AFDM:

An Advanced Fluid-Dynamics Model

Volume I: Scope, Approach, and Summary

W. R. Bohl

*D. Wilhelm**

F. R. Parker

*J. Berthier***

*L. Goutagny****

H. Ninokata†

**Visiting Scientist at Los Alamos. Institut für Neutronenphysik und Reaktortechnik, Kernforschungszentrum, 75 Karlsruhe 1, Postfach 3640, FEDERAL REPUBLIC OF GERMANY.*

***Visiting Scientist at Los Alamos. CENG/SETH, 17 Avenue des Martyrs, BP 85X, 38041 Grenoble Cedex, FRANCE.*

****Visiting Scientist at Los Alamos. IPSN/DERS/SIES, CEA Cadarache, 13108 Saint Paul Lez Durance, Cedex, FRANCE.*

†Visiting Scientist at Los Alamos. Oarai Engineering Center, Power Reactor and Nuclear Fuel Development Corporation, Oarai, Ibaraki 311-13, JAPAN.

CONTENTS

ACKNOWLEDGMENTS	vii
ABSTRACT	viii
I. COMPUTER PROGRAM OUTLINE	1
II. INTRODUCTION	3
III. DIFFERENTIAL EQUATIONS	7
A. Mass Conservation	10
B. Momentum Equations/Equations of Motion	10
C. Structure Internal Energy	12
D. Particle Internal Energy	14
E. Liquid 1 (Fuel) Internal Energy	16
F. Liquid 2 (Coolant) Internal Energy	18
G. Vapor Internal Energy	18
H. Interfacial Area Convection	21
IV. CONCEPTUAL AND NUMERICAL ASSUMPTIONS	22
A. Basic Assumptions	22
1. Dimensionality	22
2. Time-Factorization Algorithm	22
3. Use of a Semi-Implicit Convection Scheme	25
4. Computational Mesh	25
B. Options Available	26
C. Intracell Transfer Limitations	27
D. Equations-of-State	29
1. The Simplified Analytic Equation-of-State (SAEOS)	30
2. The SESAME EOS	30
V. SOLUTION ALGORITHM	32
A. Summary	32
B. Step 1: Calculation of Intracell Exchanges	34
1. The Simplified Model	34
a. Using the NOPHASE Option	34
b. Without the NOPHASE Option	35

2. The Standard Model	36
a. Topologies and Flow Regimes	36
b. Calculation of Convectible Surface Areas	37
c. Determination of Instantaneous Interfacial Areas	41
d. Heat-Transfer Coefficients	41
e. Momentum Exchange Functions	44
f. Intracell Updates for Heat and Mass Transfer	44
g. Update of Velocities and Interfacial Areas Based on Mass Transfer	46
C. Step 2: Estimation of End-of-Time-Step Values	47
D. Step 3: The Pressure Iteration	52
E. Step 4: Final End-of-Time-Step Values	56
F. Boundary Conditions and Time-Step Controls	58
VI. OBSERVATIONS BASED ON AFDM DEVELOPMENT	60
REFERENCES	62
APPENDIX A: AFDM INPUT DESCRIPTION	65
APPENDIX B: NOMENCLATURE	87

ACKNOWLEDGMENTS

The success of an international code development effort such as AFDM necessarily involves the work and cooperation of a number of people besides those directly associated with the technical details. The authors wish to acknowledge Robert Curtis and Phil Wood, US NRC; Reimar Fröhlich, Günther Kessler, and Gerhard Heusener, KfK; Akira Watanabe, PNC; Harold Sullivan, Los Alamos; the late Andre Schmitt and Antoine Meyer-Heine, CEN; and Alan Jones, ISPRA, for their efforts towards the completion of AFDM.

The word processing and editing required for the AFDM documentation was substantial. Special thanks go to Olga Rauenzahn-Grovic and Cindy Martinez for their hours spent on the preparation of the AFDM volumes, and to Karyn Ames for her patience in editing the diverse styles of the project authors and their numerous corrections into a consistent text.

..

ABSTRACT

AFDM, or the Advanced Fluid-Dynamics Model, is a computer code that investigates new approaches simulating the multiphase-flow fluid-dynamics aspects of severe accidents in fast reactors. The AFDM formalism starts with differential equations similar to those in the SIMMER-II code. These equations are modified to treat three velocity fields and supplemented with a variety of new models. The AFDM code has 12 topologies describing what material contacts are possible depending on the presence or absence of a given material in a computational cell, on the dominant liquid, and on the continuous phase. Single-phase, bubbly, churn-turbulent, cellular, and dispersed flow regimes are permitted for the pool situations modeled. Virtual mass terms are included for vapor in liquid-continuous flow. Interfacial areas between the continuous and discontinuous phases are convected to allow some tracking of phenomenological histories. Interfacial areas are also modified by models of nucleation, dynamic forces, turbulence, flashing, coalescence, and mass transfer. Heat transfer is generally treated using engineering correlations. Liquid-vapor phase transitions are handled with a nonequilibrium, heat-transfer-limited model, whereas melting and freezing processes are based on equilibrium considerations. Convection is treated using a fractional-step method of time integration, including a semi-implicit pressure iteration. A higher-order differencing option is provided to control numerical diffusion. The Los Alamos SESAME equation-of-state has been implemented using densities and temperatures as the independent variables. AFDM programming has vectorized all computational loops consistent with the objective of producing an exportable code.

AFDM: AN ADVANCED FLUID-DYNAMICS MODEL

Volume I: Scope, Approach, and Summary

by

W. R. Bohl, D. Wilhelm, F. R. Parker, J. Berthier,
L. Goutagny, and H. Ninokata

Contributors

B. Berthet, E. A. Fischer, G. Hennes, R. J. Henninger, S. Ichikawa,
S. Kleinheins, S. Kondo, L. B. Luck, P. J. Maudlin, B. D. Nichols,
F. Ruel, P. Schmuck, and P. R. Smith

I. COMPUTER PROGRAM OUTLINE

- 1. Program Identification:** AFDM (Advanced Fluid-Dynamics Model).
- 2. Computer for Which the Program Is Designed:** CRAY-1A.
- 3. Description or Function:** AFDM is a three-velocity-field, multiphase, multicomponent, Eulerian, fluid-dynamics computer code. It has been designed to test approaches for use in future code development work that will model liquid-metal fast-breeder reactor core materials during a core-disruptive accident.
- 4. Method of Solution:** A time-factorization approach is used to differentiate intracell modeling from intercell convection. In intracell modeling, rapidly varying (sensitive) quantities are treated implicitly, and slowly varying (stable) quantities are treated

explicitly. A semi-implicit procedure is used for the intercell solution with a pressure iteration that is driven by the discrepancy between the computation-cell pressures and the equation-of-state (EOS) pressures. The EOS pressures are computed by assuming that the cell smear densities and temperatures are the independent EOS variables.

5. **Restrictions:** All structure volume fractions are assumed to be cell-wise constants. Flow-regime modeling assumes unrestricted flow such that channel geometry has not been modeled. The number and types of components are limited, and transient temperature gradients inside liquids and solids and bubble/droplet deformation behavior are not followed.
6. **Running Time:** It takes approximately 2 min to create a compile file from the program library and then to compile and load AFDM on a CRAY-1A. The run times depend on the options selected and the problem size. Up to 45 000 cards are compiled, again depending on the options selected.
7. **Unusual Features of the Program:** A higher-order differencing option is provided to reduce numerical diffusion. Convection of interfacial areas is performed to follow phenomenological histories, and the equations include interfacial area source and loss terms. The SESAME tabular EOS is used to remove the restrictions inherent in an analytic EOS. All computational loops are vectorized.
8. **Machine Requirements:** The reference AFDM program requires a memory of 800 000 words that can be reduced or increased by changing parameter statements (dimensions). The ability to do vector arithmetic is required for practical calculations.
9. **Related Programs:** SIMMER-II.
10. **Material Available:** The source deck, test problems, results of executed test problems, and the eight volumes of AFDM documentation.

II. INTRODUCTION

In 1974, a project was set up at Los Alamos National Laboratory for the computer analysis of severe liquid-metal fast-breeder reactor (LMFBR) accidents.¹ The project team developed the SIMMER computer code for modeling the coupled-neutronics/fluid-dynamics behavior of a disrupted nuclear reactor core. Two versions of the SIMMER code were produced: SIMMER-I² and SIMMER-II.³ The international use of the SIMMER-II code indicated several problem areas, particularly in the heat-, mass-, and momentum-transfer modeling, the neutronics accuracy/efficiency tradeoffs, the fluid-dynamics numerical methods, the can-wall and fuel-pin representation, and the multicomponent analytic equation-of-state (AEOS) formalism. However, neither the technology nor the charter existed to construct a SIMMER-III code that could guarantee resolution of all problems. A development program was proposed in early 1985 to address some of the problems. Because even SIMMER-II is very complex, this program was designed to develop a simplified computer code that would contain new approaches in several of the SIMMER-II problem areas and that would be useful in some important application areas. The new code was called the Advanced Fluid-Dynamics Model, or AFDM. A summary of the improvements investigated is shown in Table I.

