Report on the Panel Discussion on 'Modeling of Multiphase Flow'

A. Prosperetti[1]

Department of Mechanical Engineering, The Johns Hopkins University

Baltimore MD 21218 USA

G.F. Hewitt

Imperial College of Science, Technology, and Medicine, Department of Chemical Engineering and Chemical Technology, Exhibition Road, London SW7 2AZ UK

D.D. Joseph

Department of Aerospace Engineering and Mechanics, University of Minnesota 110 Union St SE, Minneapolis, MN 55455 USA

Y. Matsumoto

Department of Mechanical Engineering, The University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113, Japan

T.G. Theofanous

Departments of Chemical and Mechanical Engineering, UC Santa Barbara, Santa Barbara CA 93106 USA

The panel on 'Modeling of Multiphase Flow' was convened by the first author (AP) and held on Monday, May 28. It was attended by well over 100 participants and the discussion could have easily gone on far beyond the 1 hr 40 mins allocated. Prof. Gad Hetsroni (Department of Mechanical Engineering, Technion, Haifa 32000, Israel) had to cancel his participation due to a last-minute commitment. The summaries that follow have been contributed by Profs. Joseph, Matsumoto, Prosperetti, and Theofanous; the summary of Prof. Hewitt's presentation has been written by the first author on the basis of notes and copies of Prof. Hewitt's transparencies.

Modeling Approaches for Single and Multiphase Systems

(G.F. Hewitt)

While single and multiphase modeling exhibit many similarities, such as the use of a few exact solutions, empirical correlations, and phenomenological and statistical models, the complexity due to the coexistence of many phases

[1]Also Faculty of Applied Physics, Twente Institute of Mechanics, and Burgerscentrum, University of Twente, AE 7500 Enschede, The Netherlands

severely hampers the task of multiphase modeling. As a consequence, the field is considerably less developed than it would be desirable and necessary for practical applications.

Most commercial nuclear safety and oil industry transient multiphase flow computer codes are based on the multifluid model and are mainly one-dimensional. These codes suffer from several problems:

- Appropriateness of the equations: How many equations should be used? Are all significant terms included? Is ill-posedness significant?
- Validity of numerical methods: Do the discretized equations faithfully mirror the original differential formulation? Are the numerical solutions grid- and time-step independent?
- Validity of the closure relationships: Do the closure methods have sufficiently generality and accuracy? Have they been validated against data?

Unfortunately the answer to many (perhaps most) of these questions is in the negative. Many examples can be made in which predictions of different codes differ substantially, and in which numerical results obtained after an experiment exhibit a marked difference with the pre-test ones.

The conclusion is thus a pessimistic one. The multi-fluid method, as applied in current commercial computer codes, is unlikely to give the right answer for several reasons:

- For economic and technical reasons, the numerical methods used in the codes may lead to results which do not correspond to a solution of the original equations.
- The equations used may be at an insufficient level of detail to capture the important phenomena.
- The closure laws used within the equations cannot be of sufficient generality for reliable prediction.

In the short term, the risk of bad predictions could be reduced by considering ‘worst-case scenarios’, but this is unlikely to be attractive in a competitive world.

A Computational Platform for Multiphase Flow and Heat Transfer (T.G. Theofanous)

Multiphase flows are ‘complex’. The complexity derives from ‘collective’ behaviors of interacting entities within such flows (bubbles, drops, interfaces), and manifests itself in their, often dynamic, spatial distributions - ‘patterns’. Predicting multiphase flows means being able to predict these patterns – everything else follows. Understanding multiphase flow means being able to capture in our mind the key mechanisms responsible for such pattern formation,

and verify by experiment/theory that this is indeed so. **This is the principal intellectual and practical content of the subject**.

The challenge of 'complexity' is compounded by the 'variability' of multiphase flows. Even pool boiling from a horizontal flat plate exhibits enough of these both, to basically remain undecipherable after more than half a century of study. Moreover, there is a chasm between 'simple' flows that are being (or presumably can be) studied, and practical flows that need to be understood. Progress has been hampered by the lack of appropriate integrative tools. Recent advances in Computational Fluid Dynamics (CFD), and explosion of computing power, offer an unprecedented opportunity to satisfy this need. While institutional support of integrative efforts remains inadequate, much can be done toward the development of such tools.

