DYNAMICS OF TWO-PHASE FLOWS

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Preface

Research in two-phase flow and heat transfer with change of phase currently emphasizes the dynamics of two-phase flows, flow boiling, and flow condensation. This work is motivated in large part by the great need to understand better the physical phenomena taking place in various conventional and nuclear energy conversion/production systems. This research is directed to developing the capability to improve thermal efficiency and to optimize the design of such systems, and more precisely evaluate the safety aspects of these systems. Major research programs are being conducted in government, industry, and university laboratories in both Japan and the United States. The Japanese work is characterized as rather fundamental whereas the U.S. workers have a tendency to deal with more applied work.

The importance and value of a joint Japan-U.S. seminar was recognized in 1979 when the first seminar on Two-Phase Flow Dynamics, cosponsored by the Japan Society for the Promotion of Science and the U.S. National Science Foundation, was held at the University Seminar House in Kansai. Five years later, the second seminar similarly cosponsored was held in Lake Placid, New York. During these intensive interaction periods, a valuable exchange of information occurred in the technology of multiphase dynamics. As a result of these seminars, considerable collaborative research and much interchange between researchers in the two countries was initiated.

The research field on two-phase flow had grown in the four intervening years to the time when this Third Japan-U.S. Seminar on Two-Phase Flow Dynamics was held in July of 1988 at Lake Biwa, Japan. This seminar, too, was jointly sponsored by the JSPS and the USNSF. Emphasis had been on developing a better understanding of the physics of the phenomena and improvements in dynamic analysis of normal transient or accident situations. Therefore, the holding of this third seminar was especially appropriate and beneficial to all parties. This volume, therefore, represents a distillation of the research reported during this meeting.

The seminar featured a broad review of the status of research relating to two-phase flow dynamics both with and without phase change. The papers fall into several categories which formed the natural grouping for the seminar, and for this volume, These major groupings are:

1. Fundamental equations and closure laws;
2. Flow regime modeling and dynamics;
3. Phase separation and distribution phenomena;
4. Wave and shock phenomena and critical flows;
5. Forced convective and post-dryout heat transfer.

In the final analysis, the value of any gathering such as this can only be judged in relation to the lasting effects as evidenced in the direction and quality of research which follows. The exchange of information by these two active nations is expected to substantially enhance progress in many areas of energy conversion including power plant efficiency, reliability, and safety. Ultimately, it is hoped that the seminar will lead to an improved understanding of process and system behavior, which in turn will lead to improved safety, longevity, and optimization of operational efficiencies of future energy conversion systems which utilize multiphase flows.

Finally, the organizers of the Japan-U.S. Seminar on Two-Phase Flow Dynamics would be remiss if they did not acknowledge the vision and foresight of Professor Arthur E. Bergles, Dean of Engineering at Rensselaer Polytechnic Institute, and Professor Seikan Ishigai, Professor Emeritus of Osaka University who jointly conceived and organized the first seminar a decade ago. It was through their efforts that this has become a successful series of quadrennial events. The second seminar in 1984 was jointly organized by Professor Koji Akagawa, Professor Emeritus of Kobe University, and Professor Owen C. Jones of Rensselaer Polytechnic Institute. In addition, the editors of this volume would also be negligent if they did not recognize the kind support of the Japanese Society for the Promotion of Science and the United States National Science Foundation, and for all institutions and companies which provided support for members of their organizations to participate in the seminar. This support provides extremely high leverage for continued collaboration and progress in the field.

In closing, the editors would like to express thanks to members of their respective organizations who provided valuable assistance and support in the planning, preparation, and conduct of the seminar. This support was the key to conducting a successful seminar and developing what we hope will be a useful compendium of research papers in the field.

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FUNDAMENTAL EQUATIONS AND CLOSURE LAW

DISCRETE MODELING CONSIDERATIONS IN MULTIPHASE FLUID DYNAMICS*

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ABSTRACT

A discussion is given of discrete modeling considerations in multiphase fluid dynamics and related areas. By the term "discrete modeling" we refer to a collection of ideas and concepts which we hope will ultimately provide a philosophical basis for a more systematic approach to the solution of practical engineering problems using digital computers. Our conception of discrete modeling is still evolving and has not yet led to useful results; thus the present paper is of the nature of a preliminary report on work in progress, and its primary purpose is to stimulate further thought and discussion. As presently constituted, the main ingredients in our discrete modeling Weltanschauung are the following considerations: (1) Any physical model must eventually be cast into discrete form in order to be solved on a digital computer. (2) The usual approach of formulating models in differential form and then discretizing them is an indirect route to a discrete model. It is also potentially hazardous: the length and time scales of the discretization may not be compatible with those represented in the model. It may therefore be preferable to formulate the model in discrete terms from the outset. (3) Computer time and storage constraints limit the resolution that can be employed in practical calculations. These limits effectively define the physical phenomena, length scales, and time scales which cannot be directly represented in the calculation and therefore must be modeled. This information should be injected into the model formulation process at an early stage. (4) Practical resolution limits are generally so coarse that traditional convergence and truncation-error analyses become irrelevant. (5) A discrete model constitutes a reduced description of a physical system, from which fine-scale details are eliminated. This elimination creates a closure problem, which has an inherently statistical character due to uncertainty about the missing details.

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Methods from statistical physics may therefore be useful in the formulation of discrete models. In the present paper we elaborate on these themes and illustrate them with simple examples.

INTRODUCTION

Multiphase flow plays a fundamental role in a wide variety of technologically important processes, systems, and devices, including nuclear reactors and other energy systems. Consequently there is great interest in analytical models for describing multiphase flow behavior. Just as in single phase flow, there is a spectrum of modeling approaches that can be taken depending upon the application. These include the atomistic simulation of behavior at the molecular level, local instant continuum modeling, and averaged macroscale modeling. It is pertinent to this discussion to note that the evolution of these modeling approaches starts with a particle formulation in terms of ordinary differential equations at the atomistic level. Then, by averaging over systems of particles, a local instant continuum model in the form of partial differential equations (PDEs) is obtained. The macroscale model is obtained by still another averaging of the local instant continuum model. These modeling approaches applied to single phase fluid dynamics yield the equations of molecular kinetics, the Navier-Stokes equations, and the Reynolds averaged Navier-Stokes equations respectively. The primary application that we address in this paper is system modeling, and the only approach that is numerically tractable for this case, considering the current state of computer capability, is the averaged macroscale model.

