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A critical reflection of computational fluid dynamics applications to fluvial sedimentary systems

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Abstract A variety of computational fluid dynamics models for fluvial flow, sediment transport and morphological evolution have been developed and are in widespread use. Yet their quality remains unclear due to poor assumptions in model formulations, implementation of sediment functions of uncertain validity, and problematic use of model calibration and verification as assertions of model veracity. This paper presents a critical reflection of computational river models. It is argued that model calibration can be subjective, verification is impossible and validation does not necessarily establish model truth. It is suggested that computational river models remain premature, and high level expertise, physical insight and experience are vital for meaningful solutions to be acquired and for limitations to be properly assessed.

Key words fluvial process; sedimentary system; sediment transport; fluvial morphology; computational fluid dynamics; mathematical modelling; river engineering; fluvial hydraulics

INTRODUCTION

The capability of making accurate calculations of fluvial flow, sediment transport and morphological evolution is becoming progressively important as the concern over river systems in response to climate change and human interventions is increasing. Modelling the strongly coupled flow–sediment–morphology systems presents a problem of considerable interest in computational fluid dynamics. The last half century has seen a significant move from comparatively simpler cross-section-averaged one-dimensional (1D) models in the early 1950s and depth-averaged two-dimensional (2D) models since the 1980s to full three-dimensional (3D) models more recently. Computational modelling has evolved to become a proactive problem-solving technology for the river environment. Nevertheless, existing models are limited because of underlying assumptions and limited knowledge of the physics of turbulence, sediment transport, and the interaction between them. Arguably computational hydraulics for fix-bed rivers, based on the St Venant equations, matured prior to 1960 and those for movable-bed rivers with sediment transport and morphological developments remain premature. To illustrate, a variety of sediment transport functions are often implemented in modelling packages (e.g. HEC-6 of the US Army Corps of Engineers; ISIS of HR Wallingford & Halcrow Ltd, UK; and MIKE11 of the Danish Hydraulic Institute, to name a few). Distinct sediment functions would probably lead to quite differing outputs (US Army Corps of Engineers, 1996). Unfortunately there is no way to convincingly choose between these outputs, but to invoke personal experience and preference etc. Apparently identifying the critical issues of computational river models is of significance for enhanced modelling quality and uncertainty assessment.

MAJOR ISSUES OF COMPUTATIONAL RIVER MODELS

A number of issues of computational models for alluvial rivers can be identified (Table 1), of which some are interrelated. These issues encompass a variety of perspectives in fluid mechanics, sediment transport mechanics, morphological considerations, computational aspects as well as the methodology of model assessment etc., and are physically related to a wide spectrum of temporal and spatial scales, varying from turbulence microscales to river-reach scales. Whilst a recent pilot study has addressed the issues of simplified governing equations, asynchronous solution procedures and implementation of river bed mobility (Cao *et al.*, 2002), this papers aims to discuss the remaining aspects that merit close attention for quality enhancement of modelling.

Table 1 Major issues of computational models for alluvial rivers.

Arena	Major issues
Fluid mechanics	Turbulence closure models and sediment effects Simplified governing equations Boundary resistance
Sediment transport mechanics	Equilibrium *vs* non-equilibrium sediment transport Sediment functions
Morphological	Implementation of river-bed mobility
Computational	Synchronous *vs* asynchronous procedures
Model assessment	Calibration and verification/validation

EQUILIBRIUM *VS* NON-EQUILIBRIUM MODELS: SEDIMENT FUNCTIONS

In equilibrium models sediment transport is assumed to be at a capacity that is prescribed by one of a range of sediment functions using local hydraulic and sediment information. Often the lumped total-load concept is used without discriminating the physically distinct mechanisms of bed load and suspended load movements. Obviously the exchange between suspended sediment, bed load and bed surface material cannot be explicitly represented. Intuitively non-equilibrium models are more advanced than equilibrium models because they account for the limited availability of sediment under some special conditions, and more notably the time and space for sediment transport to adapt to its possible capacity in line with local flow scenario. Yet because of the uncertainty associated with both types of models there has been no study of the methodology whereby non-equilibrium models can be confirmed to be superior to equilibrium ones. One of the major sources of uncertainty with equilibrium models comes with the sediment transport function that must be introduced to determine sediment transport rate and for heterogeneous sediments the size distribution of bed material being transported. In non-equilibrium models this feature is reflected by the relationships that must be incorporated to determine the net flux of sediment exchange with bed material.

