APPROACHING MULTIPHASE FLOWS FROM THE PERSPECTIVE OF COMPUTATIONAL FLUID DYNAMICS

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ABSTRACT

Thermalhydraulic simulation methodologies based on subchannel and porous-medium concepts are briefly reviewed and contrasted with the general approach of Computational Fluid Dynamics (CFD). An outline of the advanced CFD methods for single-phase turbulent flows is followed by a short discussion of the unified formulation of averaged equations for turbulent and multiphase flows. Some of the recent applications of CFD at Chalk River Laboratories are discussed, and the complementary role of CFD with regard to the established thermalhydraulic methods of analysis is indicated.

1. Limitations of Thermalhydraulic Simulation Methodologies

Multidimensional computations of internal flows and heat transfer in nuclear reactor components rely at present on two main methodologies for spatial discretization: porous-medium and subchannel approaches.[1,2] Even though both are considered to be advanced computational tools, aimed at accommodating models for single and multiphase flows, these approaches target only relatively crude resolution of flow details, and their underlying theoretical bases rest firmly on hydraulic concepts. Methods of this kind are ideally suited for the geometries of densely-packed rod bundles and tube banks, widely used in the nuclear reactor systems, but they suffer from serious *inherent* limitations.

The linear dimensions of computational cells, 'porous' control-volumes and subchannels, can be small compared to the scale of equipment size, but they must remain large relative to the scale of local flow-field variations. Whereas any subchannel layout must provide each subchannel with at least some solid-wall boundary, the lower-bound restriction on the sizes of 'porous' control-volumes stems from the requirement that they contain sufficient proportion of the solid matrix in order to smear the flow details over large enough regions. Only then can the wall effects, both mechanical and thermal, be accounted for through hydraulic means (empirical friction factors, heat-transfer coefficients, etc.) in these computational approaches.

In both the porous-medium and subchannel computations, the finite-volume balances embody approximations whose effects cannot be diminished by the use (whenever possible) of finer meshes. The universally employed representation of the fluid-solid forces in terms of distributed resistances is compatible with the control-volume selection, but it precludes the rigorous consideration of momentum diffusion within the fluid, and the no-slip or velocity-profile-based boundary conditions at solid surfaces. Wall boundary conditions for scalars, such as temperature, are similarly avoided, and the effects of near-wall flow patterns on their local gradients cannot be considered. In addition, subchannel arrangements are, in general, non-orthogonal, preventing a rigorous treatment of the transverse momentum balances.

2. Perspective of Computational Fluid Dynamics

In essence, the porous-medium and subchannel methodologies bridge the gap between the system (or component-level) thermalhydraulics and the truly *micro*-approach represented by Computational Fluid Dynamics (CFD). As a rule, the modern CFD algorithms are formulated for arbitrary multidimensional geometries, and accommodate progressively finer approximations to the continuum description of fluid flow, heat and mass transfer. When allotted sufficient numbers of degrees of freedom, the CFD analogues of continuum equations are able to capture at least some of the physics beyond the reach of hydraulics approaches, and therefore provide a framework in which the limitations imposed by the use of the latter methods may be overcome. The CFD methods for internal flows (based on finite-volume or finite-element discreatizations) adopt meshes that naturally allow for realistic representations of solid geometries, and enable the constraint of the computed fields through imposition of wall boundary conditions. In principle, the resolution of important physical and geometrical scales is then always better than that obtainable with subchannel or porous-media methods, and any empirical input to modelling is introduced at the more local level.

Among the most distinctive and industrially-important CFD methodologies developed to date are the numerical simulation methods for turbulent flows, closely allied with turbulence modelling. The advanced methods for incompressible flows comprise four categories:[3]

- One-point-average formulations are based on a hierarchy of correlation equations obtained through one-point averaging of the Navier-Stokes equations. Closure of a truncated set of these equations must rely on hypotheses regarding higher-order correlations appearing in the equations governing the evolution of lower-order correlations.
- Two-point-average methods are based on two-point averages of the Navier-Stokes equations, and were introduced to allow explicit consideration of scale information in modelling.
- Large-Eddy-Simulation Methods, three-dimensional and time-dependent, proceed with explicit computation of large-scale flow-field structures, while accounting for the small-scale turbulence through the subgrid-scale models.
- Direct (full) simulations of turbulent flows, currently feasible only for flows characterized by relatively small Reynolds numbers, attempt to resolve the flow-field at the Kolmogorov length-scale by solving the discrete analogues of the unaveraged Navier-Stokes equations.