The local instant or microscopic behavior of multiphase flow is accurately modeled by the Navier-Stokes formulation with the addition of interfaces across which appropriate jump conditions hold. A particularly elegant formulation of this problem has been developed by Kataoka (1986) to obtain a local instant formulation for multiphase flow analogous to the Navier-Stokes formulation for single phase flow. The Kataoka formulation can be solved in principle to obtain a microscopic description of a multiphase flow process. Unfortunately, just as in the case of the Navier-Stokes formulation, the application to large-scale engineering problems is numerically intractable. Therefore, to obtain macroscale solutions we must resort to further averaging and seek solutions for the average values of the system dependent variables. This second averaging operation introduces the need for additional closure models, and the details of the averaging methods have been the subject of debate. Nevertheless, the multiphase system models in use today are based on this approach and research efforts to improve these models are continuing.

In spite of significant research efforts within the past decade, existing macroscale multiphase flow models cannot yet be regarded as satisfactory in terms of either accuracy or

predictive capability. They rely heavily on empiricism, often of an ad hoc variety, important physical effects are sometimes neglected altogether, and the interplay between model and numerical solution scheme is not well characterized. This reflects, of course, the immense complexity of multiphase flow, in which all of the difficulties of single phase flow and turbulence occur in conjunction with the additional complications of interfacial dynamics, flow regime transitions, interphase transport, phase transitions, and so on.

In view of the complexity of the problem, it would be unrealistic to hope that a truly comprehensive and predictive macroscale multiphase flow model will emerge in the near future, although incremental progress toward this goal can and should be expected. Unfortunately, the rate of such progress seems to have slowed in recent years. The purpose of the present paper is to discuss a somewhat different approach which we feel holds promise for further progress in macroscale modeling.

At the Japan-U.S. Seminar on Two-Phase Flow Dynamics, Ransom and Trapp (1984) discussed the importance of well-posedness and stability of two-phase flow models with respect to constructing numerical solutions. Tacit in that discussion was the assumption that a multiphase flow model for the macroscale behavior could be formulated as a system of PDEs. That being the case, obtaining a well-posed model becomes tantamount to including appropriate and sufficient physics in differential form; numerical solutions could then be obtained in a straightforward manner. In the present paper we examine the basic premise of whether it is reasonable to expect that a sufficiently complete PDE model exists for the macroscale description and whether improved modeling can be achieved by seeking missing differential terms representing additional physics of the flow. In this context, even the well-posed models that were discussed by Ransom and Trapp (1984) were not claimed to be complete physical descriptions in the limit of short-wavelength effects, but rather merely to have benign behavior at short wavelengths. These models are not equivalent to the local instant formulation, and it is not clear that further refinement of the macroscale model within the PDE framework would ever achieve such a result. We will presently argue the premise that it may be more productive to recognize practical modeling and computational limitations from the outset and construct discrete models that are compatible with the inherently discrete numerical solution process.

Our expository task is made more difficult by the fact that our views are still evolving and have not yet resulted in a specific model. Nevertheless, our contention is that insufficient consideration has been given to certain serious and fundamental difficulties with current approaches to multiphase flow modeling and computation, and that an alternative view and approach is perhaps better suited to the construction of models suitable for implementation and solution on digital computers. For want of a better term, we

use "discrete modeling" to refer to the collection of ideas and concepts of which our current view is comprised and which constitute the subject of the present discussion.

The basic motivations for discrete modeling have already been summarized in the Abstract, and they will be amplified upon and the approach outlined in the subsequent sections. It is convenient to divide this discussion into four main parts. First we discuss continuum formulations and attempt to highlight some perspectives that are frequently lost sight of. Next we discuss numerical considerations, and then we outline the development of a discrete model. Finally, statistical concepts are introduced. This subdivision is somewhat artificial as there are numerous points of interconnection between the different sections. We shall attempt to call attention to these connections at appropriate places.

CONTINUUM FORMULATIONS

Within the framework of classical mechanics, the basic dynamical laws at the molecular level may be expressed as a system of ordinary differential equations for the coordinates and velocities of the molecules. A useful mathematical model is obtained by formulating the average space-time behavior of the system properties in terms of continuous functions. With this approach the physical laws then appear as PDEs that govern the behavior of the continuum. The dynamical description then consists of the PDEs, a specified initial state, and appropriate boundary conditions. This practice is commonplace in fluid mechanics and results in highly useful formulations. Only in extreme situations, such as highly rarified gases, is it necessary to resort to more fundamental particulate descriptions.

As a result of the averaging process used to obtain a continuum approximation, macroscopic closure laws are required. In the case of fluid mechanics, Newton's law of viscosity, Fourier's law of conduction, and Fick's law of diffusion are such closure laws for momentum, energy, and mass.

Continuum Limitations

It is apparent that such partial differential formulations are not exact; they are merely very useful approximations. For example, Fourier's law of heat conduction is very accurate for most applications, yet it predicts that thermal signals propagate with infinite speed, which is clearly unphysical. This is an illustration of the very general fact that partial differential descriptions typically break down at very short length and time scales. In particular, the familiar Navier-Stokes equations, with which we all feel so comfortable as a description of ordinary single-phase fluid dynamics, become inaccurate at sufficiently short lengths and

times; the goal of generalized hydrodynamics (Mountain, 1977; Alder and Alley, 1984) is to remedy this deficiency.

In general, the length and time scales below which continuum descriptions become inaccurate are on the order of the characteristic lengths and times associated with the microstructure of the medium. For example, the Navier-Stokes equations break down, and generalized hydrodynamics is called into play, when length and time scales approach those of a molecular magnitude. Only for lengths and times much larger than characteristic molecular lengths and times do the Navier-Stokes equations provide a quantitatively correct description of fluid dynamical behavior. Fortunately, this range of lengths and times is very wide and encompasses essentially all macroscopic fluid flow phenomena. That is to say, the differential description is useful because there is a wide separation of scales between the smallest macroscopic scales of interest and the microscopic scales associated with the internal structure of the fluid.