To date a large number of sediment transport functions have been developed. However most, if not all have been confirmed using specific laboratory and/or field measurement data sets, and there has been no universally valid function for the underlying physics of turbulent flow interaction with sediment. Also it cannot be stated which function is the "best" to use for a given situation. An assessment of the performance of the currently popular sediment transport functions can be found in, among others, Gomez & Church (1989) and Yang & Wan (1991). Distinct sediment transport functions will yield different answers, and normally the sediment rates/discharges are more sensitive to the choice of sediment function than the evolution of river morphology. Therefore model developers and end-users have to judge the computational results based on their experience and their understanding of the basis on which existing sediment transport functions were derived. Inevitably the modelling output is subject to model developers and end-users, and the lack of objectiveness is apparent. This feature is particularly aggravated when bed load transport dominates because (a) the accuracy of existing bed load formulae is dramatically lower than that of suspended load relationships; and (b) there is considerable spatial and temporal lag of bed load transport with respect to the change of flow.

Generic to all spatially dimensional models for fluvial sediment transport, a pivotal aspect of non-equilibrium models is the determination of the net flux of sediment exchange between the water column and the bed surface. The net flux of sediment exchange is the difference between the upward entrainment flux due to turbulence and the downward deposition flux under gravitational action, defined at a reference elevation near the bed. In 1D and depth-averaged 2D models, this comes as the closure of the source–sink terms in the mass conservation equation for sediment, whilst it is manifested in the bottom sediment conditions in vertical 2D and 3D models. The lack of successful formulations continues to be one of the basic constraints precluding reliable modelling.

Specifying bed sediment entrainment flux is the key to the determination of the net flux of exchange as there is little dispute that the deposition flux can be calculated practically using the local near-bed sediment concentration and fall velocity. There appears to be a plethora of empirical functions for bed sediment entrainment. However none yields generally satisfactory results for various particle sizes. A physically appealing approach to formulating bed sediment entrainment is to link it to turbulent bursting, which has been experimentally found to play a central role in picking up sediment. A formulation of this kind can be found in Cao (1999; see also discussion by Hurther & Lemmin, 2001). Further progress along this line is dependent on the experimental techniques and instrumentation that can be deployed to measure the entrainment flux so that quality data are available to back up formulations. Concurrently, it must not be forgotten that even under the idealized situations of steady uniform flows, specifying the reference elevation can be uncertain (Cao, 1999). It is vital to recognize the deficiency of a comparative or sensitivity study of how the final computed sediment transport processes are influenced by the reference elevation.

BOUNDARY RESISTANCE

A relation for hydraulic resistance must be incorporated to close the momentum equation in 1D and 2D models. This involves another important topic in fluvial hydraulics. The complexity of fluvial river resistance stems from not only the irregular boundary, vegetation and hydraulic structures, but the sediments carried by the flow. It continues to be difficult to pinpoint the friction factor especially of natural rivers. Often the Darcy-Weisbach friction factor, alternatively the Manning roughness, has to be tuned to reconcile the computational outputs with measurements. The uncertainty of this practice does merit clear recognition when assessing model performance. This holds true for 3D models, except that it is reflected by the boundary hydrodynamic roughness that is involved in the law of the wall for the bottom boundary conditions.

A relevant problem associated with hydraulic resistance, in the context of computational river modelling, is the optimal determination of distributed roughness. In natural rivers, distributed roughness appears to match the real world more closely than a single roughness value for a specific reach. However the currently popular calibration methodology involving a manual trial-and-error procedure can be subjective and extremely demanding. Most likely only local optima, rather than global optima, can often be achieved. Consequently new methodology for calibrating distributed roughness is greatly needed. The genetic algorithm seems to have the potential for applications in this subject (Coley, 1999), especially as the rapid advancement of computer technology is making costly computation realistic.