AFDM is a three-velocity-field, two-dimensional, multiphase, Eulerian, fluid-dynamics code. The components treated are shown in Table II. The problem volume can contain up to seven density-components: structure, particles, two different liquids, and three vapor species. Structure is stationary and occupies an arbitrary volume in each cell. The moving components are collected into three materials. Material 1 (usually called the fuel) can exit as a solid particulate, a liquid, or a vapor. Material 2 (usually known as the coolant) is presumed to exist in the liquid or vapor state. Material 3 is a noncondensable gas. The seven density components are assigned to five energy components, one each for the structure, the particles, each liquid, and the vapor mixture. Finally, there are three moving velocity fields. The particles and the liquid fuel move with one velocity; the liquid coolant is assigned a second velocity; and the vapor possesses a third velocity. Expansion into more density and energy components (and into more momentum fields) is feasible, but the original choices were judged to be sufficient to determine whether the proposed methods would work.

TABLE I

INVESTIGATED IMPROVEMENTS FROM SIMMER-II TO AFDM

<u>SIMMER-II</u>	<u>AFDM</u>
1. Two velocity fields used	Three velocity fields used
2. Only an AEOS operational	A SESAME EOS interface operational
3. One flow regime present (modified-dispersed flow)	Twelve geometric topologies with four distinct flow regimes present (bubbly, churn-turbulent, cellular, and dispersed)
4. Interfacial areas based on information in isolated computational cells	Interfacial areas convected over the Eulerian mesh
5. Only limited interfacial area source terms and heat-transfer mechanisms are available	A variety of bubble/droplet breakup processes and heat-transfer mechanisms modeled
6. First-order donor-cell differencing used	Higher-order donor-cell differencing available
7. No virtual mass terms used	Virtual mass terms included
8. Pressure iteration performed with a constant value for $\partial \bar{p} / \partial p$	Pressure iteration consistent with EOS nonlinearities and the single-phase/two- phase transition
9. Vapor pressure-volume work term treated explicitly (sometimes unstable)	Vapor pressure-volume work term treated implicitly (stable)
10. Momentum and energy convected with velocities different than those used for densities (mass)	All components convected consistently
11. Vaporization/condensation model iterates equations sequentially (slow to converge)	Equations for vaporization/condensation solved with an integrated implicit formulation
12. Scalar programming designed for the CDC 7600 computer	Vector programming designed for a Cray or a similar modern supercomputer

TABLE II
DENSITY COMPONENTS, ENERGY COMPONENTS, AND
VELOCITY FIELDS FOR THE AFDM CODE

<u>Components</u>	<u>Densities</u>	<u>Internal Energies</u>	<u>Velocities</u>
Structure	$\bar{\rho}_s$ ($\bar{\rho}_S$)	e_s	-
Solid Particulate	$\bar{\rho}_p$ ($\bar{\rho}_P$)	e_p	$\vec{v}_p = \vec{v}_{L1}$
Liquid	$\bar{\rho}_{L1}$ ($\bar{\rho}_{L1}$)	e_{L1}	$\vec{v}_{L1}$
	$\bar{\rho}_{L2}$ ($\bar{\rho}_{L2}$)	e_{L2}	$\vec{v}_{L2}$
Vapor	$\bar{\rho}_{g1}$ ($\bar{\rho}_{G1}$)	e_g	$\vec{v}_g$
	$\bar{\rho}_{g2}$ ($\bar{\rho}_{G2}$)		
	$\bar{\rho}_{g3}$ ($\bar{\rho}_{G3}$)		
Schematic Representation	$\bar{\rho}_m$	e_r	$\vec{v}_q$

Assume: The structure EOS is limited.

$\bar{\rho}_p$, $\bar{\rho}_{L1}$, and $\bar{\rho}_{G1}$ compose Material 1.

$\bar{\rho}_{L2}$ and $\bar{\rho}_{G2}$ compose Material 2.

$\bar{\rho}_{G3}$ is a noncondensable gas and is Material 3.

In the absence of other information,

$\vec{v}_{L1}$ can be considered as belonging to Momentum Field 1,

$\vec{v}_{L2}$ can be considered as belonging to Momentum Field 2, and

$\vec{v}_g$ can be considered as belonging to Momentum Field 3.

Three additions are required to the mass, energy, and momentum components of Table II. First, both for convection using higher-order differencing and for internal EOS operations, the vapor internal energies e_{Gm} for individual vapor density components are required. These are temporary variables obtained by assuming one temperature for the vapor field. Second, properties at material interfaces are required for evaluation of vaporization and condensation rates. When vaporization or condensation occurs, these interfacial properties are assumed to be at the saturation conditions obtained from the vapor partial pressure of the species undergoing mass transfer. These saturation conditions are obtained from the EOS. Third, AFDM convects interfacial areas per unit volume, a_f^C , between the continuous momentum component and discontinuous momentum components. Here, f may represent L1/L2, L1/G, or L2/G, using the momentum subscripts in Table II. This convection allows an approximate following of phenomenological histories, despite the Eulerian code format.

Section III gives the differential equations solved by AFDM, discusses the reasons for their selection and gives approximations implied by these equations. Section IV presents additional conceptual assumptions applied to the differential equations to produce a numerical algorithm. It also discusses EOS considerations. Section V outlines the numerical solution procedure. Section VI provides observations on the success achieved in resolving the SIMMER-II problem areas examined in AFDM. In the context of these observations, areas where additional work could be profitable are indicated. The report concludes with an appendix giving the AFDM input descriptions and a list of AFDM project nomenclature.

Volume I illustrates the scope of the AFDM code, indicates the simplifying assumptions and approximations made, and summarizes the solution procedure. Details on the formalism and the AFDM code itself may be found in other volumes of the AFDM documentation. A summary of the nomenclature used for the AFDM program is given in Appendix B of Vol. I. Volume II describes AFDM topologies, flow regimes, and interfacial area modeling. Volume III details the formulas used for heat-transfer and momentum exchange coefficients. Volume IV presents the intracell heat- and mass-transfer solution algorithm. Volume V treats the convective transport algorithm, including the pressure iteration and the equations used for "higher-order" spatial differencing. Volume VI describes the EOS formulas and the interfacing of these formulas into the AFDM numerical

algorithm. Volume VII is a programmer/user's manual giving FORTRAN details and sample problems. Volume VIII describes the T6P postprocessor, a graphics tool used to assist in diagnosing the results of an AFDM run.

III. DIFFERENTIAL EQUATIONS

This section provides the differential equations relating the densities, internal energies, and velocities given in Table II. The style of presentation is that of the SIMMER-II³ manual. An averaging procedure to derive the equations as suggested by Ishii⁴ is not included because of the lengthy manipulations involved. Work on this problem has been performed by Ruel⁵ and has resulted in equation modifications. Comments based on such considerations are included in the discussion of the equations.

The AFDM objective is to treat multiphase fluid dynamics in regions away from structures. Although AFDM has a limited structural representation with momentum and energy transport at structural boundaries, mass transport to structures is restricted to processes resulting in condensation. Melting, freezing, and other phenomena leading to structural deformation and/or changes in the structure volume fractions as a function of time were beyond the scope of this program. Although the flow topologies (possible fluid geometric configurations) necessarily must consider the existence of structural surfaces, restricted flow regimes (for fluid flow in channels) have not been defined in the AFDM code.

The smear densities (called macroscopic densities here and in SIMMER-II) are indicated with either lower- or uppercase subscripts in Table II. The use of lower- or uppercase density subscripts depends on convenience for a given application. SIMMER-II generally used lowercase subscripts to distinguish between the different density components belonging to a given energy component. In AFDM, uppercase subscripts sometimes seem more consistent in relating to energy and EOS quantities. The thermodynamic densities (called microscopic densities) are written without the bar over the symbol. Both densities can be written schematically using the subscript "m". (A second use of the symbol "m" is a material-component index, particularly when treating summations or transport operations involving two components of the same material, such as liquid and vapor.) The volume fractions α_m for the differential equations for both the structure and liquid fields are then defined by

$$\alpha_m = \bar{\rho}_m / \rho_m \quad . \quad (1)$$

The vapor volume fraction α_G is defined by the requirement that

$$\alpha_S + \alpha_P + \alpha_{L1} + \alpha_{L2} + \alpha_G = 1 \quad , \quad (2)$$

where α_S is the structure-volume fraction,

α_P is the particle-volume fraction,

α_{L1} is the liquid-volume fraction for Material 1, and

α_{L2} is the liquid-volume fraction for Material 2.

Because of the desire for the single-phase/two-phase transition to take place at some finite vapor-volume fraction in interfacing with the EOS, a second "effective" vapor-volume fraction is defined for use in the EOS and some intracell transfer operations. This definition is introduced when the approximations made to formulate a solution algorithm are discussed in Sec. IV. Equations (1) and (2) furnish the appropriate definitions for the differential equations.

The individual internal energies are designated by uppercase subscripts indicating energy components. A schematic representation for an individual internal energy component uses the subscript r .

The form of the energy equations adopted here is similar to SIMMER-II in that they are written in terms of the internal energy of the materials, not the total energy. Using the form of the equations that includes the kinetic energy terms becomes significantly more difficult to solve numerically with the staggered mesh and semi-implicit algorithm to be used.