If the microscales were always of a molecular magnitude then questions of scale separation would seldom arise. But in many of the descriptions employed for engineering purposes, the characteristic scales of the internal structure being modeled are themselves macroscopic in nature. For example, the microstructure in a porous medium consists of the detailed geometry of the individual pores. Flow in porous media is usually described by equations in which the effects of this microstructure are modeled in terms of distributed porosity, frictional drag forces, etc. (Whitaker, 1986). The resulting PDEs are clearly valid only on length scales much greater than a characteristic pore size, even though they in principle possess solutions on all length scales. In such situations the desired separation between the calculated and modeled scales is much less clear cut, and one must be careful not to attribute quantitative significance to any predicted solution features with scales comparable to the internal microscales.

A word is in order about the nature of the inaccuracies that occur when a continuum description is pushed too far; i.e., applied on scales too small. Ideally one hopes that such inaccuracies, while necessarily quantitative, are not qualitative or catastrophic. For example, the Navier-Stokes equations predict profiles for strong shock waves which are qualitatively reasonable even though quantitatively inaccurate. If, however, viscosity is neglected while thermal conductivity is retained, the profiles acquire a qualitatively unphysical discontinuity (Zel'dovich and Raizer, 1967).

There are also situations in which the inaccuracies of a continuum model are catastrophic in nature. In the present context, the relevant example is the one-dimensional two-phase flow equations with both viscosity and surface tension neglected, which constitute an improperly posed problem characterized by violent and unbounded instabilities at short wavelengths (Ramshaw and Trapp, 1978). These

instabilities make it impossible to calculate even longer wavelength components of the solution (unless they are controlled by introducing artificial diffusion, as is often done in practice). Thus for a continuum model to be useful at all, even over a restricted range of length and time scales, it is necessary that its inaccuracies at smaller scales be benign in nature, and that it exhibit at least qualitatively reasonable behavior in spite of the inaccuracies.

In nonlinear problems there may be even more stringent requirements concerned with the necessity to prevent errors at small scales from contaminating larger scales. The obvious example is the rate of energy dissipation, which must be correctly represented in both shock waves and turbulence in spite of any other inaccuracies which may be present at small scales. Both artificial shock viscosities of the Von Neumann-Richtmyer type and subgrid scale (large eddy simulation) eddy viscosities for turbulence, when implemented conservatively, possess this essential property (Von Neumann and Richtmyer, 1950; Ramshaw, 1979). In both cases, the effect of the artificial viscosity is to artificially expand the microscale on which the energy dissipation occurs until it becomes large enough to resolve in the calculation. This expansion is done in such a way as to preserve the rate at which energy is dissipated. It seems likely that similar considerations will apply to discrete modeling in more general contexts as well.

It should be emphasized that the breakdown in continuum descriptions at small scales does not imply that the various continuous variables in the problem, such as velocities, densities, etc., become in any sense ill-defined. The implication is rather than when such variables vary too rapidly in space and/or time they no longer satisfy PDEs of a simple structure. The further implication is that it may not in fact be useful to define and deal with quantities which cannot be calculated in any simple way. That is to say, continuous quantities may not be the most natural description of the system at small length and time scales. The statistical mechanics literature provides additional support for this view. Statistical theories of continuous systems frequently encounter short-wavelength divergences (sometimes referred to as ultraviolet catastrophes by analogy to quantum electrodynamics), particularly in the treatment of thermal fluctuations of continuous quantities. These difficulties are commonly circumvented by adopting some sort of coarse-graining procedure such as dividing the system into little cells (Bedeaux et al., 1982; Gunton and Droz, 1983; Visscher, 1978, 1985), which is tantamount to replacing a continuum model by a discrete one. We shall presently argue more generally that this is indeed the simplest and most natural approach to avoid difficulties with continuum models at short scales (cf. Visscher, 1978).

In this regard, it is interesting to note that there are increasingly frequent speculations to the effect that the fundamental laws of nature on the most basic level, and

perhaps even space and time themselves, may be discrete in nature (Feynman, 1982; Namsrai, 1985; Lee, 1987). However, we shall resist any temptation to draw support for our discrete modeling ideas from this source, as our motivation stems more from the scale separation considerations discussed above and from the computational considerations discussed below. For our purposes we are entirely content to accept Newton's laws for molecular motion and the Navier-Stokes equations for fine-scale fluid motion as starting points.

Multiphase Formulations

We now consider the implications of the above considerations for multifluid descriptions of multiphase flow, in which each phase is described by its own fluid dynamical variables and equations coupled appropriately to those of the other phases (Banerjee, 1986; Drew, 1983; Bedford and Drumheller, 1983; Stewart and Wendroff, 1984; Drew and Wood, 1985; Ishii, 1975). The basic idea is that these variables and equations refer to some sort of appropriate averages over the detailed fine-scale structure of the multiphase flow. For example, in a bubbly flow one may have a cloud of bubbles of various sizes and shapes, each with its own position, orientation, and velocity, and one seeks a reduced description in which only a mean velocity, void fraction, and perhaps a few bubble size distribution parameters are retained. The central point now is that the length and time scales associated with the detailed flow structures are not always widely separated from the macroscopic length and time scales on which one would like to predict the average behavior. That is to say, the desired separation of scales upon which the validity of a continuum description depends rarely obtains in multiphase flow, where the scales of the internal structures over which we desire to average may be comparable to the macroscopic scales over which the desired averaged quantities vary. This is precisely the sort of situation in which a simple partial differential description may be expected to break down. Thus it is somewhat doubtful whether PDEs for the averaged flow variables, however arrived at, can realistically be expected to accurately predict the variations of those variables on the length and time scales of interest.

A related concern emerges from a consideration of how these types of averaged multiphase flow equations are usually obtained. The usual procedure is to apply space and/or time averaging to the local instantaneous equations (Banerjee, 1986; Drew, 1983; Bedford and Drumheller, 1983; Stewart and Wendroff, 1984; Drew and Wood, 1985; Ishii, 1975). These types of averaging are subject to certain fundamental objections, which will be discussed below, but this is not the point at issue here. (A related concern is that when all the dust settles the averaging scales seem frequently to have disappeared from the model, whereas the model must in fact still depend on which scales have been modeled and which are represented directly.) The point is rather that the characteristic lengths and times over which these averages are performed clearly define lower limits for the scales over which the equations accurately represent differential

variations. Yet this point is often lost sight of and it is tacitly assumed that the continuous solutions of the resulting equations are significant even at smaller scales. Of course, the hope is that if the equations are properly formulated they will not predict any structure at scales less than the averaging scales; i.e., that the solutions will in fact be smooth on those scales. Unfortunately, one has no real assurance that this in the case. The converse danger also exists, namely that the model will be solved with resolution lengths and times that exceed the averaging scales, so that the physical scales are insufficiently represented in the model.