TURBULENCE CLOSURE MODELS

For single-phase flows the current state-of-the-art for turbulence closure models can be found in recent literature (Jaw & Chen, 1998; Hanjalic, 1999; Leschziner, 2000). Often the more complicated closure models (e.g. the complete Reynolds stress model) can be expected to give better resolution of the turbulent flow structure than simpler closures. However, no significant advantage is ensured if only the mean flow quantities are sought (Jaw & Chen, 1998). Also the higher computational cost of the complete Reynolds stress closure models can make them less attractive for large-scale river problems. Thus a viable balance between the complexity and capacity of turbulence closure models is essential. Although turbulence closure models have seen successful applications in a wide range of engineering areas, it is essential to recognize the particular prominence of turbulence closure as a major source of errors. Computational river models, whilst offering increasing predictive power and potential, are not yet sufficiently well established to be applied on a routine basis to complex 3D fluvial flows, unless only a rough qualitative knowledge is pursued. This is determined by the complicated channel topography, boundaries and composition of bed materials, in sharp contrast to flow problems with adequately clearly resolved boundaries seen in other industrial areas such as aircraft, automotive, heating and ventilation design etc. The behaviour of turbulence interaction with complicated boundary remains poorly understood and formulated, which is why considerable expertise and experience are vital for practical applications.

For a long time it has been known that sediments alter the structure of the turbulent flow, by which they are carried, which in turn affects the transport of sediments. The sediment effects can be appreciable as the volumetric sediment concentration reaches about an order of magnitude of 10^{-6} (Crowe *et al.*, 1996), which is quite common in natural rivers. There has been much controversy over the behaviour of turbulence modulation by sediment. This topic has been the theme of a large number of experimental studies, which have generated a plethora of conflicting results. For particle–air two-phase flows that share considerable similarity to suspended sediment-laden flows, turbulence may be enhanced when the suspended particles are larger than the turbulence length scale, or suppressed when they are so fine as to be enclosed within the turbulent eddies. In particular, it has been shown that turbulence is attenuated or enhanced by suspended particles respectively in relation to small or large values of particle Stokes number *St* and relative particle size *Rd*. The critical values of *St* and *Rd* for transition between turbulence attenuation and enhancement are about 1.0 and 0.1 respectively (Crowe *et al.*, 1996). Based on these observations, Fig. 1 summarizes the effects of particle size on turbulence. For enhanced river modelling, the role of sediment in modulating turbulence must be properly incorporated. The significant variability of parameters in stratification analogy-based models (Villaret & Trowbridge, 1991) appears to characterize the existence of additional mechanisms, in addition to stratification, that are responsible for turbulence modification. Most plausibly the role of particle size in relation to turbulence scales needs to be properly incorporated.

MODEL CALIBRATION AND VERIFICATION/VALIDATION

The above observations have clearly demonstrated that deterministic computational models for alluvial rivers are open systems, and various empirical constitutive relations have to be incorporated to close the models. Current practice of applying these models involves two separate stages, i.e. calibration and verification/validation. In the first stage (calibration) the various empirical parameters are tuned so that the model reproduces results in agreement with measurements. In the second stage (verification/validation) the model, along with the empirical parameters calibrated in the first stage, is run on a separate data set for the same or similar river problem. If the calibrated model, without resorting to further adjustment of parameters, reproduces the measured data with acceptable error tolerance, then it is considered verified or validated by many.