Consistent with their integrative role, such tools need to be centered at the Effective Field (EF) level of treatment. Direct Numerical Simulations (DNS) can, and in fact then need to be, in a supportive role. Further down the scale, we have available Molecular Dynamics (MD). In between, arguably, we can address mesoscopic scales with Discrete Particle methods such as Lattice Gas, Dissipative Particle Dynamics, and the Lattice Boltzmann Method, although so far applications have been limited to DNS. This hierarchy of tools is consistent with the multiscale nature of these flows. The question is how to strategically approach their integration and use, toward understanding and prediction.

In fact, the key question is how to approach the Effective Field treatment. In general this would involve an appropriate sort of averaging (Ishii,1975; Drew and Passman, 1998; Zhang and Prosperetti, 1994), and a set of constitutive laws that describe the interaction between the fields, as well as the evolution of interfacial area through which these interactions occur. We found great value in such an approach, and brought it to practical use for a class of flows involving the mixing and thermal detonation of high-temperature melts poured into a pool of volatile liquid, such as water (Theofanous et al., 1999a; 1999b). This experience taught us that the EF treatment provides only a high-level framework that needs to be significantly embellished by the key physics relevant to a particular application. This brings us to the general vision of a 'computational platform' from which one launches efforts addressing individual 'classes of problems'. This contrasts with the idea of a generally applicable multiphase flow 'code'. **From this experience we also developed ideas suggesting that EF should not be regarded in the restrictive sense in which it has been classically developed/employed**. In particular, this experience led us to an EF interpretation based on explicitly tracking the 'Large Scale Discontinuities' (LSD) within the flow, and a quite general computational framework thereof. This is the centerpiece of our approach toward a Computational Platform for Multiphase Flows as embodied in our Multiscale Simulation Code (MuSiC) (Nourgaliev et al., 2000; 2001a; 2001b).

Briefly, by LSD's we mean the dynamic demarcation lines (surfaces) between rheologically homogeneous subdomains (i.e., liquid-continuous vs vapor-continuous). The idea is that, in this way, we capture the major distinctions in describing local mechanical and thermal non-equilibrium. Reflecting the extent of these domains explicitly would

be a major step toward describing the internal systemic dynamics (the collective behavior noted above) of such flows. Clearly, in this way we have the basic ingredients to describe patterns as well. Moreover, since transport across such large-scale discontinuities is often critical to behavior, we should wish for explicit treatment along with their tracking. Most importantly, such 'interfaces' are susceptible to smearing by numerical diffusion and this capturing would remove major difficulties with constitutive treatment in their neighborhood. All this applies to gas-liquid flows, and other multiphase systems as well.

In MuSiC we track these LSD's explicitly, including their generation or disappearance as dictated by the flow (and heat transfer). The important implication is that this 'localized' EF treatment requires consideration of dispersed flows only. This simplifies both the conceptual and practical aspects of averaging, as well as the constitutive treatment within such dispersed flows. On the other hand, this requires the constitutive treatment of the LSD's, and this is a new task. Another advantage is that the numerical treatment of consistently coupling disperse flows, or even deforming/moving solid boundaries across such LSD's, is quite general, and we have shown it to be robust. So, automatically, we have fluid-structure interaction capability as well, ability to model large number of objects moving though such flows (and vice versa) and, at the DNS level, the capturing of physical interfaces.