A simple illustration of these considerations is provided by the separated or stratified flow of two immiscible incompressible fluids between parallel plates (Ramshaw and Trapp, 1978). Viscosity will be neglected so that potential flow theory can be applied, while surface tension will be retained to make the problem well posed. Attention is further restricted to small perturbations about a uniform steady-state solution, so that the problem may be linearized. Within these restrictions the exact dispersion relations for the two-dimensional problem are determined by (Ramshaw and Trapp, 1978)

$$\alpha_1\rho_2 F(\alpha_2 kH)(ku_2-\omega)^2 + \alpha_2\rho_1 F(\alpha_1 kH)(ku_1-\omega)^2 - \alpha_1\alpha_2\sigma Hk^4 = 0 \qquad (1)$$

where α_i, ρ_i, and u_i (i=1,2) are respectively the volume fraction, density, and velocity of phase i, σ is the surface tension, H is the plate spacing, k is the wave number, ω is the angular frequency, and $F(z) = z \coth z$. This problem may also be described using the one-dimensional area-averaged two-phase flow equations (Ramshaw and Trapp, 1978), and in this description the dispersion relations are determined by

$$\alpha_1\rho_2(ku_2-\omega)^2 + \alpha_2\rho_1(ku_1-\omega)^2 - \alpha_1\alpha_2\sigma Hk^4 = 0 \qquad (2)$$

Equations (1) and (2) are essentially equivalent provided that $kH \ll 1$; i.e., that the wavelength of the disturbance is long compared to the plate spacing. (In this limit $F(\alpha_1 kH)$ and $F(\alpha_2 kH)$ both tend to unity.) The plate spacing here plays the role of an internal characteristic length scale. When the wavelength becomes comparable to the plate spacing, the one-dimensional description becomes quantitatively inaccurate, in spite of the fact that the equations may possess solutions with structure on that scale. Because the full problem is nonlinear, there is also a danger that these inaccurate small-scale structures will feed back into and contaminate the longer wavelength components of the solution. Thus the mere fact that a differential formulation is able to generate continuous solutions on all scales does not imply that all scales are represented with equal

fidelity, or indeed that inaccuracies on small scales will not eventually contaminate the solution on larger scales as well. The smallest length scales in the problem are effectively determined by the value of the surface tension. For physical values these length scales are much shorter than the plate spacing. Thus we have a situation where the solution does in fact contain components on length scales below the internal scale, and these components are inaccurate. This can be circumvented by artificially increasing the surface tension (Ramshaw and Trapp, 1978), but again one must be concerned with the effect this may have on the accuracy of the longer wavelengths as well.

In summary, the absence in multiphase flow of a clear separation between the scales associated with the microstructure and the scales of macroscopic interest makes it somewhat doubtful that the latter can be accurately described by means of PDEs which implicitly assume that such a separation exists. In such a situation it may be more appropriate to formulate the model directly in discrete terms based on the averaging scales that one wishes to employ, e.g., by constructing control volumes of a given size and considering their contents as the discrete variables in the description. We will later elaborate on this suggestion, and argue that the size of such volumes should be defined with respect to the resolution employed in a practical numerical calculation.

COMPUTATIONAL CONSIDERATIONS

A further and purely pragmatic argument for formulating models in discrete terms from the outset is that it will eventually be necessary to cast or convert the models into discrete form in any case so that they can be solved on digital computers. From a practical point of view, what is wanted is a discrete model corresponding to the resolution that can be employed in practice for the solution of a given problem, and one would like this model to be as faithful as possible to the physics within those constraints. Formulating a differential model and then discretizing it is a rather indirect route to such a model, and it is fraught with pitfalls. Perhaps the main danger is that the length and time scales of the eventual discretization may not be compatible with those implicit in the averaging procedure on which the model was based. A further difficulty is that the inevitable discretization errors are not taken into consideration during the process of model formulation, which might conceivably have been done in such a way as to reduce them. It therefore seems sensible to eliminate the continuum middleman, so to speak, and to attempt to formulate such discrete models directly, in a single step, rather than by discretizing a continuum model whose fidelity is questionable even if it were solved exactly.

One might argue that discretization errors can be separately analyzed and dealt with by conventional techniques for doing so, such as convergence and truncation-error analyses

(Roache, 1972). The problem is that these traditional methods of assessing the size and effects of discretization errors are largely irrelevant in practical calculations because of the coarse resolution limits imposed by computer time and storage constraints. Such analyses are based on the low-order terms in Taylor series expansions in the space and time increments, and when these increments are not small the low-order terms bear little or no relation to the overall errors. Indeed, high-order difference schemes can yield highly inaccurate solutions in problems with large gradients, and conversely schemes that are formally of zeroth-order accuracy (i.e., inconsistent schemes) can nevertheless yield accurate results under certain conditions (Pike, 1987; Levermore et al., 1987). In practice one is hardly ever in a position to keep refining the resolution until the solution no longer changes, and one must seek other means of obtaining the most accurate results possible under the circumstances. In any case, there is clearly no point in examining the behavior of the system in the limit of infinitely fine resolution when the models themselves do not apply on scales less than those over which the averaging is performed in their derivations.