This formalism ignores the possible use of entropy as a field variable, based on the Kernforschungszentrum Karlsruhe (KfK) suggestion⁶ that the use of entropy gives simpler differential equations than the internal energy variables used here. The four reasons for not adopting an entropy approach in the AFDM effort are as follows.

- (a) Entropy is not conserved. This leads to greater difficulty in debugging. Also, a solution procedure that forces errors to zero cannot be used for nonconservative equations, as is presently done with the conservation relationships.

- (b) The EOS becomes more complex with entropy as an independent variable. Another integration is involved. Although an appropriately simplified EOS could eventually be formulated for reactor materials, code flexibility in treating other material systems would be limited.
- (c) Entropy increases from nuclear heating would depend directly on temperature, instead of indirectly on temperature through the neutronics. In other words,

$$\dot{s} \sim Q/(\bar{\rho}T) \quad , \quad (3)$$

where $\dot{s}$ is the rate of entropy increase,

$\bar{\rho}$ is the density of the component being heated,

Q is the nuclear heating rate (per unit volume), and

T is the temperature.

This situation apparently leads to even greater EOS accuracy requirements for calculation of temperatures. Also, entropy additions would not obey the intuitive relationships generally associated with nuclear heating such as a modified "chopped cosine" heating rate in the axial direction.

- (d) We lacked experience in applying entropy as an independent variable in the multidimensional, multicomponent problem to be addressed. With the tight AFDM schedule, we have had little room for mistakes. A completely novel approach on such a basic issue was anticipated to significantly lower the chances for success.

The individual velocities are designed by uppercase momentum field subscripts. Velocities can be written schematically with the subscript q or q' . The general idea to be followed in any expansion of this formalism to more components is that each velocity field can consist of several energy components. Each energy component can consist of several density components. Differing energy components of the same material, for example, hot and cold liquid sodium or inner and outer regions for a liquid drop, must be accommodated by appropriate EOS and intracell transfer relationships.

The differential equations approximated and solved by AFDM are now given by the following relationships.

A. Mass Conservation

For the structure, $\bar{\rho}$ is assumed to be constant. For the liquid and vapor components, the mass conservation equations are

$$\frac{\partial \bar{\rho}_m}{\partial t} + \nabla \cdot (\bar{\rho}_m \vec{v}_q) = -\Gamma_m, \quad (4)$$

where Γ_m is the total mass-transfer rate per unit volume from component m .

Three (reversible) mass-transfer paths exist in AFDM:

- (1) Liquid fuel can freeze into particles, and fuel particles can melt.
- (2) Fuel vapor can condense, and fuel liquid can vaporize.
- (3) Coolant vapor can condense, and coolant liquid can vaporize.

B. Momentum Equations/Equations of Motion

A momentum equation is required for each velocity field. If the convective term is expressed in a conservative form, these can be given by

$$\begin{aligned} \frac{\partial (\bar{\rho}_q \vec{v}_q)}{\partial t} + \sum_{m \in q} \nabla \cdot (\bar{\rho}_m \vec{v}_q \vec{v}_q) + \alpha_q \nabla p - \bar{\rho}_q \vec{g} + K_{qS} \vec{v}_q \\ - \sum_{q'} K_{qq'} (\vec{v}_{q'} - \vec{v}_q) - \vec{v}_q \vec{M}_q = - \sum_{q'} \Gamma_{qq'} [H(\Gamma_{qq'}) \vec{v}_q + H(-\Gamma_{qq'}) \vec{v}_{q'}], \end{aligned} \quad (5)$$

where $\bar{\rho}_q$ is the sum of the density components for momentum field q ,
 $m \in q$ includes all density components, m , existing in momentum field q ,
 p is the locally averaged pressure,
 $\vec{g}$ is the gravitational acceleration,
 K_{qS} is the exchange function for momentum transfer to structure,
 $\Gamma_{qq'}$ is the mass-transfer rate from velocity component q to velocity component q' ,
 $K_{qq'}$ is the exchange function for momentum transfer between velocity field q and field q' ,

$\vec{VM}_q$ is the virtual mass term, and

$H(x)$ is the Heaviside unit function defined by

$$H(x) = 0 \text{ for } x < 0, H(0) = \frac{1}{2}, \text{ and } H(x) = 1 \text{ for } x > 0.$$

No explicit viscous terms or terms for the modeling of turbulent momentum fluxes are considered. Fully liquified reactor materials have low viscosity. The principal influence of viscosity near wall surfaces can be represented by friction terms. In a case where representation of viscosity away from walls is required, the coding might be modified in a manner similar to SIMMER-II. Unfortunately, if large velocity gradients are imposed on the SIMMER-II algorithm when large viscosity is assumed, the explicit formulae adopted exhibit instability. Programming an algorithm sufficiently implicit to be stable in this situation was beyond the scope of the AFDM program. The modeling of turbulent mixing is even more complex. The smearing from donor-cell differencing has been sufficient to cause excessive mixing with reactor scale nodes in the past; however, for situations where small-scale experiments are modeled with small nodes, the neglect of momentum diffusion perpendicular to the velocities in Eq. (5) becomes particularly important. Turbulence modeling is desirable for such simulations and for addressing small-node to large-node scaling questions; nevertheless, derivation of the appropriate turbulence closure relationships still requires a research program.

For liquid-continuous flow, numerical studies revealed the desirability of including virtual mass terms for some situations. A general discussion on the virtual mass considerations made for AFDM is in Appendix A of Vol. V. The conclusion of this discussion is to define virtual mass terms in Eq. (5) by

$$\vec{VM}_{L1} = -\alpha_{L1,eff} \vec{VM}_G, \quad \vec{VM}_{L2} = -\alpha_{L2,eff} \vec{VM}_G, \quad \text{and} \quad (6)$$

$$\vec{VM}_G = -\alpha_{GP,eff} C_G \frac{\alpha_{L1} + \alpha_{L2}}{\alpha_P + \alpha_{L1} + \alpha_{L2}} \left[\frac{\partial \vec{v}_G}{\partial t} - \alpha_{L1,eff} \frac{\partial \vec{v}_{L1}}{\partial t} - \alpha_{L2,eff} \frac{\partial \vec{v}_{L2}}{\partial t} \right], \quad (7)$$

where $\alpha_{L1,eff} = (\alpha_P + \alpha_{L1})/(\alpha_P + \alpha_{L1} + \alpha_{L2})$,

$$\alpha_{L2,eff} = \alpha_{L2}/(\alpha_P + \alpha_{L1} + \alpha_{L2}),$$

$$\rho_{L,eff} = \alpha_{L1,eff} \rho_{q=L1} + \alpha_{L2,eff} \rho_{q=L2},$$

$$\rho_q = \bar{\rho}_q/\alpha_q, \text{ and}$$

α_P , α_{L1} , and α_{L2} are the energy component volume fractions of Eq. (2).

The C_G term is adopted from Ishii and Mishima⁷ as a function of the flow regime. It is defined when used in Eq. (44), Sec. V.C. The volume fraction ratio also appearing as a coefficient in Eq. (7) limits the influence of particles on the acceleration of bubbles. Convective contributions are sometimes added to the virtual mass relationships. However, numerical studies suggested that the appropriate convective terms depend on the problem being considered. Consequently, no convective terms have been programmed into the AFDM virtual mass algorithm.

The mass-transfer terms on the right side of Eq. (5) more correctly should appear with a velocity normal to the interface between the two moving momentum fields. However, these terms are generally small, and transfers using the bulk velocity avoid numerical problems when the fraction of mass transferred from a given velocity field approaches unity.

In planning the AFDM code, consideration was given to using the nonconservative form of Eq. (5) for momentum convection. Significant simplifications are possible, and greater accuracy has been claimed for calculation of quasi-steady-state flow with non-uniform mesh intervals. However, the nonconservative form seems to give inaccurate results in postulated highly transient situations. Also, the AFDM effort was limited, and the necessity of producing a product dictated that a choice be made. The final arguments leading to the selection of Eq. (5) were (a) the improved consistency of the coupled mass/momentum convection algorithm obtained, and (b) the reduction of difficulties when liquid is filling a previously voided cell, which occurs with the use of the selected, staggered computational mesh.

