane *et al.* argue that it may be difficult, both philosophically and practically, to establish that such evidence provides conclusive validation of a model. The chapter then proceeds to develop this notion of validation and discuss surrounding issues of calibration, sensitivity analysis and benchmarking. As a result of this discussion, a series of guidelines are proposed to replace ASME criterion 10 for environmental applications.

Despite our best efforts, almost all aspects of CFD modelling (choice of conceptual model, boundary conditions, topography, model parameters and validation data) will contain uncertainty. Techniques are therefore required to estimate the impact of these uncertainties on model predictions. This area is addressed by Horritt in his chapter on model parameterization, validation and uncertainty analysis. Horritt discusses emergent techniques for uncertainty analysis with a focus on the use of new technologies, such as remote sensing, to provide essential data to constrain model calibration. He concludes that the spatial heterogeneity of natural environments is a significant challenge for CFD modellers that can only be partially overcome with current technologies. Thus, in addition to criteria proposed by Lane *et al.*, full evaluation of a CFD study requires an evaluation of uncertainty propagation through the model system.

1.3 Part Two: Application potential for fluvial studies

Part Two of the book provides an overview of particular applications of CFD to fluvial and estuarine environments. We specifically chose not to consider marine, aeolian or atmospheric issues due to space limitations, although there is much to be learnt from comparing and contrasting aeolian, atmospheric, marine, fluvial and estuarine studies. For example, all four environments have to address the very severe difficulty of how to represent boundary shear stress effects in near surface cells. Many traditional modelling approaches share methods based upon roughness height specification and associated modification of the turbulent velocity profile in the near wall region. Part Two therefore begins with general reviews of the two most common current applications of CFD to the study of fluvial and estuarine flows: (a) reach-scale modelling of fluvial processes (Lane and Ferguson); and (b) floodplain inundation modelling (Bates *et al.*). Lane and Ferguson (Chapter 10) show how CFD has resulted in a much deeper understanding of flow, sediment transfer and ecological processes at the reach scale. This has now included application of CFD to understanding each of the major river channel facets (riffle–pool sequences, meanders, confluences or tributary junctions) and has been extended to include consideration of instream habitat. They argue that these kinds of applications have required innovation in terms of process representation, notably in terms of the strongly related issues of discretization and boundary roughness. However, they also argue that a major change is still needed to extend research from a consideration of flow to also include sediment transport and channel change, where the presence of a deforming boundary can lead to severe numerical instabilities. It is in relation to deformable boundaries that some of the most innovative applications of reach-scale CFD are being explored.

In Chapter 11, Bates *et al.* provide a similar overview of treatments of floodplain inundation. Floodplains represent an environment of particular importance to the riparian manager, and one that is currently moving through a paradigm change in terms of the practical application of flood inundation modelling methods with adoption of approaches that have a strong grounding in CFD. Bates *et al.* review the complexity of the inundation process, which involves the complex lateral transfer of mass and momentum from the river channel to the floodplain, involving flows that may be strongly three dimensional. Away from the channel, shallow water flows become dominant that are more strongly two dimensional. These flows are a challenge as the inundation front can move rapidly across the floodplain (during wetting and drying) interacting strongly with the floodplain topography and vegetation as it does so. This can result in computational difficulties due to the large number of elements that play no part in the solution for much of the time, until they are inundated. It is also associated with numerical stability issues as during wetting and drying flow depths are commonly very small, which can lead to severe numerical diffusion and sometimes instability. Bates *et al.* develop two important themes in CFD applications to floodplain flows. First, they emphasize the need to nest models of different complexity according to the part of the environment being simulated. For instance, they describe the potential utility of nesting a 1D solution of the St Venant equations in a 2D diffusion wave treatment of floodplain flow, as the former is sensitively dependent upon getting the correct flux from channel to floodplain, which in turn requires a good estimate of in-channel water levels. This kind of approach has much potential and it implies that CFD solutions will need to be developed that recognize our own understanding and observations of the system that is to be modelled in developing innovative modelling strategies. Second, they demonstrate the crucial progress that has been made in CFD modelling of floodplain flows as a result of progress in our ability to measure floodplain topography, notably using laser altimetry. As the flows are generally shallow, and provided the river floodplain system does not convey as a two-stage channel system, the topographic forcing of flow is likely to dominate the inundation process. This is where there has been a fundamental improvement in our ability to model flood inundation, one that has led to a situation where progress in CFD is now being driven by the high-quality topographic data available to apply to models rather than an explicit concern over existing modelling methods: with the barrier to topographic representation removed, 2D modelling approaches have become both cost-effective and preferred to their 1D counterparts.