DISCRETE MODEL FORMULATION

Our research has not progressed to the point of a complete formulation, let alone numerical experimentation. However, based on the preceding discussion, we can now outline the approach that is envisioned. A direct derivation, or perhaps construction, of a discrete model might proceed along the following outline. Begin by dividing the system of interest into a number of computational elements (possibly control volumes), the number of which is to be determined by computer time and storage considerations. Let the discrete variables in the description be appropriate integral parameters associated with the computational elements (for example, the total mass, momentum, and energy of each phase within each control volume). Then postulate and/or derive a time advancement procedure by which the values of these discrete variables on each time level may be calculated from those on the previous time level. Ideally this procedure would be developed on the basis of appropriate accuracy- or error-based criteria to attain the maximum accuracy possible within the constraints of the discrete description adopted and for a given level of algorithmic complexity. Statistical methods might be employed for this purpose, as will be discussed below. In practice a more heuristic approach will usually be required, based on such considerations as postulated fluxes of conserved quantities between computational elements, the length scales of the various physical processes and whether they are larger or smaller than the resolution length, and so on. For example, in a bubbly flow various interphase exchange effects can be expressed in terms of the bubble size distribution, and the portion of that distribution corresponding to bubble diameters less than the resolution length would need to be modeled while larger bubbles could be represented directly.

Cascade phenomena (e.g., drop or bubble breakup), in which larger length scales evolve into scales too small to be further resolved, would clearly require special consideration. The effects of unresolved scales back on resolved ones would also require consideration and formulation. The way in which such effects are represented will depend strongly on the physics; no general statements appear possible. For example, coalescence of subgrid scale drops or bubbles may produce drops or bubbles large enough to be resolved directly, which would then need to be properly introduced into the calculation. In other circumstances a stochastic approach analogous to "eddy noise" in subgrid scale turbulence modeling (Rose, 1977; Yakhot et al., 1985) might be more appropriate. The general hope is that by focusing directly on the discrete quantities that are actually being computed, one can formulate models in which the relevant physics is represented within the constraints of the available resolution in a more harmonious manner.

It will be noted that this proposed approach bears more than a passing resemblance to the control-volume approach to deriving difference equations (Roache, 1972). Because of this resemblance, the existing one-dimensional two-phase thermal-hydraulic systems codes already possess something of the character that we think should be associated with discrete models, although many of the elements that such models should possess are simply ignored or omitted. Some of the mathematical manipulations will also bear a close resemblance to those of the conventional volume-averaging approach, in spite of the fact that there are irreconcilable philosophical differences between the two approaches. One essential difference is that in conventional volume averaging, the control volume is not considered as a fixed finite region corresponding to a discretization element, but rather as a sliding control volume which can be centered at any point in the region. Another is that ensemble averaging plays an essential role in the approach proposed here, as will be discussed in the next section.

The general philosophy underlying the approach proposed above is very much in line with that of the subgrid scale or large eddy simulation turbulence models (Ramshaw, 1979; Rose, 1977; Yakhot et al., 1985; Ferziger, 1983), the basic idea of which is that scales large enough to resolve are directly calculated while scales below the resolution are necessarily modeled. In this way minimum demands are placed upon the model, and the less that we ask of it the more likely it is to measure up to our expectations. The modeling process then largely consists of formulating subgrid scale models for physical processes occurring on scales below the resolution scales, and coupling them to the computed scales in a consistent and computationally efficient manner.

STATISTICAL CONSIDERATIONS

Averaging

It is commonly recognized that most multiphase fluid flows have a statistical character, and that the macroscopic equations describing them should be based on some appropriate averaging procedure. In spite of this, explicitly statistical considerations have played almost no role in the modeling of the various fluctuation terms that arise from the averaging. This may be symptomatic of the fact that as a general rule, there has been a tendency to become overly preoccupied with formal manipulations while neglecting the conceptual foundations of the averaging procedures themselves. In particular, the usual running space and/or time averaging procedures are not in our view well founded; the appropriate averaging procedure for general use is ensemble averaging. To be sure, lip service is sometimes paid to the idea that space and time averages are really only substitutes for ensemble averaging, to which they are hopefully equivalent by virtue of some ergodic theorem. But any such equivalence is possible only for a system which is statistically homogeneous and steady in time. In transient inhomogeneous systems, the usual running space and time averages over finite regions are not really averages at all, as they are not superpositions or weighted combinations of different realizations or possible outcomes. It is therefore not really sensible to attempt to model the fluctuation terms that thereby arise in terms of the averaged variables, for this presupposes a relation between quantities that are inherently unrelated. The values of the fluctuation terms clearly depend on information about the fine-scale details of the flow. To model these terms as functions of the averaged variables is to assume a closure where none can possibly exist--there can be no closure within a single realization. If closure occurs at all, it can occur only "on the average;" i.e., only after performing an appropriately weighted ensemble average over all possible realizations of the flow. Thus the various closure relationships which have been proposed and studied become sensible only when an underlying ensemble average is regarded as having been implicitly performed. It then becomes questionable what the space and/or time averaging originally adopted is contributing to the desired final formulation, a question that has been almost universally ignored.

Indeed, in contrast to the common view, it is not even correct to think of the usual sliding space- and time-averaging operations as discarding any information about the small-scale flow features. Such averages attenuate short-wavelength and high-frequency components (i.e., the amplitude of those components is reduced) but do not eliminate them (see Appendix A). The situation is analogous to early attempts to derive the Boltzmann equation from statistical mechanics using a running time average, where it was eventually recognized that the formal time smoothing operation was not having the assumed and intended effect

(Zwanzig, 1967). For an averaging operation to do its job some information must be discarded, and this is not done by sliding averages.

Yet the intent of the usual averaging procedures is basically sound. The intent is to somehow lump together the effects of detailed dynamical processes taking place on length and time scales too small to resolve, and this must surely be done in any practical multiphase flow model. Our contention here is that the simplest and most direct way to do this is to integrate over fixed nonsliding control volumes, and to let the ensemble averages of the integrated contents of these control volumes be the discrete variables of which the description is comprised. In contrast to a running average, an integration over fixed regions does discard information, and the problem acquires a legitimately statistical character because of uncertainty about the missing details. It is these missing fine-scale details over which ensemble averaging averages.

The Closure Problem

Once a conceptually well-founded averaging procedure is adopted one can confront the closure problem in a proper setting. There are two fundamental aspects to the closure problem. The first is to decide what variables are to be included in the desired macroscopic description. For example, suppose we have divided a two-phase system up into control volumes of a size corresponding to the resolution we wish to employ in a practical calculation. Based on past experience, we will probably want to include the mass, momentum, energy, and volume fraction of each phase within each control volume in our set of macroscopic variables. But this will rarely be sufficient; other parameters will be necessary to specify information about the flow regime. In a bubbly flow, for example, information equivalent to a number density of bubbles will be required to determine whether a given void fraction corresponds to many small bubbles or a few large bubbles. Information about the distribution of bubble sizes will probably also be required. Interfacial area has been suggested as an additional variable (Ishii, 1975; Ishii et al., 1982), but while it is clearly a critical parameter whose value must be known to predict interphase transfer rates, it is not clear whether it is a fundamental or a derived variable. The latter seems more likely for bubbly flow, where the bubble number density seems more fundamental.