C. Structure Internal Energy

A separate energy equation is written for each of the five energy components. The structure energy equation is

$$\begin{aligned} \frac{\partial(\bar{\rho}_S e_S)}{\partial t} - \sum_q K_{qS}(\bar{\mathbf{v}}_q \cdot \bar{\mathbf{v}}_{qS}) &= Q_S + h_{PS} a_{PS}(T_P - T_S) \\ &+ \sum_{m=1}^2 \left\{ h_{LmS} a_{LmS}(T_{Lm} - T_S) + h_{SG} a_{GS} Y_{Gm} [\max(T_{Sat,Gm}, T_S^l) - T_S] \right\} x_{Lm} \end{aligned}$$

$$+ \sum_{m=1}^3 h'_{GS} a_{GS} Y_{Gm} (T_G - T_S)(1 - X_{Lm}) \quad , \quad (8)$$

where $\vec{v}_{qS}$ are the fluid/structure interfacial velocities,

Q_S is the heat-transfer coefficient between energy component r and the structure,

a_{rS} is the interfacial area per unit volume between energy component r and the structure,

T_r is the temperature of energy component r ,
 r can be P , $L1$, or $L2$,

h_{SG} is the structure-side heat-transfer coefficient for vapor-structure energy transfer,

a_{GS} is the interfacial area per unit volume between the vapor field and the structure,

Y_{Gm} is the mole fraction of vapor component m ,

$T_{Sat,Gm}$ is the saturation temperature corresponding to vapor component m ,

T_S is the structure temperature,

$$T_S^I = \frac{h_{GS} T_G + h_{SG} T_S}{h_{GS} + h_{SG}} \quad ,$$

h_{GS} is the vapor-side heat-transfer coefficient for vapor-structure energy transfer,

$$h'_{GS} = \frac{h_{GS} h_{SG}}{h_{GS} + h_{SG}} \quad ,$$

$X_{Lm} = 1$ when liquid Lm exists,

$X_{Lm} = 0$ when liquid Lm does not exist (for example, it is all vaporizing or cannot condense), and

$X_{L3} = 0$ because vapor component 3 does not possess a corresponding liquid.

A term resulting in fluid frictional heating of the structure is included in the left side of Eq. (8). This term requires a nonzero interfacial velocity, as defined in Sec. V.E. More correctly, such energy is deposited in the fluid boundary layer such that the interfacial velocity is zero. However, such detailed modeling was judged not to be cost effective in AFDM.

The structure nuclear heating Q_S is the product of five terms. There is a basic heating rate input on a unit mass basis. This is multiplied by an input radial distribution, an input axial distribution, and an input time-dependent normalization factor. The resulting heating rate is then converted to a per unit volume basis by multiplication with the macroscopic density. Similar operations are performed for the particle, liquid, and vapor components. The per unit volume notation is used because neutronics reaction rates are determined from the products of the macroscopic cross sections and the neutron flux giving units of events/(m³-s).

The energy transfer terms on the right side of Eq. (8) are modeled to give bulk energy transfers (in other words, transfers involving cell-averaged values) between the structure and the particle/liquid energy fields. Terms are also present for the energy transferred during condensation when the structure surface temperature is assumed to be at $T_{Sat,Gm}$. For those vapor components that cannot condense on the structure surface (where using the actual low value of $T_{Sat,Gm}$ would imply vaporization), an interface temperature or a heat-transfer coefficient is defined that balances the heat flows. Because a transient, diffusion-limited heat-transfer model required more time (and technology) than that available to the AFDM program, each vapor component is assumed to contact a fraction of a_{GS} proportional to its mole fraction. A more detailed discussion of the approximations used to treat vaporization and condensation is in Vol. IV.

D. Particle Internal Energy

The particle internal energy equation solved by AFDM is given by

$$\begin{aligned}
 & \frac{\partial(\bar{\rho}_P e_P)}{\partial t} + \nabla \cdot (\bar{\rho}_P e_P \bar{\mathbf{v}}_{L1}) + p \left[\frac{\partial \alpha_P}{\partial t} + \nabla \cdot (\alpha_P \bar{\mathbf{v}}_{L1}) \right] \\
 & - \frac{\bar{\rho}_P}{\bar{\rho}_P + \bar{\rho}_{L1}} \left[\sum_{q'} K_{q'L1} (\bar{\mathbf{v}}_{L1} - \bar{\mathbf{v}}_{q'}) \cdot (\bar{\mathbf{v}}_{L1} - \bar{\mathbf{v}}_{q'L1}) \right. \\
 & \left. + K_{L1S} \bar{\mathbf{v}}_{L1} \cdot (\bar{\mathbf{v}}_{L1} - \bar{\mathbf{v}}_{L1S}) - \bar{\mathbf{v}}_{L1} \cdot (\bar{\mathbf{v}}_{L1} - \bar{\mathbf{v}}_{GL}) \right] \\
 & = Q_P + I_{L1P} \{ H(I_{L1P}) e_{Sol,L1} + H(-I_{L1P}) e_{Li q,L1} \} + h_{PSaps} (T_S - T_P)
 \end{aligned} \tag{9}$$

$$\begin{aligned}
& + \sum_{m=1}^2 \left\{ h_{LmP} a_{LmP} (T_{Lm} - T_P) + h_{PG} a_{GP} Y_{Gm} \left[\max(T_{Sat,Gm}, T_P^I) - T_P \right] \right\} X_{Lm} \\
& + \sum_{m=1}^3 h'_{GP} a_{GP} Y_{Gm} (T_G - T_P) (1 - X_{Lm}) ,
\end{aligned}$$

- where $\vec{v}_{q'L1}$ is the interfacial velocity between momentum fields q' and $L1$,
 $\vec{v}_{GL}$ is the effective liquid/vapor interfacial velocity,
 Q_p is the particle nuclear heating rate,
 Γ_{L1P} is the freezing (positive) or melting (negative) rate for mass interchange between liquid 1 and particles,
 $e_{Sol,L1}$ is the solidus energy for fuel,
 $e_{Liq,L1}$ is the liquidus energy for fuel,
 h_{rp} is the heat-transfer coefficient between energy component r and the particles ($h_{sp} = h_{ps}$),
 a_{rp} is the interfacial area per unit volume between energy component r and the particles ($a_{sp} = a_{ps}$),
 r can be S , $L1$, or $L2$,
 h_{pG} is the particle-side heat-transfer coefficient for vapor-particle energy transfer,
 a_{pG} is the interfacial area per unit volume between the particle field and the vapor,
 $T_P^I = \frac{h_{GP} T_G + h_{PG} T_P}{h_{GP} + h_{PG}}$,
 h_{GP} is the vapor-side heat-transfer coefficient for vapor-particle energy transfer, and
 $h'_{GP} = \frac{h_{GP} h_{PG}}{h_{GP} + h_{PG}}$.

Because pressure is determined from an EOS, all moving components are treated as compressible in AFDM. Indeed, ignoring the compressibility of high-temperature liquid would be a serious error. For consistency, a pressure-volume work term is included for particles, liquids, and vapor. Experience with SIMMER-I suggests that treating particles and low-temperature liquids as incompressible is not a profitable approach if single-phase ($\alpha_G < 0$) cells can exist.

The interfacial velocities for the interfield frictional heating terms are defined in Sec. V.E. These drag terms apply to a momentum field and are proportioned to fuel and particles based on mass. (A surface area allocation would be more accurate, but raise potential stability questions.) The virtual mass contribution comes from (a) the assumption that a contribution of the form $\vec{v}_{q'} \cdot \vec{v}_{GL}$ should appear in the appropriate total energy equation, and (b) the acquisition of a $\vec{v}_{q'} \cdot \vec{v}_q$ term when the mechanical energy equations are subtracted from the total energy equations to obtain the internal energy equations. As in the case of structure, the conversion of kinetic energy to internal energy by frictional dissipation is presumed to change the bulk particle energy directly, instead of appearing in the boundary layer.

The terms in the heat-transfer expressions are defined similarly to the structure equation with the P (particle) subscript replacing the S (structure) subscript for liquid/vapor to particle transfers, and H, again, represents the Heaviside function. The additional term results from the production of particles by freezing and their loss by melting. An equilibrium model for melting/freezing is used in AFDM such that the heat of fusion in melting is taken from the particles, whereas the heat of fusion in freezing is added to the liquid fuel.

E. Liquid 1 (Fuel) Internal Energy

The internal energy equation for the molten fuel is

$$\begin{aligned}
 & \frac{\partial(\bar{\rho}_{L1}e_{L1})}{\partial t} + \nabla \cdot (\bar{\rho}_{L1}e_{L1}\vec{v}_{L1}) + p \left[\frac{\partial\alpha_{L1}}{\partial t} + \nabla \cdot (\alpha_{L1}\vec{v}_{L1}) \right] \\
 & - \frac{\bar{\rho}_{L1}}{\bar{\rho}_P + \bar{\rho}_{L1}} \left[\sum_{q'} K_{q'L1} (\vec{v}_{L1} - \vec{v}_{q'}) \cdot (\vec{v}_{L1} - \vec{v}_{q'L1}) \right. \\
 & \left. + K_{L1S} \vec{v}_{L1} \cdot (\vec{v}_{L1} - \vec{v}_{L1S}) - \vec{v}_{L1} \cdot (\vec{v}_{L1} - \vec{v}_{GL}) \right] \\
 & = Q_{L1} - \Gamma_{L1P} \left[H(\Gamma_{L1P}) e_{Sol,L1} + H(-\Gamma_{L1P}) e_{Li,q,L1} \right] \\
 & + \Gamma_{GL1} \left[H(\Gamma_{GL1}) i_{Con,G1} + H(-\Gamma_{GL1}) i_{L1} \right]
 \end{aligned} \tag{10}$$

$$\begin{aligned}
& + \left[h_{L1S} a_{L1S} (T_S - T_{L1}) + h_{L1P} a_{L1P} (T_P - T_{L1}) \right. \\
& \left. + h_{L1L2} a_{L1L2} (T_{L2} - T_{L1}) X_{L2} + h_{L1G} a_{GL1} (T_{Sat,G1} - T_{L1}) \right] X_{L1} \quad ,
\end{aligned}$$

- where Γ_{GL1} is the condensation (positive) or vaporization (negative) rate for mass interchange between liquid 1 and vapor,
- $i_{Con,G1}$ is the enthalpy of saturated liquid for vapor component 1 (fuel),
- i_{L1} is the enthalpy of liquid component,
- h_{L1L2} is the heat-transfer coefficient between liquid 1 and liquid 2,
- a_{L1L2} is the interfacial area per unit volume between liquid 1 and liquid 2,
- h_{L1G} is the liquid 1-side heat-transfer coefficient for liquid 1-vapor energy transfers, and
- a_{GL1} is the interfacial area per unit volume between vapor and liquid 1.