Falconer *et al.* (Chapter 12) address the issue of estuarine flows. As with floodplains, these are zones of particular importance. For instance, they are commonly depositional zones. As rivers invariably pass through them, they can become the repository of any kind of waste material in transport in the river system. Estuarine flows are distinct for a number of reasons. First, and although this may also apply to very wide floodplains, the spatial scale of estuaries can be larger, and this reintroduces important source terms into the momentum balance equations: the effects of the earth's rotation and surface wind stresses. Second, they may have important buoyancy effects, largely associated with gradients of density in the horizontal and vertical, which can lead to important mixing processes. Indeed, important field observations in estuaries have shown that the freshwater–saltwater interface can be a crucial component of the sediment entrainment-deposition process (e.g. Uncles *et al.*, 1998). Falconer *et al.* describe the key processes that must also be incorporated to represent water quality in estuaries. This involves a series of general transport equations (Chapter 3) but with additional processes and parameters introduced to describe non-conservative aspects of water quality dynamics. For instance, faecal coliform modelling requires treatment of the coliform decay rate. Falconer *et al.* present a series of case studies of estuarine modelling. The choice of the Ribble example is interesting as it contrasts nicely with Hankin and Beven's consideration in Chapter 17 of the same system from an uncertainty perspective. This illustrates two complementary approaches to modelling, one emphasizing process complexity and the other emphasizing process uncertainty. It is important to recognize that complexity and uncertainty are neither positively nor negatively correlated, but that (Chapter 9) the relationship between the two is one that merits much further consideration. Falconer *et al.* show that their model could reproduce daily variation in point faecal coliform counts. The Mersey estuary provided a second case study, focusing on salinity and sediment transport. As is commonly the case, predictions of hydrodynamics were excellent, but those of suspended particulate matter only good, and this emphasizes the very great difficulties associated with modelling the sediment transfer process noted previously in Chapter 4.

In Chapters 13 and 14, consideration turns to two very different classes of river problem: gravel-bed (Nicholas) and sand-bed (Wiele and Torizzo) rivers. Whilst this distinction is not necessarily a useful one in substantive terms, it is crucial in CFD terms as the two environments are associated with very different modelling challenges. Gravel-bed rivers are a particular problem because of the complex geometry of the bed surface, which not only raises data acquisition challenges but also requires innovative representation of surface complexity in CFD models. Consideration of a gravel-bed river immediately turns one's attention to the strong spatial and vertical gradients in flow associated with individual clasts or groups of clasts. However, as Nicholas shows, there is a larger scale of consideration where this process detail has to be sacrificed if reach-scale sediment transport and flow problems are to be resolved. Nicholas emphasizes that a key theme in gravel-bed river modelling, especially when trying to scale up, is the specification of appropriate wall functions. This is a sub-grid-scale problem (Chapter 10) and Nicholas presents a range of alternative roughness models which do not require the assumptions associated with conventional wall treatments. These include random perturbation of bed surface topography as opposed to implicit representation of topography in wall treatments and discrete element models, similar to the porosity treatment described by Lane and Ferguson (Chapter 10) but parameterized using geostatistical methods. The modelling approach was particularly successful as it was able to represent known deviations from predicted wall treatment cases. Nicholas extends consideration to 3D modelling of braided rivers which is of particular importance. He presents a particularly novel method for determining distributed patterns of drag, which merits much further exploration. He also confirms the work of Lane and Ferguson (Chapter 10) which shows that roughness is a much less effective calibration parameter in 3D models as compared with 2D and 1D models.