The difficulty in identifying a complete set of macroscopic variables is forcefully illustrated by the observation that such a set of variables would permit the prediction of flow regime transitions, and this is clearly a very difficult proposition. We are usually in the less satisfactory position of dealing with a less complete set of variables which suffices to describe a restricted class of flow situations (e.g., bubbly flow). Unfortunately, to our knowledge there is no general theoretical approach to the determination of a complete set of macroscopic variables in

any particular situation. This has been and remains a question on which the present statistical theories are silent, although certain insights and general guidelines have evolved. As a practical matter, one must simply introduce variables corresponding to one's conception of what is needed to characterize the important physics on the small-scale level and proceed to work out the consequences.

The second aspect of the closure problem is simpler to deal with in principle, but in practice the complications are so great that the required procedure can rarely be explicitly carried out. Once the macroscopic variables are identified, it is necessary to derive or postulate a closed system of equations which these variables satisfy. The usual approach to this problem has been the hierarchy approach (Leslie, 1973), in which one systematically derives equations for the moments of fluctuating quantities that appear in the equations for the variables of interest. These equations then contain unknown higher moments of the fluctuating quantities, for which further equations can be derived, and so on ad infinitum. This process must be truncated at a low order to obtain equations sufficiently simple to be useful, and this truncation has been an arbitrary and unsystematic process.

An alternative and more systematic approach to this aspect of the closure problem is provided by a non-hierarchial closure method based on information theory; i.e., the maximum entropy formalism (Levine and Tribus, 1979; Rosenkrantz, 1983). This formalism provides a very general way of assigning probability distributions over microstates subject to constraints embodying known macroscopic information (see Appendix B). This approach can in principle be used to derive closed reduced descriptions in a single step, without the necessity of generating or truncating an infinite hierarchy of moment equations. It has recently been used to give a formal derivation of closed nonlinear dissipative evolution equations in Hamiltonian statistical mechanics (Ramshaw, 1986a). However, further theoretical developments are needed before this approach will be applicable to multiphase flow phenomena. The Navier-Stokes equations are dissipative rather than Hamiltonian in structure, and if they are adopted as the starting point the theory will need to be generalized to a non-Hamiltonian microscopic dynamics. This will entail, among other things, addressing the well-known ambiguity in defining the appropriate volume element in state space (Ramshaw, 1986b,c). This difficulty can be circumvented by adopting the Hamiltonian equations of motion for the constituent molecules as the microscopic starting point, but one has the feeling that it should not be necessary to go all the way down to the molecular level to find a sound foundation for the theory. And even if this were done, it is not yet clear how to properly identify the "parameter of slowness" appearing in the general theory in the case of a spatially distributed system.

Work to overcome these theoretical obstacles is in progress. Even if it is fully successful, however, there will be

practical limitations to the use of the results. The resulting closed descriptions will contain complex formal expressions involving the detailed microscopic dynamics in a rather intractable way; they will be essentially multiphase analogs of the familiar Green-Kubo time-correlation function expressions for molecular transport coefficients (Ramshaw, 1986a). Such expressions can yield valuable information about the structure of the theory and what variables appear in the constitutive relations, but they will seldom be amenable to quantitative evaluation. The situation is analogous to that of the ordinary molecular transport coefficients of a dense fluid, which can in principle be calculated from the intermolecular force law by means of the Green-Kubo expressions, but which in practice must be measured experimentally. Such theories will therefore never completely eliminate the need for empirical data; their proper function is rather to provide a suitable framework within which experimental data can be compiled, interpreted, and utilized, and to provide a well-founded starting point for approximations.

Stochastic Models

Our discussion so far has centered on deterministic models for the determination of ensemble averaged quantities. An alternative approach is to formulate equivalent stochastic models, in which only a single (hopefully representative) realization of the ensemble is simulated. In this approach the evolution equations for the macroscopic variables of interest contain stochastic terms, which in the present context would represent part or all of the effects of the unresolved small-scale motions back on the resolved larger-scale motions. The evolution equations then assume the character of nonlinear Langevin equations, which may be solved by stochastic simulation methods (Suzuki, 1981; Murthy, 1983; Gerling, 1984; Tartaglia and Chen, 1984; Heermann, 1986). The stochastic approach has the potential major advantage that it automatically accounts for fluctuation-renormalization effects (Zwanzig, 1980; Rodriquez and Pena-Auerbach, 1984) without the necessity for explicitly including the nonlocal terms to which such effects typically give rise. When fluctuations are large, as is frequently the case in multiphase flow, the equivalent deterministic models for ensemble averaged quantities may be expected to contain terms which are nonlocal in both space and time, in the sense that constitutive relations depend on information from an entire region of space and a finite time interval rather than just on information from the immediate neighborhood of the space-time point in question (Zwanzig, 1980; Rodriquez and Pena-Auerbach, 1984). Such nonlocal terms are very inconvenient to deal with in practical calculations, and if they turn out to be essential for accuracy then stochastic models may well be preferable to deterministic models.

CONCLUSION

As previously emphasized, our ideas on discrete modeling are still in a formative stage, and the present discussion is not intended to be the last word on the subject. We recognize that the picture we have presented is still incomplete, as we do not yet have a well-defined universal procedure that one can follow to generate models of the type we advocate. Indeed, no such procedure may exist; it may always be necessary to adopt different approaches tailored to different physical circumstances. Needless to say, at this stage we do not recommend that existing models be discarded, nor that attempts to improve them by the conventional approaches be terminated. Progress should proceed on a wide front by a variety of approaches. What we do hope is to promote a greater awareness of some of the difficulties with the current approaches and with some of the issues we have discussed, many of which do not seem to be very widely appreciated. And while we do not expect to be joined on the discrete modeling bandwagon by a mass exodus of passengers from more conventional modes of transportation, we would be pleased to hear from and interact with occasional more adventurous travelers who might consider themselves kindred spirits.