The left side of Eq. (10) is similar to the particle energy equation. The right side allows vaporization/condensation (V/C), as well as melting/freezing. The expression for the V/C rate, Γ_{GL1} , is developed so as to achieve energy conservation when summed over all interfaces where V/C can occur. Then, the choices for the energy transfer to be associated with mass transfer are as follows. In condensation, the liquid appears at the enthalpy of the interface (that of saturated liquid). In vaporization, the bulk enthalpy of the liquid is used such that the difference between the interface conditions and the bulk conditions increases (or decreases) the effective heat of vaporization. The AFDM code has insufficient information to calculate a time-dependent temperature gradient within a liquid. Associating an interfacial energy with mass leaving the liquid would spuriously decrease (or increase) the liquid temperature.

The other terms on the right side of Eq. (10) model bulk energy transfers from structure/particles to liquid 1, bulk energy transfers from liquid 2 to liquid 1, and energy transfers based on the temperature difference between the vapor/liquid 1 interface and the cell-averaged liquid 1 value.

F. Liquid 2 (Coolant) Internal Energy

The internal energy equation for the coolant is

$$\begin{aligned}
 & \frac{\partial(\bar{\rho}_{L2}e_{L2})}{\partial t} + \nabla \cdot (\bar{\rho}_{L2}e_{L2}\vec{v}_{L2}) + p \left[\frac{\partial\alpha_{L2}}{\partial t} + \nabla \cdot (\alpha_{L2}\vec{v}_{L2}) \right] \\
 & - \left[\sum_{q'} K_{q',L2}(\vec{v}_{L2} - \vec{v}_{q'}) \cdot (\vec{v}_{L2} - \vec{v}_{q',L2}) \right. \\
 & \quad \left. + K_{L2S}\vec{v}_{L2} \cdot (\vec{v}_{L2} - \vec{v}_{L2S}) - \vec{v}_{L2} \cdot (\vec{v}_{L2} - \vec{v}_{GL}) \right] \\
 & = Q_{L2} + \Gamma_{GL2} \left[H(\Gamma_{GL2})i_{Con,G2} + H(-\Gamma_{GL2})i_{L2} \right] \\
 & + \left[h_{L2S}a_{L2S}(T_S - T_{L2}) + h_{L2P}a_{L2P}(T_P - T_{L2}) \right. \\
 & + h_{L1L2}a_{L1L2}(T_{L1} - T_{L2})X_{L1} \\
 & \left. + h_{L2G}a_{GL2}(T_{Sat,G2} - T_{L2}) \right] X_{L2} ,
 \end{aligned} \tag{11}$$

where the terms are defined similarly to the preceding equations, and the only mass transfer allowed is vaporization and condensation.

G. Vapor Internal Energy

The vapor internal energy equation used is

$$\begin{aligned}
 & \frac{\partial(\bar{\rho}_G e_G)}{\partial t} + \sum_{m=1}^3 \nabla \cdot (\bar{\rho}_{Gm} e_{Gm} \vec{v}_G) + p \left[\frac{\partial\alpha_G}{\partial t} + \nabla \cdot (\alpha_G \vec{v}_G) \right] \\
 & - \left[\sum_{q'} K_{q',G}(\vec{v}_G - \vec{v}_{q'}) \cdot (\vec{v}_G - \vec{v}_{q',G}) + K_{GS}\vec{v}_G \cdot (\vec{v}_G - \vec{v}_{GS}) - \vec{v}_G \cdot (\vec{v}_G - \vec{v}_{GL}) \right] \\
 & = Q_G + \sum_{m=1}^2 -\Gamma_{GLm} \left[H(-\Gamma_{GLm})(i_{Con,Gm} + h_{lg,Gm})X_{Lm} + H(\Gamma_{GLm})i_{Gm} \right]
 \end{aligned}$$

$$\begin{aligned}
& + \sum_{m=1}^2 h_{GLm} a_{GLm} (T_{Sat,Gm} - T_G) X_{Lm} \\
& + \sum_{m=1}^2 Y_{Gm} \{ h_{GS} a_{GS} [\max(T_{Sat,Gm}, T_S^I) - T_G] \\
& + h_{GP} a_{GP} [\max(T_{Sat,Gm}, T_P^I) - T_G] \} X_{Lm} \\
& + \sum_{m=1}^3 \{ Y_{Gm} [h'_{GS} a_{GS} (T_S - T_G) + h'_{GP} a_{GP} (T_P - T_G)] \\
& - T_{GLm} e_{Lm} \} (1 - X_{Lm}) \\
& + \sum_{m=1}^2 A_m \min(T_{Sat,Gm} - T_G, \Delta T_h) (T_{Sat,Gm} - T_G) H(T_{Sat,Gm} - T_G) ,
\end{aligned} \tag{12}$$

where e_{Gm} is the internal energy of vapor component m ,
 i_{Gm} is the enthalpy of vapor component m ,
 $h_{lg,Gm}$ is the heat of vaporization of component m ,
 h_{Gr} is the vapor-side heat-transfer coefficient at the interface of
 the vapor and energy component r ,
 r can represent S , P , $L1$, or $L2$,
 A_m is an input coefficient for homogenous condensation, and
 ΔT_h is a code-computed limiting temperature difference.

The left side of Eq. (12) is similar to the other energy equations. A major departure from SIMMER-II is the use of vapor internal energies for individual density components in determining convection. This is required with higher-order differencing. In other words, the internal energy convected in/out of a cell must reflect the convected component composition. Using higher-order differencing, this convected composition depends on the gradients of the individual density components, not simply the average over a donor cell.

There are five summations on the right side of Eq. (12). First, the energy transfers associated with V/C mass transfers are evaluated. As in Eqs. (10) - (11), that treat removal of liquid by vaporization, the removal of vapor by condensation in Eq. (12) is at the bulk vapor enthalpy. Second, the heat transfer into the vapor at liquid/vapor interfaces is evaluated. Third, the heat transfer into the vapor at structure and particle interfaces is calculated for the case where the liquid of a given vapor density component exists or condensation can occur. Fourth, direct heat transfer between structure/particles and vapor is determined for vapor density components where no liquid is possible. This summation also includes a term for direct liquid-to-vapor mass transfer when all of a liquid component is predicted to vaporize, but the resulting saturation temperature is too low to calculate a T_{GLm} by the energy balance approach. Fifth, a homogenous condensation term has been included in the vapor energy equation because the AFDM V/C model does not allow condensation of one vapor species on the liquid surface of a different material. Unusual situations such as fuel vapor expanding in a pool of liquid sodium can result in highly subcooled vapor without such a term. The form chosen is based mainly on numerical considerations. The quadratic allows a continuous derivative at the inception of condensation, and the linear approximation at high-temperature differences limits excessive values. Theoretically, homogeneous condensation, like homogeneous nucleation, might be limited to situations near the critical point. Perhaps a better analogy is to conduction-controlled flashing in liquids. The AFDM code is simulating an artificial surface because condensation cannot be represented on the real surface. The process is limited by conduction through the fluid to the surface. At constant pressure and superheat, flashing vapor production has been described by the square of the difference between the bulk liquid temperature and the vapor saturation temperature,⁸ and a similar temperature dependence involving the bulk vapor temperature could be appropriate here.

The form of the work term in the energy equations was taken from Stewart.⁹ If all liquids would be assumed to possess constant microscopic densities, the work term in these equations would simply vanish and that of the vapor equation could be reduced to the SIMMER-II form by using

$$\frac{\partial \alpha_P}{\partial t} + \frac{\partial \alpha_{L1}}{\partial t} + \frac{\partial \alpha_{L2}}{\partial t} = - \frac{\partial \alpha_G}{\partial t} \quad (13)$$

H. Interfacial Area Convection

The SIMMER-I code convected radii for bubbles and liquid drops. This procedure was prudently deleted in SIMMER-II. Such convection has no relationship with the associated liquid- and vapor-volume fractions. However, the lack of convection in SIMMER-II also resulted in distortions. For example, the progressive breakup of moving liquid by a gas stream was approximated by finding (independently for each computational cell) the "steady-state" droplet radii that will satisfy a Weber number criterion in the presence of the existing (transient) pressure gradient. Ishii⁴ proposed that interfacial areas be convected with the velocities of the interfaces. This seems to be conceptually correct, but such an algorithm is impractical in AFDM. The Eulerian code format does not allow the retention of sufficient information to construct the phenomenological history required to determine real interfacial velocities.