The challenge for sand-bed river modelling is different. Wiele and Torizzo explore the issue of how sand transport adjusts to a dam release and changes in sediment delivery. Modelling sand-bed rivers is a challenge as sediment transport can occur at almost any flow discharge, resulting in the continual interaction between the bed of the river and its flow. Wiele and Torizzo use a depth-averaged model for flow but with a quasi-3D sand transport treatment, the latter driven by depth-averaged flow predictions combined with a near-bed boundary condition for shear stress. The modelling was supported by high-quality data collection as part of the work of the Grand Canyon Monitoring and Research Centre and the model was applied in steady state form to two flows: the highest post-dam closure flow; and the test release flow. Model results are interesting as they show that deposition volumes vary in relation to not only discharge and sand supply but also channel shape.

Many rivers are influenced by instream and bank-side vegetation. Given the volume of research into bed roughness issues in rivers, it is surprising that vegetation has been given so little attention. Wilson *et al.* (Chapter 15) address this issue. The chapter begins with a review of different means of vegetation representation in hydraulic models using conventional experimental–conceptual approaches. Many of these approaches have been based upon manipulation of conventional roughness parameters to allow vegetative resistance effects to be incorporated. Wilson *et al.* show the importance of carefully designed experiments in providing the conceptual underpinning for development of more effective numerical modelling approaches. They show that this leads to better models for practical application but also the development of CFD as a research tool, which in turn leads to new ways of developing models for practical application. Thus, they apply a drag-force approach to two different 3D FV formulations of the Navier–Stokes equations, and then consider how their approach can be upscaled for practical application. The work emphasizes the importance of vegetation in relation to turbulence, something that is often overlooked when CFD models are applied to vegetated systems and only vegetation-roughness issues are considered.

The importance of considering vegetation in rivers partly stems from a changing legislative context in which protection of the biota is now given as much, if not more, importance as management of the abiota. Thus, Leclerc (Chapter 16) continues the ecological theme introduced by Wilson *et al.* but extends consideration to ecohydraulics and the associated use of CFD in habitat management. Numerical habitat modelling, as with studies of floodplain flows, is going through somewhat of a paradigm shift as the conventional 1D approaches to hydraulics implicit in models like IFIM and PHABSIM are being displaced by 2D analyses. This shift was well illustrated by the work of Leclerc in the 1990s and reflects what we now know about the biology of habitat preference curves where what matters is the range of habitat available in a given spatial unit, which requires some form of 2D characterization. Leclerc sets the problem up by doing something that we do not do sufficiently in CFD applications: he considers the problem from the perspective of the goals of the project (in this case – fish) and then asks what must an associated modelling approach deliver as a result. He demonstrates that the amount of modelling complexity that is required depends sensitively upon the goals of the study. Thus, Leclerc provides an important overview of the state of the art in terms of how habitat preference curves, and derivatives, can be developed. This leads into a critical review of how CFD can be used to deliver the necessary environmental variables for populating these methods. This begins with a convincing review of the inadequacies of approaches based upon 1D treatments. He then explores 2D approaches, emphasizing that they will give more useful results but this is at the expense of additional data requirements. As other chapters have shown (Chapters 10 and 11) remote data acquisition will help here. But so will innovative ways of topographic parameterization (Chapter 13) which may in turn make 2D approaches standard in this kind of application. Leclerc emphasizes that 2D and 3D approaches are crucially underpinned by digital elevation models, and shows that these in themselves represent important methodological challenges but also substantial ecologically relevant process knowledge.