The key technical aspect of the LSD approach is the use of a characteristics-based method of solution in the EF regions, and a characteristic-base coupling across the LSD's — this we call Characteristics-Based Matching (CBM) (Nourgaliev et al., 2001b). Further, in implementation we found the additional benefit that this allows the proper specification of boundary conditions, which allows us robust solutions that do not depend on numerical diffusion for stability – that is to refine the grid, $dr \rightarrow 0$, with no ill effects. Along the same lines, we have a highly efficient incompressible solver based on Numerical Acoustic Relaxation (NAR) (Nourgaliev et al., 2001c) that moreover allows for conveniently coupling compressible and incompressible regions (Nourgaliev et al., 2001b). Further, NAR could be applied to DNS with interface tracking (not LSD, but actual gas-liquid interfaces) robustly enough to handle realistic density ratios (over 1,000 , as compared to $\sim$10 being the current state of the art for Eulerian-based methods).

All the components of this computational platform (which includes LBM and MD) and their status of verification can be seen at `http://www.crss.ucsb.edu/music`. We envisage that an appropriate subset of these tools will be needed to be 'assembled' as required for any particular class of problems being examined. Initially constitutive descriptions will be passed up this hierarchy (from MD and DNS to EF), 'by hand'. Ultimately, all will communicate while running in parallel, the DNS focusing on each particular region of the flow as needed.

We emphasize the importance of carefully thought-out experiments integrally connected to such efforts, and in particular to the thus-created well-focused needs for constitutive laws at the Large Scale Discontinuities.

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Multi-Scale Analysis of Turbulent Bubbly Flows

(Y. Matsumoto)

Bubbly flow has multiple structures in time and spatial scales. The macro-scale flow structure is affected by both meso-scale and micro-scale phenomena. The multi-scale analysis is required to solve a bubbly flows reasonably. It is

Figure 1: Streamlines around a clean and a contaminated bubble.

well known that a very small amount of surfactant can drastically change the terminal velocity of a bubble. When the liquid is contaminated, the bubble motion is affected by the Marangoni effect due to the variation of surface tension along the bubble surface caused by the gradient of the contaminant concentration. Figure 1 shows the streamlines around the clean bubble and the contaminated one. The numerical results reveal that the flow pattern around the contaminated bubble becomes similar to that of a rigid particle and the drag coefficient increases from that of a clean bubble to that of a rigid particle.

The behavior of rising bubbles in quiescent contaminated water was calculated by Direct Numerical Simulation (DNS), as an example of a bubbly flow, where meso-scale phenomena are clearly observed. The Navier-Stokes equation is solved by the finite difference method and the bubble motion is tracked on a rectangular grid system. The relation between drag coefficient, Reynolds number, and void fraction is investigated at moderate Reynolds numbers. Present results for the void fraction dependence on the drag coefficient show a good agreement with experimental and theoretical ones. The flow around many spherical bubbles rising in a periodic box was simulated and information on the turbulence structure in the bubbly flow was obtained. Using the DNS results of multi-bubble system, some averaged quantities were extracted. The turbulent energy in the surrounding liquid increases with the void fraction. To simulate a large-scale turbulent bubbly flows by Large Eddy Simulation (LES), a Sub-Grid Scale (SGS) model was developed. The two-fluid simulation by LES was also carried out under the same conditions as the present DNS. Constitutive equations, where not only the SGS stresses but also boundary conditions of the pressure and the vorticity

Figure 2: One-dimensional vertical energy spectrum in bubbly flow with a void fraction of 0.833%.

on the interface are taken into account, were derived for the LES. Figure 2 shows a snapshot of a bubbly flow and the one-dimensional vertical energy spectrum in bubbly flow with a void fraction of 0.833%. The energy spectrum obtained by the present bubbly flow model reproduces the DNS result well, while the result by the conventional model, where the SGS stress and the boundary conditions on the interface are neglected, shows considerable difference with the DNS one. 20

Correlations from Numerical Experiments

(D.D. Joseph)

In my presentation and in the discussion that followed I took a too extreme position against modeling. I was motivated to do so by my general impression that many models fail to achieve their stated goals and by our recent success with the generation of correlations from direct numerical simulations of solid-liquid flow. (A list of papers is given in my paper ‘Power law correlations for lift from direct numerical simulation of solid-liquid flow’ in the Proceedings of this meeting.)