AFDM convects interfacial areas with the bulk fluid velocities. The general equation is

$$\frac{\partial a_f^C}{\partial t} + \nabla \cdot (a_f^C \vec{v}_q) = \sum_A S_{A,f} + \sum_B S_{B,f} + S_{C,f} \quad , \quad (14)$$

where a_f^C is the surface area per unit volume for interface f to be convected,

$\vec{v}_q$ is velocity of momentum field q to be used to convect interface f ,

$S_{A,f}$ represents interfacial source terms for the case of continuous liquid,

$S_{B,f}$ represents interfacial area source terms for the case of continuous vapor,

$S_{C,f}$ represents an interfacial area source resulting from mass transfer, and

f represents interfaces L1/G, L2/G, and L1/L2.

Two models for interfacial area convection exist in AFDM. In the first model (ARCV1), each a_f^C is uniquely assigned to a momentum field. In the second model (ARCV2), the a_f^C (representing interfacial areas between the continuous and discontinuous phases) are convected with the velocity of the discontinuous

phase. The phenomena providing contributions to $S_{A,f}$ are nucleation, dynamic forces, turbulence, and coalescence. The $S_{B,f}$ contributions come from dynamic forces, coalescence, and flashing. A full definition of the determination of the a_f^C and the models for $S_{A,f}$ and $S_{B,f}$ are given in Vol. II.

IV. CONCEPTUAL AND NUMERICAL ASSUMPTIONS

This section gives some basic assumptions and simplifications for the numerical solution of the conservation equations in the AFDM.

A. Basic Assumptions

Four introductory topics are treated here. First, there is the dimensionality of the mesh used to discretize the equations. Second, the time-factorization philosophy used to construct a numerical algorithm is discussed. Third, the reasons to use semi-implicit differencing in performing convection are presented. Last, we give the assignment of variables to the finite-difference mesh.

1. Dimensionality. The AFDM code was programmed in two-dimensional r - z cylindrical geometry. A reduction to one-dimensional slab or cylindrical geometry is available. Although fast reactor core geometry is recognized to be best modeled by a triangular- z configuration, treatment of such a three-dimensional non-orthogonal system was beyond the scope of the AFDM effort. Even the task of writing the finite-difference equations in three-dimensional orthogonal geometry was judged to be excessive, and r - z geometry was believed to be sufficient (and necessary) to test the desired models and methods. (A one-dimensional representation can be very misleading both in terms of the capabilities of the numerical methods used and in the phenomenological implications that may be drawn from the calculations.) Other options such as x - y geometry and one-dimensional spherical geometry were not programmed. Experience with SIMMER-II suggests that other options could be added to a future version of AFDM, if desired.

2. Time-Factorization Algorithm. The solution algorithm adopted in AFDM is given in Fig. 1. Except for the momentum exchange resulting from drag (from fluid-structure, fluid-fluid, and virtual mass terms), a time-factorization (time-splitting) approach is used where intracell mass and energy transfers are evaluated separately from intercell transfers. Mathematically, the

differential equations are solved using the time derivatives and the right side of each equation. Then, the updated variables are convected using the differential equations in the form where the right sides have been set to zero. Any SIMMER-III code will possess so many components and such complexity that a more integrated approach appears impractical, so the disadvantages should be investigated by AFDM. Also, generally accepted intracell models do not exist, and the ability to modify mass and energy exchanges should be facilitated to the extent possible. Changing an integrated implicit formulation is much more difficult than changing a more modular approach. A drawback of the time-factorization algorithm is that feedback from convection on intracell mass and energy transfer will not occur within one time step. This lack of feedback has been criticized by Stewart⁹ as leading to inaccuracies. For example, if one cell is vaporizing and an adjacent cell is condensing, a balanced flow will not be obtained in one time step.

One implication of the time-factorization algorithm is the necessity to use α_0 , a small, non-zero vapor volume fraction at which two-phase to single-phase transitions are presumed to occur. All vapor is treated as noncondensable during the calculation of convection. Consequently, as with real noncondensables, derivatives with respect to vapor smear (macroscopic) densities may assume very large, rapidly changing values if the vapor volume fraction is allowed to go to zero. The formalism adopted assumes that vapor exists in every cell in an effective vapor-volume fraction, α_{ge} , defined so that conversion of structure into a liquid field component (such as particles) would not change the pressure and so that the two-phase/single-phase transition takes place with the correct liquid smear densities. The mathematical expression is

$$\alpha_{ge} = \max [\alpha_0(1 - \alpha_S), 1 - \alpha_S - (1 - \alpha_0)(\alpha_P + \alpha_{L1} + \alpha_{L2})] \quad , \text{ or} \quad (15)$$

$$\alpha_{ge} = \max [\alpha_0(1 - \alpha_S), \alpha_G + \alpha_0 (\alpha_P + \alpha_{L1} + \alpha_{L2})] \quad , \quad (16)$$

where α_S , α_P , α_{L1} , and α_{L2} are given in Eq. (1) and α_G is defined by Eq. (2).

Fig. 1.
Schematic of the AFDM numerical algorithm.

3. Use of a Semi-Implicit Convection Scheme. The anticipation of some relatively quiescent time periods in situations where the environment may have a high-sonic velocity, for example, a pool, leads to the desire to calculate sonic-wave propagation implicitly. However, to keep the multicomponent, multidimensional algorithm tractable, use of beginning-of-time-step values are desired for mass, momentum, and energy in computing convection. This leads to a general approach known as semi-implicit differencing, which was pioneered by Liles and Reed.¹⁰ This choice means that the pressure is approximated by end-of-time-step values everywhere, and convective terms are treated using $\nabla(\psi_i^n \vec{v}_q^{n+1})$, where ψ_i^n is a beginning-of-time-step value for a quantity, ψ , of an arbitrary species, i , to be convected with end-of-time-step velocity, q . When the semi-implicit approach is combined with the differential equations previously assumed, the changes in velocities during the pressure iteration shown in Fig. 1 depend only on the changes in pressure. Further, the series of linearized approximations used in the pressure iteration can be reduced to the solution of pressure errors involving systems of N equations for an N cell array.

In the AFDM version of semi-implicit differencing, only five selected relationships containing sensitive variables "drive" the pressure iteration. This significantly reduces the computational effort. Of course, an accuracy penalty exists in some situations. The basis for the judgements made is in Sec. V.D.

4. Computational Mesh. A staggered mesh has been selected for AFDM with velocities defined on the cell boundaries, whereas densities, internal energies, and pressures are defined at cell centers. This is similar to SIMMER-II. The main advantages of such an arrangement are related to the use of the semi-implicit algorithm and the equations for the internal (rather than the total) energy. Only two pressures are required to obtain a given axial or radial velocity change. Consequently, the composition of one cell only depends on pressure changes in itself and its four neighbors. With the avoidance of the convection of kinetic energy, a donor-cell approximation is not required for treating velocities, except in the convective terms of the momentum equations.

Although the staggered mesh greatly facilitates evaluation of the pressure iteration by limiting the number of off-diagonal matrix elements, disadvantages do exist. Momentum convection is difficult to perform consistently, complete energy conservation is sacrificed, and decisions must be reached on averaging

quantities at cell boundaries. One illustration of these difficulties is the so-called "water packing" problem mentioned in the TRAC manual.¹¹ It is most severe when a channel is filling with liquid from the bottom and vapor is flowing downward to be condensed in the cold lower part of the channel. In this situation, nonphysical pressure pulses develop when a cell is filled with liquid and the downward velocity at the top of the cell must be reversed. Even though there is no liquid momentum associated with the downward moving vapor (from the donor cell), the required averaging to solve the momentum equations means that one-half of the liquid in the filling cell is assumed to possess a downward velocity on the time step when the cell is full of liquid. An impulse must be given to this liquid so that it possesses the same upward velocity as the liquid below. This impulse creates a brief pressure pulse. The TRAC solution to this problem is to reduce the liquid inertia, thus minimizing the size of the impulse required. Although the different momentum convection scheme in AFDM reduces the magnitude of the problem, it does not disappear. Any future code development effort needs to evaluate the benefits and problems associated with the use of a staggered mesh carefully.

B. Options Available

As facilitated by the modular approach, the exploratory nature of the AFDM code has resulted in the implementation of several compiler options, which allow the user to investigate the effect of different algorithms and run the code at different installations. Options that change the models/methods used are as follows.

(a) Two versions of the intracell transfer functions exist: a simplified version (KQOM1) and a more sophisticated version (KQOM2). In KQOM1, the drop and bubble radii are input. In KQOM2, interfacial areas are determined from differential equations.

(b) In the KQOM1 option, mass-transfer modeling can be eliminated by using the NOPHASE option. Using NOPHASE, only sensible heat transfer occurs from the liquids to the vapor.