Whilst this two-stage calibration–verification process has been widely employed in many other areas, some basic problems with respect to fluvial applications have been ignored. A computational river model encompasses a number of parameters to be determined. One primary question is whether there is a unique combination of these parameters. From time to time the same or essentially similar results are produced using differing combinations of model parameters. Usually there is no way to choose between these sets of parameters, other than to invoke extra-evidential considerations such as symmetry, simplicity, flexibility, personal, political or metaphysical preferences (Oreskes *et al.*, 1994) as well as prejudices and financial factors. A secondary question arises as to how the overall performance of modelling can be objectively judged in comparison with measurement. This is especially critical for 3D modelling as normally there are many megabytes of numbers, and it is almost impossible for model developers and end-users to assimilate and interpret even a small

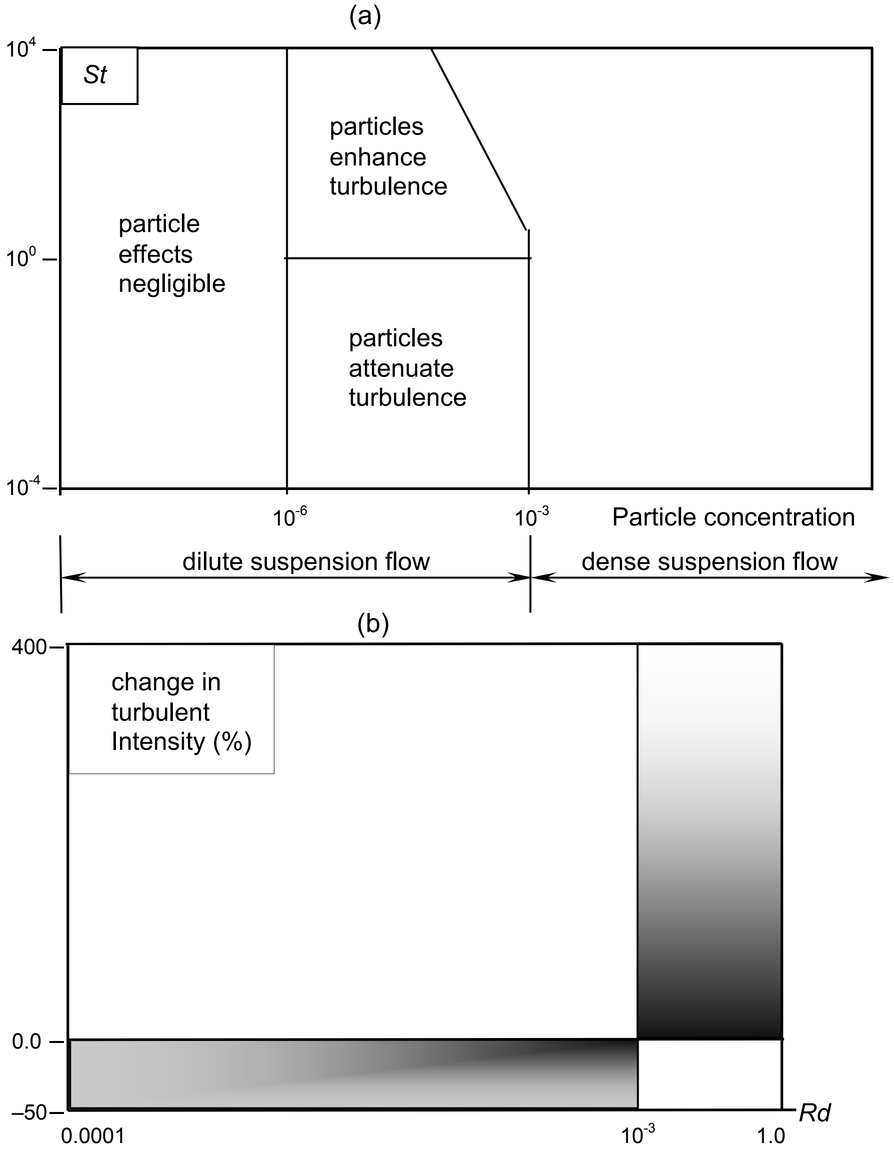

Fig. 1 Illustration of particle effects on turbulence. (a) Particle-turbulence interaction as influenced by particle Stokes number *St* and concentration; and (b) effect of relative particle size *Rd* on turbulence intensity (the shaded area denotes distribution of experimental data).

fraction of the output. That way, the judgement of acceptable agreement with measured data is virtually on the basis of a limited portion of information, e.g. some selected verticals and cross-sections etc. Thirdly, it is hard to specify the initial conditions, whereas the computation can be sensitively influenced by the initial status in nonlinear systems. Therefore the agreement between computed and measured results in general can be subjective.