Generating correlations from experiments is an old method on which many industrial applications are based but it has come to have a bad name, viewed as empirical and not fundamental. The great example is the Richardson-

Zaki correlation which is the cornerstone of fluidized bed practice. My enthusiasm for correlations has to do with the surprising emergence of correlations from the simplest kind of post-processing of our numerical experiments. We have done lift correlations for single particles and for the bed expansion of many particles in slurries. The procedure we follow is to plot the results of our simulations in log-log plots of the relevant variables. The surprise for us is that these plots frequently come up as straight lines giving rise to power laws. For example, a single particle will lift-off in a Poiseuille flow at a certain Reynolds number $R = pUd/\nu$ for a given settling Reynolds number $R_G = \rho_f(\rho_p - rho_c)gd^3/\eta^2$. When we plotted the lift-off criterion from about 20 points we found that

$$R = a\, R_G^n\,,$$

with an intercept a and slope n in the log-log plot. The straight lines are impressively straight and we generated such correlations for lift to equilibrium, for the bed expansion of many particles and in non-Newtonian fluids. The existence of such power laws is an expression of self-similarity, which has not been predicted from analysis or physics. The flow of dispersed matter appears to obey those self-similar rules to a large degree.

We can get power laws when only two variables are at play; when there are three variables or more, it would appear that we get different power laws separated by transition regions. This is certainly the case for the Richardson-Zaki correlation; it has one power law relating the fluidization velocity to the solids fraction at low Reynolds number and another at high Reynolds with a Reynolds number-dependent transition between. We got such correlations between three variables for slurries, and from experiments (see 'Power law correlations for sediment transport in pressure driven channel flow,' by Patankar, Joseph, Wang, Barree, Conway and Asadi, submitted to Int. J. Multiphase Flow).

We have generated 3D calculations from simulation for a fluidized bed with 1204 spheres (to appear in J. Fluid Mech.), but it is very expensive. The direction of our work is to develop simulations to get efficient computation leading to 3D correlations. This will happen. Then we will get real engineering correlations from numerical experiments. I like this approach since it uses numerical simulations in a natural way evolving from their intrinsic properties rather than trying to fit them into a more familiar frame. I think that processing of data for correlations, from experiments, field data or simulations is a great new opportunity of the computer age and ought to be vigorously pursued.

The problem faced by models is how to get the various interaction terms right. Much of the time the guesses made for these interaction terms are poor and the predictive power of the model is not there. Better models must also make use of correlations for the interaction terms. For example, the Richardson-Zaki correlation gives an excellent correlation for bed expansion, but leaves the modeling of the drag force needed for a mechanist's model to imagination.

My position in the round table was too extreme; let it be said that the active pursuit of correlations is an excellent direction for future research using computers in a new way with direct applications to both engineering practice and model construction.

The Systematic Derivation of Averaged Equations by Direct Numerical Simulation (A. Prosperetti)

Modern computational methods enable us to effect direct numerical simulations of relatively simple problems involving disperse particle flows. Certainly, what we can do still falls far short of realistic situations of practical interest. Nevertheless, from the simulations that are currently feasible, it is possible to gain the insight and the quantitative information necessary for a systematic closure of the averaged equations for such systems, at least in some situations.

We have studied the case of a suspension of equal spheres in (locally) Stokes flow (Marchioro et al. 2000, 2001; Wang & Prosperetti 2001; Tanksley & Prosperetti 2001). Schematically, our procedure consisted of the following steps: (1) Set up an ensemble of macroscopically equal systems; (2) Simulate the same physical process (e.g., sedimentation, shear, etc.) for all the realizations of the ensemble; each such process will be characterized by a certain number of parameters $\Pi_1, \Pi_2, \ldots$ (e.g., the applied force for sedimentation, the applied shear, etc.); (3) Take the ensemble average of the results; all the average quantities will depend on the same parameters $\Pi_1, \Pi_2, \ldots$; (4) Choose some quantities as fundamental; in our case we take the mean volumetric flux $\mathbf{u}_m$, the mean particle velocity $\overline{\mathbf{w}}$, the disperse-phase volume fraction β_D and the mixture pressure p_m; other average quantities of interest will be the mean stress $\mathbf{\Sigma}$, the mean inter-phase force $\mathbf{f}$, etc.; (5) Eliminate the parameters $\Pi_1, \Pi_2, \ldots$ between the dependent variables $\mathbf{\Sigma}_C$, $\mathbf{f}$, etc. and the primary variables. The result of this step is the formulation of constitutive relations such as $\mathbf{\Sigma} = \mathbf{\Sigma}(\mathbf{u_m}, \overline{\mathbf{w}}, \beta_D \ldots)$, $\mathbf{f} = \mathbf{f}(\mathbf{u_m}, \overline{\mathbf{w}}, \beta_D \ldots)$, which are the required closure relations.