APPENDIX A

REMARKS ON SLIDING VOLUME AND TIME AVERAGES

Our purpose here is to call attention to some properties of sliding volume and time averages that are sometimes lost sight of. For brevity the mathematical development will be restricted to volume averaging, but entirely analogous results and statements hold for time averaging.

A general sliding volume average of an arbitrary function of position $f(\underset{\sim}{r})$ may be defined by

$$\bar{f}(\underset{\sim}{r}) = \int d\underset{\sim}{r}'\, W(\underset{\sim}{r}-\underset{\sim}{r}')\, f(\underset{\sim}{r}') \qquad \text{(A-1)}$$

where $W(\underset{\sim}{r})$ is a weighting function. The function $W(\underset{\sim}{r})$ is assumed to be everywhere positive, to be localized in the vicinity of $\underset{\sim}{r} = 0$ (and therefore to tend toward zero for large $|\underset{\sim}{r}|$), to have a characteristic width on the order of the desired spatial averaging length L, and to satisfy

$$\int d\underset{\sim}{r}\, W(\underset{\sim}{r}) = 1 \qquad \text{(A-2)}$$

The latter property ensures that when $f(\underset{\sim}{r})$ is uniform

its value is not changed by the averaging. Frequently $W(\underset{\sim}{r})$ is taken to have the simple box or step function form $W(\underset{\sim}{r}) = (1/L^3)\, B(x)B(y)B(z)$, where $B(s)$ is unity for $-L/2 \leq s < L/2$ and zero otherwise.

Since Eq. (A-1) is of convolution form, it may be Fourier transformed to yield

$$\hat{\bar{f}}(\underset{\sim}{k}) = \hat{W}(\underset{\sim}{k})\, \hat{f}(\underset{\sim}{k}) \qquad \text{(A-3)}$$

where $\hat{F}(\underset{\sim}{k})$ denotes the Fourier transform of $F(\underset{\sim}{r})$. As is well known, $\hat{W}(\underset{\sim}{k})$ will have a characteristic width of order $1/L$. Now even if $W(\underset{\sim}{r})$ is taken to have the simple box form given above, its Fourier transform $\hat{W}(\underset{\sim}{k})$ will in general be nonzero for all finite values of $\underset{\sim}{k}$, although it must of course tend to zero as $|\underset{\sim}{k}|$ tends to infinity. Equation (A-3) may therefore be solved for $\hat{f}(\underset{\sim}{k})$ from a knowledge of $\hat{\bar{f}}(\underset{\sim}{k})$, so that $f(\underset{\sim}{r})$ may be determined from a knowledge of its spatial average $\bar{f}(\underset{\sim}{r})$. The sliding spatial averaging of Eq. (A-1) therefore does not discard or suppress any information contained in $f(\underset{\sim}{r})$. In particular, it does not remove or destroy the short-wavelength components; it merely attenuates them. The averaged function $\bar{f}(\underset{\sim}{r})$ contains exactly the same information as the unaveraged function $f(\underset{\sim}{r})$. It therefore cannot be expected to satisfy equations of any simpler structure than $f(\underset{\sim}{r})$, and moreover it clearly cannot be assumed to be smooth on scales less than the averaging length L unless the original function $f(\underset{\sim}{r})$ was already smooth on those scales. For an averaging procedure to have the desired effect it must discard some information, and since the present procedure does not do so it cannot be regarded as a satisfactory basis for multiphase flow modeling.

Two remedies for this difficulty suggest themselves. The first is to define $W(\underset{\sim}{r})$ in such a way that its Fourier transform is a box function in $\underset{\sim}{k}$-space; e.g., $\hat{W}(\underset{\sim}{k}) = (\text{const.})D(k_x)D(k_y)D(k_z)$, where $D(s)$ is unity for $-2/L < s < 2/L$ and zero otherwise. Equation (A-3) then shows that the short-wavelength components of $f(\underset{\sim}{r})$ are actually removed by the averaging, and that $f(\underset{\sim}{r})$ can no longer be reconstructed from a knowledge of its average $\bar{f}(\underset{\sim}{r})$. But now a new difficulty appears; when the inverse transform of this $\hat{W}(\underset{\sim}{k})$ is taken it is found to have negative regions, so it is not acceptable as a weighting function.

The second remedy is to no longer permit the volumes over which the averaging is performed to slide continuously around, but rather to fix them in space; e.g., to identify them with the cells in a fixed grid. The spatial averaging then no longer has the convolution form of Eq. (A-1) and the above objections no longer apply. In particular, integration over such fixed cells clearly discards information about the fine-scale structure contained within those cells, as we would like an averaging procedure to do.

Nevertheless, spatial averaging over fixed cells is still not sufficient in itself for the reasons already discussed. It is still not really an averaging in the sense that it is applied only to a single realization of the flow and is not a weighted combination of different possible realizations or outcomes. It is therefore more appropriate to think of it as a lumping procedure; i.e., an operational procedure for generating integral variables corresponding to the continuous variables of the fine-scale differential description. As discussed in the text, it is still necessary to ensemble average these integral variables before one can have any hope that they constitute a closed macroscopic description of the system.

APPENDIX B

OUTLINE OF MAXIMUM ENTROPY CLOSURE

Here we wish to indicate how the maximum entropy formalism (Levine and Tribus, 1979; Rosenkrantz, 1983) provides a very simple route to closure in terms of whatever macroscopic variables are utilized to describe a physical system. We consider a system whose microstate is denoted by $\underset{\sim}{X}$ and whose relevant macroscopic variables are $\underset{\sim}{A}(\underset{\sim}{X}) = (A_1(\underset{\sim}{X}), A_2(\underset{\sim}{X}), \ldots)$. The ensemble average values of the variables $\underset{\sim}{A}(\underset{\sim}{X})$ are presumed to be known and are denoted by $\underset{\sim}{a} = (a_1, a_2, \ldots)$. The maximum entropy formalism supplies the least biased or maximally noncommittal (in the sense of information theory) probability distribution in $\underset{\sim}{X}$ consistent with the specified values of $\underset{\sim}{a}$. This distribution is of the generalized canonical form