Clearly, for flows characterized by realistic Reynolds numbers, the resolution limitations on present-day computers make it necessary to engage averaged formulations and turbulence models. Complex (and often poorly understood) physics, such as that encountered in the presence of multiple phases, adds additional burden. It has been argued recently by Boris[4] that the CFD methods available today can simulate flow either in complex geometry with simple physics or with complex physics in relatively simple geometry, but they cannot do both. Notwithstanding the difficulties, the goal of extending the CFD approach to multiphase flows continues to be steadily pursued, and general formulations that are not directly linked to any specific geometry, and refrain from using hydraulic concepts at the outset, are still in demand.

3. Averaged Descriptions of Turbulent and Multiphase Flows

The one-point averaging procedures yield turbulent-flow descriptions that form the basis of engineering computations and virtually all the commercially developed CFD simulation software to date. Essentially the same procedures are also used to derive the averaged *multifluid* transport equations, which lead to models underlying a large class of numerical simulation methods for multiphase flows. While all multifluid formulations are based on the treatment of individual phases as interpenetrating continua coexisting in the flow domain, they differ in many details. It appears that most derivations can be put on a common ground by tracing their origin to the distributional form of the local instant (differential) balances for a multifluid continuum.[5,6]

In the Eulerian description of a mixture of Newtonian fluids, the property balances accounting for transport within the bulk fluid are cast as partial differential equations, while transport across the interfaces (treated as singular massless surfaces) is accounted for by supplementary jump conditions. Denoting the density by ρ, the velocity field by $\mathbf{u}$, the diffusive flux by $\mathbf{J}$, and the source density of a given property, ψ, by ϕ, both balances can be written in the generic forms:

$$\frac{\partial(\rho\psi)}{\partial t} + \nabla\cdot(\rho\psi\mathbf{u} - \mathbf{J}) = \rho\phi, \tag{3.1}$$

$$[\![\rho\psi(\mathbf{u} - \mathbf{u}_s) - \mathbf{J}]\!]\cdot\mathbf{n} = \phi_s. \tag{3.2}$$

Eqs. (3.1) and (3.2) yield balances of mass, momentum, and energy, respectively, for $\psi = 1$, $\mathbf{u}$, and e, where e denotes the specific energy. In addition, $[\![\ ]\!]$ denotes the property difference across the interface, $\mathbf{n}$ is the unit vector normal to the interface, $\mathbf{u}_s$ is the interfacial velocity, and ϕ_s is the interfacial source of property ψ (e.g., surface tension).

In the multifluid formulation of n-phase problem, a set of n binary *phase-indicator* functions, θ_k $(k = 1, \ldots, n)$, is introduced to determine which of the phases is present at a given time and position. Considering all differential operations in the distributional sense, the gradient of θ_k and its transport equation may be written as:[6]

$$\nabla\theta_k = -\mathbf{n}a_k, \tag{3.3}$$

$$\frac{\partial\theta_k}{\partial t} + \mathbf{u}_s \cdot \nabla\theta_k = 0, \tag{3.4}$$

where the scalar delta-function, a_k, is conveniently interpreted, in the limit, as the interfacial area per unit volume of the fluid mixture.[6] Using Eqs. (3.3) and (3.4), the distributional balances describing the dynamics of the k-th phase may be cast in the form,

$$\frac{\partial(\theta_k\rho\psi)}{\partial t} + \nabla \cdot [\theta_k(\rho\psi\mathbf{u} - \mathbf{J})] = \theta_k\rho\phi + [-\rho\psi(\mathbf{u} - \mathbf{u}_s) + \mathbf{J}] \cdot \mathbf{n}a_k. \tag{3.5}$$