The last two chapters in the book both take up the theme of real-world application of CFD codes. Barry Hankin and Keith Beven (Chapter 17) continue the theme developed by Horritt in Part One of the book, namely how to begin to quantify some of the uncertainties that are inevitably present in practical applications. To date this has been an under-researched area, given the computational cost of simulations and the need to undertake multiple realizations of a model, usually in a Monte Carlo framework, to begin the uncertainty analysis process. Hankin and Beven suggest a risk-based approach to environmental CFD modelling should now be adopted and that both the methods and computational capacity now exist to allow this change to take place. Hankin and Beven illustrate this point by comparing a study of a complex system with uncertain inputs where limited computational time was available to an academic study where uncertainty analysis via the Generalized Likelihood Uncertainty Analysis (GLUE) method was used. In the first study it was only possible given the timescales available to carry out a limited sensitivity analysis, and the chapter makes the limitations of this approach all too apparent. Nevertheless, as Hankin and Beven note, complex CFD models are being used to inform billion pound expenditure programmes in the water industry, yet interpretative tools for assessing the degree of belief in these model predictions are not yet seen as integral to the process. This will clearly be a developing theme over the next decade for environmental applications of CFD codes, and studies of the type outlined by Hankin and Beven are likely, through the impact of legislation such as the EU Water Framework Directive, to become increasingly common.

The book concludes with a chapter by Gareth Pender *et al.* (Chapter 18) on the use of CFD methods for environmental design and management. Pender *et al.* take a different approach from that of Hankin and Beven, and instead of showing what may be possible in the future they seek to provide an insight into the quality of the simulations that can now be achieved when CFD tools are placed in the hands of competent design engineers with access to typical field data. Pender *et al.* summarize the issues involved in setting up a CFD applications (including free surface representation, boundary conditions, roughness, geometry and turbulence) and seek to demonstrate how decisions over how these are represented may impact on simulation quality and show the constraints on practical application.

1.4 Where next for environmental CFD?

The chapters in this book clearly demonstrate the rapid recent development of environmental applications of CFD techniques. Integration of data from newly emergent sources, such as remote sensing, with CFD models and the availability of cheap yet powerful desktop computing has yielded an ability to construct multi-dimensional models of flow and transport at a resolution and level of detail that would, even 10-years ago, have seemed unattainable. With hindsight, however, the fact that the controlling equations of these models have been well known for over a century and that numerical techniques to solve them have been available since the 1960s meant that this was, in large part, a development waiting to happen and was only prevented by logistical not theoretical constraints. An unintended consequence of this development has been the democratization of hydraulics research, and its dissemination beyond the limited group of practitioners who were able to secure access to the large-scale flume facilities that were previously necessary to conduct significant science in this area. Such facilities are expensive to maintain, time consuming to use and can only support a limited number of experiments at a time, and hence can only be found within a limited number of institutions. The ability to do significant hydraulic science on a desktop PC has fundamentally revolutionized just who is able to undertake hydraulics research and led to new interest in the subject from scientists such as geographers, earth and environmental scientists, ecologists and meteorologists who lie well beyond the traditional engineering/mathematical focus of the discipline. This development has the potential to be incredibly important, not just because it may increase the volume of hydraulics research conducted but also because scientists from these different disciplines may bring new insights and skills, such as uncertainty analysis, which may be highly relevant to environmental applications of CFD.

Despite this progress, key research questions remain. A particularly central issue is how we validate these newly emergent models. A newly arrived extraterrestrial might view this as a somewhat strange preoccupation, given that all of our other research approaches (fieldwork, experimental data collection in the laboratory, analytical solution of equations) require us to make simplifications that result in the delimitation of our spatial and temporal horizons and the exclusion of possibly important processes (Lane, 2001). However, these philosophical debates aside, we do need to be able to choose between different model formulations, and to advise when the benefits of a more sophisticated process representation outweigh the associated increase in computational and data collection costs. Data, with all their problems, still help us to do this, although as a number of chapters in this book show, other approaches are also of value. It is perhaps here, where CFD meets the real world, that the new challenges are emergent, as we deal with real rivers and floodplains that have complex structure and hence strong horizontal and vertical process gradients, and where traditional simplification of model geometry removes the critical aspects of the processes that are driving the system.