$$\rho(\underset{\sim}{X};\underset{\sim}{a}) = Q^{-1}(\underset{\sim}{a})\, g(\underset{\sim}{X}) \exp\left[\underset{\sim}{\chi}(\underset{\sim}{a})\cdot\underset{\sim}{A}(\underset{\sim}{X})\right] \tag{B-1}$$

where the partition function $Q(\underset{\sim}{a})$ is given by

$$Q(\underset{\sim}{a}) = \int d\underset{\sim}{X}\, g(\underset{\sim}{X}) \exp\left[\underset{\sim}{\chi}(\underset{\sim}{a})\cdot\underset{\sim}{A}(\underset{\sim}{X})\right] \tag{B-2}$$

and the Lagrange multipliers $\underset{\sim}{\chi}(\underset{\sim}{a})$ are functions of $\underset{\sim}{a}$ implicitly determined by the requirement that

$$\int d\underset{\sim}{X}\, \rho(\underset{\sim}{X};\underset{\sim}{a})\, \underset{\sim}{A}(\underset{\sim}{X}) = \underset{\sim}{a} \tag{B-3}$$

Here $g(\underset{\sim}{X})$ is the probability distribution of complete ignorance (Levine and Tribus, 1979; Rosenkrantz, 1983); i.e., the distribution that would be assigned by an unbiased observer with no knowledge whatever of $\underset{\sim}{X}$. It is not always clear how to determine $g(\underset{\sim}{X})$, but in many cases it may be found by group-invariance arguments (Levine and Tribus, 1979; Rosenkrantz, 1983), the rough idea of which is that truly complete ignorance should remain complete under changes of viewpoint. The distribution of Eq. (B-1) maximizes the information entropy

$$S = - \int d\underset{\sim}{X}\ \rho(\underset{\sim}{X};\underset{\sim}{a})\ \ln\ [\rho(\underset{\sim}{X};\underset{\sim}{a})/g(\underset{\sim}{X})] \tag{B-4}$$

subject to the constraints of Eq. (B-3).

Since $\rho(\underset{\sim}{X};\underset{\sim}{a})$ depends parametrically on $\underset{\sim}{a}$, so will any average evaluated using it; i.e.,

$$\langle F(\underset{\sim}{X})\rangle = \int d\underset{\sim}{X}\ \rho(\underset{\sim}{X};\underset{\sim}{a})\ F(\underset{\sim}{X}) \equiv f(\underset{\sim}{a}) \tag{B-5}$$

The distribution $\rho(\underset{\sim}{X};\underset{\sim}{a})$ therefore provides a method of closure; i.e., for expressing the average f of any desired microscopic quantity $F(\underset{\sim}{X})$ as a function of the relevant macroscopic variables $\underset{\sim}{a}$. Further, this closure is effected in a single step, without the necessity of forming an infinite hierarchy of moment equations and arbitrarily truncating it.

This procedure is appealingly simple in concept, but it is by no means a straightforward matter to apply it to two-phase flow modeling. There is as yet no satisfactory general procedure for identifying $g(\underset{\sim}{X})$, and there are mathematical difficulties in dealing with microstates described in terms of continuous fields. Moreover, in dynamical problems one does not strictly have the freedom to apply the maximum entropy formalism at different times during a transient (although it may nevertheless be a useful approximation to do so), because the time evolution of the probability distribution $\rho(\underset{\sim}{X})$ is governed by a Liouville equation (Ramshaw, 1986a). The maximum entropy distribution may be invoked only as an initial condition, following which the evolution proceeds according to the microscopic dynamics of the system. This circumstance is in fact the essential reason why nonequilibrium statistical mechanics is more difficult than, and differs in structure from, equilibrium statistical mechanics.

In spite of these highly nontrivial difficulties, the fact that the maximum entropy formalism effects a systematic non-hierarchial closure in a single step makes it an appealing alternative to more traditional hierarchy procedures. It therefore seems worthy of further consideration in connection with multiphase flow modeling.

NOMENCLATURE

English

$\underset{\sim}{A}$	=	macroscopic system variables
$\underset{\sim}{a}$	=	ensemble average of macrostate variables
$B(x)$	=	box function in position space
$D(k)$	=	box function in Fourier transform space
$F(z)$	=	z coth z, or arbitrary function
$f(x)$	=	arbitrary function
$g(\underset{\sim}{X})$	=	probability distribution of complete ignorance
H	=	plate spacing
k	=	wave number
L	=	spatial averaging length
Q	=	partition function
$\underset{\sim}{r}$	=	position variable
S	=	information entropy
s	=	dummy variable
u	=	velocity
$W(\underset{\sim}{r})$	=	weighting function
$\underset{\sim}{X}$	=	microscopic variables
x	=	spatial coordinate
y	=	spatial coordinate
z	=	dummy variable, or spatial coordinate

Greek

α	=	volume fraction
$\underset{\sim}{\gamma}$	=	Lagrangian multipliers
ρ	=	density or probability distribution
σ	=	surface tension
ω	=	complex angular frequency

Subscripts

i	=	phase index: liquid=1, vapor=2
x,y,z	=	denotes components of wave vector

Overscore

$\bar{}$	=	spatial average
$\hat{}$	=	Fourier transform

Underscore

$\sim$	=	vector quantity

Other

$\langle\ \rangle$	=	ensemble average over microstates

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channel diameters and flow directions. The effect of the superheating on the heat transfer coefficient becomes smaller with increasing channel diameters, and the effect of quality becomes smaller with decreasing channel diameter.

(3) The heat transfer coefficient increases with increasing liquid jet velocity only in horizontal flow, and the effects of the flow rate on the heat transfer coefficient are identical, regardless of different channel diameters. However, changing the liquid jet velocity has little influence on the heat transfer coefficient in vertical flow.

(4) The effects of flow rate, superheating and quality on wall shear stress can be correlated for one channel diameter with dimensionless vapor film thickness, channel diameter and flow direction. The wall shear stress increases with an increase in the dimensionless thickness and with a decrease in the channel diameter.

(5) The wall shear stress in inverted annular flow with a smooth interface having a thin vapor film, is less than that in liquid single-phase flow, but increases as the interface becomes wavy.

(6) Assuming inverted annular flow in the same channel diameter, the wall shear stress in vertical flow is larger than that in horizontal flow, because of the wavier interface.

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