This set of balances represents the multifluid counterpart of the single-fluid continuity, Navier-Stokes, and energy equations (to which it reduces in the absence of interfaces), and constitutes an ideal starting point for any kind of averaging (temporal, volumetric, statistical, etc.). In fact, Eq. (3.5) permits the development of higher-level approaches (multi-point averages or Large-Eddy-Simulation concepts) for multiphase flows. The averaging operators are usually assumed to satisfy a set of *Reynolds rules*,[5] of which the commutativity with the differential operators, $\partial/\partial t$ and ∇, can be proven for a large class of averaging operations. In general, the action of a one-point averaging operator, $\langle\ \rangle$, on both sides of Eq. (3.5), yields:

$$\frac{\partial\langle\theta_k\rho\psi\rangle}{\partial t} + \nabla \cdot \langle\theta_k\rho\psi\mathbf{u}\rangle - \nabla \cdot \langle\mathbf{J}\rangle = \langle\theta_k\rho\phi\rangle + \langle[-\rho\psi(\mathbf{u} - \mathbf{u}_s) + \mathbf{J}] \cdot \mathbf{n}a_k\rangle. \tag{3.6}$$

Further transformations of Eq. (3.6) must involve expressing the averages of products in terms of products of averages. It is at this step where the traditional approaches to turbulence and multiphase flows diverge. Due to large uncertainties regarding the underlying physics, the correlations of fluctuations have been usually neglected in the three-dimensional modelling of multiphase flows. Only recently has the modelling of correlational terms started to be successfuly addressed within the scope of multifluid closure schemes.[7,8] While this line of development is likely to continue, more experimental work of a fundamental nature is indispensable to assure reasonable validity of any new models.

4. Recent Applications of CFD at Chalk River Laboratories

The utility of CFD-based prediction methodologies, and their complementary role with regard to the more traditional thermalhydraulic analyses, are well illustrated by the recently launched project concerning the assessment of fuel-bundle appendage effects on the pressure drop and heat-transfer characteristics of a typical CANDU fuel channel. While it is well known that the price paid for higher heat-transfer rates (attained on account of bearing pads, spacers, end-plates, etc.) is an increase in pressure drop, an experimental quantification of these effects is difficult even in the single-phase flow regime. Adequate characterization of individual appendage contributions to those effects is required as part of the input information in thermalhydraulic analyses utilizing system and subchannel codes.

The application of CFD tools to predict the integral effects, such as additional pressure drop or a change of average heat-transfer rate, caused by relatively minor perturbations of channel geometry, is a viable alternative to experimental testing. The initial phase of the project has demonstrated that the standard k-ϵ model of turbulence transport (in which the turbulent *Reynolds stresses* are represented by the two-parameter gradient model, and the parameters themselves are computed by solving their modelled transport equations) is adequate for predicting the form drag coefficient for a simple obstacle mounted on a fuel rod. The predicted flow patterns lead in turn to plausible estimates of heat-transfer enhancement, which can be characterized by the correction factor to the average heat-transfer coefficient for an unobstructed-rod surface.

5. Conclusions

The contributions of CFD to thermalhydraulic design are recognized, and continue to gain in importance with the increase of available computing power. As anticipated, modern tools of computer graphics make the CFD analyses more accessible and more widely appreciated by non-specialists. While these factors are expected to steadily enhance the supporting role of CFD, the real hope for its future seems to rest with the incorporation of additional physics into the available mathematical algorithms and computer codes. Only then can some of the thermalhydraulic analysis tools be gradually replaced by the CFD technology in nuclear engineering applications.

6. References

1. M.B. Carver, "Multidimensional computational analysis of flow in nuclear reactor components", *Trans. SCS* 1 (1984) 147.
2. N.E. Todreas, and M.S. Kazimi, *Nuclear Systems*, (Hemisphere, 1990).
3. J.H. Ferziger, "Simulation of incompressible turbulent flows", *J. Comput. Phys.* **69** (1987) 1.
4. J.P. Boris, "New directions in Computational Fluid Dynamics", *Ann. Rev. Fluid Mech.* **21** (1989) 345.
5. D.A. Drew, "Mathematical modelling of two-phase flow", *Ann. Rev. Fluid Mech.* **15** (1983) 261.
6. I. Kataoka, "Local instant formulation of two-phase flow", *J. Multiphase Flow* **12** (1986) 745.
7. S.L. Lee, R.T. Lahey, Jr., and O.C. Jones, Jr., "The prediction of two-phase turbulence and phase distribution phenomena using k-ϵ model", *Jap. J. Multiphase Flow* **3** (1989) 335.
8. M. Lopes de Bertodano, S.J. Lee, R.T. Lahey, Jr., and D.A. Drew, "The prediction of two-phase turbulence and phase-distribution phenomena using a Reynolds stress model", *Trans. ASME, J. Fluids Engng.* **112** (1990) 107.

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