This leads on to a related theme that is again reflected in many of the above chapters. What is the sufficient physics (and biology and chemistry) when we wish to use CFD to understand and to manage the water environment? The word 'sufficient' will clearly depends on what CFD is to be used for and there remains considerable debate over this issue. This is well illustrated in debates over braided river modelling (e.g. Paola, 2001; Lane, 2005) where a model that is based upon a rudimentary flow routing treatment (that cannot be derived from simplification of the 2D shallow water equations) and mass-conservative, but physically realistic sediment transport rules, appears to reproduce the generic properties of river braiding. Does this mean that CFD is not necessary as a research tool? Some would argue that this is the case for certain classes of problems. When this debate is taken into the management arena, where practical considerations provide additional complexity, debates over CFD move beyond strictly technical considerations. It is in this sense that model validation and verification become crucial, as decisions over sufficiency in process representation become bound with social and economic considerations, including commercial development of code.

One way forward in relation to sufficient process representation is to develop nested modelling strategies. This reflects the idea that process complexity is defined by the components of the system that are being studied and that these vary in space, and potentially in time. Thus, what is sufficient process representation depends where you are in the model's space and time, and process complexity can be allowed to vary. This kind of coupling can be a numerical challenge, but it is probably going to be the main way forward in reconciling our growing process sophistication with the practical constraints imposed by data availability and computational demands.

Despite the progress made to date, many research challenges remain and should prove fruitful grounds for research in the coming years. Different researchers would likely come up with different priorities; however, certain key themes are obvious. First, applications to date have tended to consider only single river reaches and a likely avenue for future development will be the consideration of flow and sediment transport along multiple reaches for catchment-wide risk analysis and management. Legislation such as the EU Water Framework Directive will provide further impetus to the adoption of a holistic approach to river basin management that can only be accomplished by the application of modelling tools at a commensurate scale. Data to drive these and other applications will become an increasingly important focus, and studies that examine the use of remotely sensed data for automatic or near-automatic model discretization and parameterization will become increasingly common. This will lead in turn to a more comprehensive consideration of scale effects in CFD modelling and the impact of scale on dominant processes and parameter sensitivity. Remotely sensed data may also improve our ability to calibrate and validate the distributed predictions made by CFD models and a move to multi-criteria validation will also require an increasing level of sophistication in the techniques applied to evaluate uncertainty in CFD codes. Uncertainty will be a further dominant theme, and despite a reductionist tendency in CFD modelling, whereby increases in computer power are most often used to increase process specification or reduce model resolution, the next decade is likely to see a significant move away from a reliance on single deterministic solutions and a move to the analysis of ensembles of simulations. Further technical developments are likely to come in a number of areas including the use of porosity treatments and other boundary representation methods and in particular their extension to erosion and deposition problems. The generation of turbulence and friction by vegetation also requires much further study if we are truly to represent flows over natural surfaces. Methods are required that will enable turbulence and friction generation by plants to be estimated and these effects aggregated to the model grid scale. Data on plant geometry and biomechanics, possibly acquired from remote sensing instruments, will also be required to parameterize these process models in a physically plausible way (e.g. Mason *et al.*, 2003).

Ways of using CFD models may also change, and in particular as we gain further understanding into how to construct models for particular flow problems to yield results that are adequately realistic we may be able to begin to use our models as 'numerical laboratories'. In this way we will be able to conduct computer-based experiments that analyse, for example, how flow in generic situations depends on parameters of channel geometry, what would happen to particular channel and substrate types in the 100-year flood and so on. Lastly, as advances are made in the component areas of flow, sediment transport and ecology modelling, the barriers to model coupling will reduce and codes which can simulate complex assemblages of environmental processes will become more common. Particular examples of such multi-process approaches may include the linkage of flow and sediment transport models in a more closely coupled way than has hitherto been possible and the linking of flow simulations with ecologic processes.

In summary, much progress has been made in environmental applications of CFD which has posed new research questions for hydraulic modellers and resulted in significant new science. Such work is, however, only the beginning of what we may be able to accomplish with CFD techniques in the coming years and the interplay between computational approaches, data collection and focused experimentation is capable of yielding new insights into environmental hydraulics. The chapters in this book testify to the vitality of environmental CFD research and demonstrate the considerable potential for use of these techniques in the future.