As far as the second stage is concerned, it is worthwhile to note the arguments by Oreskes *et al.* (1994) on earth science modelling. They claim that verification and/or validation of numerical models of natural systems is impossible because of logic considerations on a philosophical basis. According to Oreskes *et al.* (1994), both verification and validation are affirmative terms. Strictly, verification is an assertion or establishment of truth. A verified model is thus useful as a prediction tool because of its demonstrated truth, and implies its reliability as a basis for decision-making. Equally correct is the term validation, which usually connotes legitimacy. It can, but does not necessarily, denote an establishment of truth. Instead, it indicates the establishment of legitimacy, generally in terms of contracts, arguments, and methods. Validation means making legally valid, granting official sanction to or confirming the validity of something. A valid model contains no known errors or detectable flaws and is internally consistent.

Succinctly speaking, verification is possible only in closed systems, in which all components of the system are established independently and are correct. Its application to natural systems is misleading (Oreskes *et al.*, 1994). Alluvial river models are never closed systems, and thus it is incorrect to use the term verification for such models. Two specific factors, *inter alia,* make river models open. Firstly the model requires a number of input parameters not completely known. Secondly the observation and measurement of both independent and dependent quantities are laden with inferences and assumptions. Although in some cases these can be justified with experience, the degree to which the assumptions hold in independent studies can never be established *a priori*.

The restricted sense of the term validation must not be ignored. Legitimacy, official sanction, or being free of apparent errors and inconsistency are not necessarily identical to truth, albeit truth is not excluded. Nevertheless it is fairly popular for river modellers to use interchangeably the terms verification and validation. Thus they misleadingly imply that validation establishes model veracity. Even more critically the term validation is used to suggest that the physical river process is accurately represented by computational models.

From the above statements, there exist critical problems with the model calibration and verification/validation phases, both logically and practically. The most significant comes with the verification/validation phase, where the model is claimed a success. This is virtually committing the basic logic error of affirming the model output, which Oreskes *et al.* (1994) describe as follows: "*To claim that a proposition (or model) is verified because empirical data match a predicted outcome is to commit the fallacy of affirming the consequent. If a model fails to reproduce observed data, then we know that the model is faulty in some way, but the reverse is never the case.*"

The misuse of the terms verification and validation in computational river modelling can be risky with respect to public interests. It is the responsibility of model developers and end-users to correctly inform the decision-makers of what computational models can realistically reflect, and more essentially the degree to which the modelling results can be relied upon.

The criticisms advanced above aim to help stimulate a wider awareness of the limitations of computational river models, rather than being a rejection of their potential use. Computational river modelling is nothing but a semi-empirical approach, which embeds enhanced understanding of the physics of the problem and is therefore more advanced than earlier crude, yet simpler, methods. More experience should lead to better modelling practice. The greater number and diversity of confirming observations by computational models, the more probable the computational models are not flawed. However, overestimation of its capability is misleading the public and can carry risks for decision-making. The common usage of the so-called calibration–verification/validation process is often nothing more than a self-evident statement that an acceptable match between model results and observations is obtained by tuning the various parameters. Rarely do computational river models have the predictive role that is frequently claimed. There is no guarantee that the calibrated models will reproduce results in agreement with measurements for other independent river problems.

CONCLUSIONS

Computational models for fluvial flow–sediment–morphology systems are at best imperfectly constructed, and at worst invalid. A number of crucial issues can be identified, which comprise the simplified equations, asynchronous solution procedure, sediment transport and entrainment functions, resistance relation, turbulence closure models and bottom boundary conditions etc. The significance of these issues may vary from river to river, but the awareness of these issues is generally meagre. For some of these issues (turbulence closures, resistance, sediment functions etc.), definitive solutions may be far in the future, while for the remainder, solutions can be found shortly from technical perspectives. The calibration and verification/validation methodology commonly used in current modelling practice is questionable. Model performance is overstated by using the affirmative terms verification and validation, which can mislead the public and decision-making. Asserting a predictive role of computational river models can be risky at least currently and in the foreseeable future.

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