(c) Using the KQOM2 approach, the ARCV1 option associates interfacial area convection with momentum fields, whereas the ARCV2 option uses the discontinuous phase, as explained in discussing Eq. (14). As an example, consider the area being convected from a cell with bubbly flow to one with droplet (dispersed) flow. The ARCV1 approach would move the interfacial area

with the liquid such that the droplet source in the dispersed cell would correspond to the bubble size in the liquid-continuous cell. The ARCV2 approach would move the interfacial area with the vapor velocity so that the droplet source would likely be larger or smaller than the bubble size in the donor cell.

(d) A tabular EOS can be obtained by using the SESAME. The default EOS is a simplified version of the SIMMER-II AEOS.

(e) Two methods exist for solving the system of N linear equations produced during the pressure iteration, where N is the number of cells. The PSOL1 option uses the MATSOL routine from SIMMER-II. The MATSOL routine is recursive and cannot be vectorized. The PSOL2 option uses the fastest of three trial approaches. These are a Banded Matrix Direct-Solution Method, a Conjugate Gradient Residual Method, and a Chebyshev Polynomial Iterate Method. More storage is required, but these routines are vectorized.

(f) The default option is to use higher-order donor-cell differencing. A DONOR option exists for first-order donor-cell differencing. The higher-order differencing approach to the reduction of numerical diffusion is based on the CSQII code¹² and originates with van Leer.¹³ It calculates a shape of the variables to be convected in each donor cell in each direction based on values of these variables in the neighboring cells. Limiters are applied to the slopes of these shapes. This approach can be applied to the semi-implicit algorithm without excessive effort because of only forming shapes with beginning-of-time-step variables.

(g) The inclusion of virtual mass terms is obtained with the IVIS option. Use of the IVIS option is recommended to reduce momentum coupling problems at the transition between single-phase and bubbly flow.

Figure 2 illustrates these compiler options. The remaining options, which allow the code to execute on differing computer systems, are described in the code user's manual (Vol. VII).

C. Intracell Transfer Limitations

The fluid-dynamics modeling in AFDM is far more detailed than that of SIMMER-II. Twelve topologies are treated, representing the various geometric configurations that are possible. Both liquid- and vapor-continuous flow regimes are treated within these topologies. The SESAME EOS removes the inaccuracies in pressures and internal energy calculations. The V/C model

The Version Tree for AFDM
64 Model Combinations

Fig. 2.
Compiler options available in AFDM.

treats the liquid temperatures implicitly, removing oscillation problems caused by small liquid volumes. The use of three moving velocity fields with the convection of interfacial areas allows modeling based more on actual interactions.

However, significant limitations are present, resulting from the number of components selected and from the time, resources, and technology available to the AFDM effort. Some of the limitations involved with the number of components are obvious, such as those from a single structure. Others are more subtle. For example, one density component for each liquid means that no transport of distorted drop or compound bubble/drop configurations can be performed. All discontinuous liquids are consequently spherical drops. Because films are not separately modeled, there can be no differentiation between film and droplet condensation based on the presence of liquid films. Also, one liquid energy component per material means that transient temperature profiles cannot be maintained within liquid drops. The use of only one vapor energy field means that some phenomena occurring during rapid transients will not be represented. Fuel bubbles cannot grow while steel bubbles condense, and bubbles cannot grow inside of a liquid drop isolated from the other vapor in a cell. The limitations coming from time, resources, and/or technology are the limiting of flow regimes to unrestricted flow, assuming equilibrium melting/freezing, representing V/C as driven by heat-transfer differences, not modeling phenomena for temperatures near the liquid critical point, and taking most source terms for bubble/drop surface areas as based on rates for approaching equilibrium conditions using time constants.

Some of the restrictions can be removed in any future development effort. However, the basic philosophy has to be one where the dominant details of complex phenomena can be represented by relatively simple models. Where this type of modeling is inadequate, the value of multifield Eulerian fluid-dynamics calculations is limited.

D. Equations-of-State

Two types of EOS information are required in AFDM. First, thermophysical properties (thermal conductivities, viscosities, and surface tensions) are needed for the Step 1 models. These are obtained using theoretical models where available (for example, the Chapman-Enskog kinetic theory of gases) and user-specified polynomials where the situation is more speculative. Second,

thermodynamic properties are required. The differential equations cannot be solved without an EOS to relate the densities and temperatures to internal energies and pressures. Also, intracell transfers, particularly the calculation of mass transfer, require EOS information. Two EOS options exist in AFDM: a simplified analytic EOS and an interface to the Los Alamos SESAME EOS library.

1. The Simplified Analytic Equation-of-State (SAEOS). The SAEOS is based on a SIMMER-1² modified polytropic gas equation to compute the pressure in two-phase cells and a formulation suggested by Fischer¹⁴ to obtain single-phase pressures. For two-phase cells, this evaluation depends on input gas constants for each material. For single-phase cells, input sonic velocities are used to represent particle and liquid compressibilities. Structure, particle, and liquid temperatures are related to internal energies by assuming constant heat capacities. Microscopic densities for structure, particles, and the liquids are input and assumed to be constant. Volume fractions for these components are determined by using Eq. (1). The saturation temperature for a vapor component is related to the partial pressure of that component by integrating the Clausius-Clapeyron equation. The internal energy for saturated vapor of a given component is determined by assuming a constant enthalpy of vaporization. For a condensable component, the vapor internal energy is computed by starting with the saturation energy and adding the difference between the vapor temperature and the saturation temperature multiplied by a constant heat capacity. A perfect gas relationship is used for the noncondensable gas. The internal energies for the three vapor components are then mass-averaged to compute the mixture vapor internal energy.

2. The SESAME EOS. In AFDM, the tabular EOS option enables a code user to retrieve data from the EOS library, SESAME.¹⁵ This library provides a wider and more realistic data base than can be obtained with an analytic representation.

The set of independent variables with which the AFDM solution algorithm proceeds is composed of macroscopic densities and temperatures ($\bar{\rho}$ and T). An independent variable vector for the AFDM algorithm can be written as

$$\vec{x}_F = (\bar{\rho}_P, \bar{\rho}_{L1}, \bar{\rho}_{L2}, \bar{\rho}_{G1}, \bar{\rho}_{G2}, \bar{\rho}_{G3}, T_P, T_{L1}, T_{L2}, T_G)^T . \quad (17)$$

This vector represents the time-dependent information normally available for EOS interrogations.

The main complexity in the implementation of the SESAME EOS is in the transformation of the macroscopic density information appearing in $\vec{x}_F$ to microscopic density information needed for EOS evaluations. This is dealt with by assuming that the materials are immiscible and that mechanical equilibrium (in pressure) exists in a numerical cell. Physical volume fractions are defined by

$$p_G(\vec{\rho}_G, T_G) = p_{L1}(\rho_{L1}, T_{L1}) = p_{L2}(\rho_{L2}, T_{L2}) = p_P(\rho_P, T_P) \quad , \quad (18)$$

$$\text{where } \vec{\rho}_G = \vec{\rho}_G / \alpha_{ge} \quad , \quad (19)$$

α_{ge} is defined by Eqs. (15) or (16), and

Eqs. (1) - (2) determine the other volume fractions.

Assuming that the EOS provides all the pressures appearing in Eq. (18) and given $\vec{x}_F$, then the system of Eqs. (1), (15), (18), and (19) represents 10 equations containing 10 unknowns,

$$(\rho_{G1}, \rho_{G2}, \rho_{G3}, \rho_{L1}, \rho_{L2}, \rho_P, \alpha_{ge}, \alpha_{L1}, \alpha_{L2}, \alpha_P) \quad ,$$

and can, therefore, be solved to determine all the α s. With algebraic substitution, this system can be reduced to three equations containing the three liquid-field volume fractions, which then can be solved numerically using a Newton-Raphson iteration.

If the α_G determined by this calculation is negative, an additional iteration is required to determine the cell volume fractions. This iteration describes mechanical equilibrium between the single-phase liquid components and the particles:

$$p_{L1}(\rho_{L1}, T_{L1}) = p_{L2}(\rho_{L2}, T_{L2}) = p_P(\rho_P, T_P) \quad , \quad (20)$$

$$\alpha_{L1} + \alpha_{L2} + \alpha_P + \alpha_S = 1 \quad . \quad (21)$$

These equations combine with the volume fraction definitions and the SESAME EOS to form a system of six equations containing six unknowns. Algebraic substitution reduces this to two nonlinear equations and two unknowns, α_{L1} and α_{L2} , that can be solved with a Newton-Raphson iteration.

Once the component volume fractions are determined, the remaining required EOS information can be obtained in a straightforward (but tedious) fashion. For example, derivatives of the macroscopic densities require $\partial \rho / \partial \bar{\rho}$ for the various components. These expressions are obtained from differentiating the equations describing mechanical equilibrium.

Finally, because unique EOS information is required in various parts of the AFDM code, the philosophy followed in AFDM is to establish several different EOS subroutines that obtain the specialized information required. The makeup of these subroutines and other EOS details are in Vol. VI.

V. SOLUTION ALGORITHM

This section presents the major steps in the AFDM solution algorithm that was shown in Fig. 1. A summary is provided first, followed by sections containing more explanation. Details are to be found in subsequent AFDM volumes.