We have found that, in the case of spatially non-uniform systems, the mixture stress and the inter-phase force acquire several new terms that happen to vanish identically in the uniform case previously considered in the literature. Furthermore, the results show that the closure coefficients for sedimentation, imposed couple, and imposed uniform shear are consistent among themselves (in the sense that, for example, the same effective viscosity is applicable to all three situations), but are systematically different from those for flow through a porous medium or when the same angular velocity is imposed on the particles. It thus appears that these latter two situations differ from the others in an essential way that cannot be captured by a set of averaged equations formulated solely in terms of two velocities, pressure, and volume fraction. Mathematically, the root of this difference is that, while the mobility matrix is the exact inverse of the resistance matrix at the microscopic level, the same relation is not satisfied after averaging. In the context of an averaged-equations description, this circumstance implies that at least one more quantity (and the related evolution equation) is necessary for a unified description of all these cases. A likely guess for this additional "hidden variable" is the "granular temperature" of the particles.

The previous results require a clear definition of the quantity to be identified with the mixture pressure p_m, as p_m must be calculated from the averaged equations rather than closed. We have attacked this problem by using the

fact that, at the microscopic level, the potential ψ of the external forces (e.g., $\psi = -\rho \mathbf{x} \cdot \mathbf{g}$ in the case of gravity) can be eliminated from the equation of motion by replacing the continuous-phase pressure p_C by a modified pressure $\hat{p}_C = p_C + \psi$. By defining the mixture pressure as that part of the average stress that transforms in the same way, one is led to a unique expression for p_m; in the case of a uniform system this is

$$p_m \;=\; (1-\beta_D) < p_C > + \beta_D \overline{p}^s$$

where $< p_C >$ is the ensemble-averaged continuous-phase pressure and

$$\overline{p}^s \;=\; \frac{1}{S} \overline{\int dS \; p_C} \,,$$

in which the integral is over the particle surface S and the overline indicates an average over all the particles (Marchioro et al 1999). This quantity has appeared before in averaged equations analyses, where it is referred to as *interfacial pressure*. This result (complemented by additional terms that arise in the non-uniform case) is valid also at finite Reynolds number, and even for non-Newtonian systems.

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Concluding Comments

The different tone of Prof. Hewitt's remarks as compared with those of the other speakers reflects the split between people who need reliable models for pressing practical needs and people involved in the development of models with

a somewhat longer (although not necessarily long-term) time horizon. Similar differences were clear in the remarks made by the audience: while some took issue with pessimistic statements, others apparently were attending the session in the hope of obtaining very definite suggestions as to which models to use for the solution of their immediate practical problems.

While it cannot be denied that accurate models are currently unavailable, except in special situations, the cautious optimism expressed by several speakers appears to have a serious basis. In the first place, the progress in computational hardware enables us to 'interrogate' more and more accurate direct numerical simulations to better understand the physics and develop closure relations. Secondly, the ambition of developing general-purpose models and codes has been recognized by and large as unrealizable and, indeed, dangerous. A variety of more specialized tools, each one with its own applicability and capabilities, seems to represent a more realistic way to tackle various problems with an acceptable degree of physical realism, at least for the foreseeable future. Even with this reduction in scope, great difficulties remain which will be overcome more easily by synergizing the efforts of groups of investigators.