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Part One

An Overview of Computational Fluid Dynamics Schemes

2

Fundamental equations for CFD in river flow simulations

D.B. Ingham and L. Ma

2.1 Introduction

Modern CFD techniques emerged between the late 1960s and early 1970s when fluid flow investigations were largely experiment based and only very simple fluid flow problems could be accurately numerically solved. With the rapid development of modern computational techniques and numerical solution methodologies over the last few decades, CFD has now been widely used in various industrial applications for investigating a vast range of industrial and environmental problems. However, compared to industrial applications, using CFD to model morphology and hydrology problems is relatively new, research on river flow CFD modelling has been very active, particularly in recent years (e.g. Nezu and Nakagawa, 1993; Lane, 1998; Ma *et al.*, 2002; Cao *et al.*, 2003, etc.). This can be largely attributed to the availability of adequate computational resources at a reasonably low cost. CFD has increasingly acted as an alternative and/or supplementary tool to the more traditional methods in the systematic investigations of various controls in river morphology, flow structure and sediment transport, and it has increasingly played an important role in river management and flood prediction. However, it should be noted that the flow structures in river flows are inherently very complex due to the effects of irregular bank and bed topographies in natural river flows. Further, considering the large scales that are involved, the modelling of natural rivers has itself become computationally

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very demanding. However, major issues of river flow modelling are in the appropriate representations of the complex river flow conditions in the CFD model. Issues such as grid resolution, grid dependence, representation of wall roughness, appropriate turbulence models, etc., are all currently under intensive discussion (e.g. Hardy *et al.*, 1999). Nevertheless, with a numerical model and the boundary conditions which provide adequate representations of the key proceses of the river flow investigated, CFD simulations may provide considerable insight into, and clearer explanations of, the structure of the flow and the interactions of the key components of the processes than do the traditional field and/or laboratory measurements.

As a basis for the CFD modelling, this chapter gives an outline of the fundamental governing equations of fluid flow and fine sediment/solute transport which are widely used in CFD simulations of river flows. Various turbulence models adopted in the modelling of turbulent flows, and the boundary conditions which are required to define a specific situation under investigation, are discussed. Then two examples of 3D numerical CFD simulations of river flow and pollutant transport in a river channel are presented.

2.2 Basic equations for river flows

The constituent equations for fluid flows are well established and they are basically in the form of a coupled set of partial differential equations, known as the Navier–Stokes equations (e.g. Batchelor, 1967), which are appropriate to river flow modelling. CFD techniques simulate physical fluid flow by numerically solving these coupled partial differential equations. Different ways of numerically solving these equations give rise to different CFD techniques in which various forms of these equations may be employed. In the framework of the finite difference/volume technique, the most fundamental solution method is referred to as the Direct Numerical Simulation (DNS). In the DNS method, the transient form of the Navier–Stokes equations is solved numerically by means of spectral and pseudospectral techniques. However, because of the complexity of general industrial, as well as environmental, problems and the limitation in the capabilities of present computer systems, DNS is nowadays still primarily limited in its use to the study of some of the very simple but fundamental flow problems, such as simple turbulent channel and pipe flows, flow in plane mixing layers, etc. When DNS is employed for simulations of high Reynolds number turbulence flows, such as river flows, a prohibitively large number of computational cells must be employed in order to resolve the smallest turbulence vortices, and usually this is not practical within the present levels of computer techniques.

A more common approach to model turbulent river flows is to use the Reynolds-averaged Navier–Stokes equations incorporating an appropriate turbulence model. This has the advantage that a relatively coarse computational grid may be employed. However, it is evident that even when using the Reynolds-averaged Navier–Stokes equations, it is sometimes very difficult to solve large scale, complex unsteady river flows in a fully 3D model due to the limitations in computer power. This is particularly true when the problem investigated is part of a real river where the flow is turbulent with irregularly shaped banks and beds. Therefore, various simplifications to the governing equations have to be made in order to reduce the dimensions of the problem.