A. Summary

Step 1 starts with the beginning-of-time-step densities, temperatures, convectible interfacial areas, velocities, and pressures ($\bar{\rho}_m^n$, T_r^n , $(a_f^C)^n$, u_q^n , v_q^n , and p^n) and updates these densities, temperatures, and velocities from mass and energy transfers. Several paths exist through Step 1, depending on the option selected. The standard path (KQCM2) has nine parts, as follows.

1. Evaluate the EOS for thermodynamic and thermophysical properties.
2. Select the topology and the flow regime. Note that the topology selection implies a continuous phase, but a given topology may possess more than one flow regime.
3. Calculate the source terms and update the convectible interfacial areas.
4. Define instantaneous interfacial areas for heat-transfer processes.
5. Obtain heat-transfer coefficients.
6. Calculate momentum-exchange coefficients.

7. Perform heat- and mass-transfer operations updating densities and internal energies.
8. Invert the EOS to obtain temperatures.
9. Modify velocities and convectible interfacial areas based on the mass-transfer results.

The Step 1 heat- and mass-transfer algorithmic idea is to treat rapidly varying (sensitive) quantities implicitly and the slowly varying (stable) quantities explicitly. The implicit part is treated using a multivariate Newton-Raphson algorithm. At the conclusion of Step 1, the modified variables are denoted by a tilde ($\sim$), or $\tilde{\rho}_m^n$, $\tilde{T}_r^n$, $(\tilde{a}_f^c)^n$, $\tilde{u}_q^n$, and $\tilde{v}_q^n$.

Step 2 is a calculation of estimated end-of-time-step values. The first operation is to calculate $\tilde{e}_r^n$ ($\tilde{e}_m^n$ for higher-order differencing) and $\tilde{\alpha}_r^n$ from $\tilde{\rho}_m^n$ and $\tilde{T}_r^n$ using the EOS. Then, the convective terms in the conservation equations are evaluated explicitly to allow a determination of $\tilde{\rho}_m^{n+1}$, $\tilde{e}_r^{n+1}$, $\tilde{u}_q^{n+1}$, and $\tilde{v}_q^{n+1}$. The density equations can be evaluated directly. The energy equations use estimated end-of-time-step values from the density equations update to obtain the $\partial\alpha/\partial t$ terms. The momentum equations assume $\tilde{p}^{n+1} = \tilde{p}^n = p^n$. Otherwise, the transfers from Step 1 could give rise to unrealistic velocity changes. The interfield drag terms are either evaluated using the SIMMER-II formulation or iterated using the time-averaged velocities, $(\tilde{v}_q^{n+1} + \tilde{v}_q^n)/2$ and $(\tilde{u}_q^{n+1} + \tilde{u}_q^n)/2$. The selection is based on stability with the purpose of obtaining a compromise with the effects of drag modifications resulting from flow-regime changes. After the velocities are determined, velocity derivatives with respect to pressure are evaluated for use in Step 3. An iteration is also performed to invert the EOS to obtain $\tilde{T}_r^{n+1}$.

Step 3 is an iteration to obtain consistency between the estimated end-of-time-step values for $\tilde{\rho}_m^{n+1}$, $\tilde{T}_r^{n+1}$, $\tilde{u}_q^{n+1}$, and $\tilde{v}_q^{n+1}$, with an updated pressure, $\tilde{p}^{n+1}$. Each step of the iteration attempts to eliminate the deviations in the conservation relations for each momentum density, a modified conservation equation for the vapor internal energy, and the difference between the pressure from the EOS and the current value of $\tilde{p}^{n+1}$. Assuming that the independent variables are the estimated end-of-time-step values for the densities, temperatures, and pressure, on each iteration a Taylor series expansion is performed on the expression for each deviation. This sets up a simultaneous set of linear equations. The derivatives in these expansions are obtained from the EOS, the derivatives of the conservation equations, and the velocity derivatives with respect to pressure computed in Step 2. Step 3 is known as

the pressure iteration because the main computational step is a solution for a set of N-coupled equations for the pressure changes, where N is the total number or real (nonboundary) cells in a problem. Step 3 is simplified by assuming that liquid internal energies do not change, that vapor energy convection is adequately described by the Step 2 estimates, and that the component density ratios within a given momentum field remain constant.

Step 4 determines the final end-of-time-step values for all variables. The main operation is to convect the initial tilde quantities $\tilde{\rho}_m^n$, $(\tilde{a}_f^c)^n$, $\tilde{e}_r^n$, $\tilde{\rho}_q^n \tilde{u}_q^n$, and $\tilde{\rho}_q^n \tilde{v}_q^n$ with the Step 3 velocities $\tilde{u}_q^{n+1}$ and $\tilde{v}_q^{n+1}$. These same Step 3 velocities are used to calculate mass and energy inflows/outflows at the problem boundaries. The convection operations give the final densities, $\tilde{\rho}_m^{n+1}$, and convectible interfacial areas, $(\tilde{a}_f^c)^{n+1}$. The final pressures, p^{n+1} , are simply the converged values from the pressure iteration. End-of-time-step velocities are used in the interfield drag terms for a momentum equation iteration to obtain the full effects of any change in flow regime. The final internal energies in Step 4 are obtained with the addition of the energy sources from the interfacial drag and the virtual mass terms. These are computed using the end-of-time-step velocities because of the necessity to be consistent with the interfield forces and structure drag used in the momentum equations. The final operation in Step 4 is the inversion of the EOS to obtain T_r^{n+1} .

B. Step 1: Calculation of Intracell Exchanges

This section provides more information on the treatment of the phenomenology within a computational cell. The idea is to treat the right side of Eqs. (4) - (5), (8) - (12), and (14) along with the time-derivative term and to ignore the remaining terms on the left side. The time-derivative term is updated using the other left-side terms in Steps 2, 3, and 4. Two different models are available--a simplified (KQOM1) model and the standard (KQOM2) model.

1. The Simplified Model. The simplified model was constructed to allow checkout of the AFDM heat and mass transfer, convection, and the EOS interface without the complications introduced by the "standard" interfacial area modeling. There are two possible ways of executing AFDM with the KQOM1 model, with or without the NOPHASE option.

a. Using the NOPHASE Option. The NOPHASE option contains the initial zero-order model used to check out Steps 2 - 4 of the AFDM algorithm. Momentum-exchange coefficients are determined, but mass transfer is ignored, and only

liquid-vapor heat transfer is modeled to limit the production of unrealistic conditions from an adiabatic vapor calculation. The NOPHASE option contains three steps.

First, products of the interfacial areas and heat-transfer coefficients for liquid-vapor heat transfer are defined based on volume fractions, input droplet radii, input thermal conductivities, and an input multiplication coefficient.

Second, the mathematical form for the AFDM momentum-exchange function between moving velocity fields is

$$K_{qq'} = a_{qq'} + b_{qq'} | \vec{v}_{q'} - \vec{v}_q | \quad (22)$$

In Step 1, the quantities $a_{qq'}$ and $b_{qq'}$ must be determined. For liquid-liquid interactions in the simplified models, the $a_{qq'}$ term comes from Stokes law for viscous flow, and the $b_{qq'}$ term is taken from a relationship postulated by Amsden, Butler, and Harlow¹⁶ for arbitrary two-phase flow ignoring viscosity considerations. For liquid-vapor coupling, the simple model has been divided into four flow regimes. These are given as a function of the vapor-volume fraction existing in the fluid, $\alpha_{G,f} = \alpha_G / (1 - \alpha_S)$, as

- (a) single-phase (all liquid) flow for $\alpha_{G,f} < 0$
- (b) bubbly flow for $0 \leq \alpha_{G,f} < 0.3$,
- (c) churn-turbulent flow for $0.3 \leq \alpha_{G,f} < 0.7$, and
- (d) dispersed flow for $0.7 \leq \alpha_{G,f} < 1.0$.

The KOCM1 model uses expressions for $a_{qq'}$ and $b_{qq'}$ that will allow AFDM to reproduce simple bubble column relative velocities in the absence of a second liquid using the appropriate input radii.

Third, three simplified energy conservation equations are solved for the two liquids and the vapor. An iteration with the EOS is programmed to allow for a nonlinear temperature-energy relationship. Convergence of the iteration gives the $\tilde{T}_r^n$.

b. Without the NOPHASE Option. Here, the parts of Step 1 defined in Sec. V.A. are followed with simplified models for interfacial areas and the heat-transfer and momentum-exchange coefficients.

Ten interfacial areas are required describing binary contacts between the five different volume fractions, α_S , α_p , α_{L1} , α_{L2} , and α_G . These are based on (a) the input radii for each KOCM1 flow regime defined above, (b) a switch from

liquid-continuous to vapor-continuous flow at $\alpha_{G,f} = 0.5$, (c) the SIMMER-II³ model for liquid-liquid contacts, and (d) an input structure surface area. The 14 heat-transfer coefficients required for Eqs. (8) - (12) are obtained using input parameters, a conduction approximation (where appropriate), and correlations of the form

$$h = k \left[C_1 Re^{C_2} Pr^{C_3} + C_4 \right] / d \quad , \quad (23)$$

where k is a thermal conductivity,

Re is a Reynolds number,

Pr is a Prandtl number,

d is a length scale such as a droplet diameter, and

C_1 , C_2 , C_3 , and C_4 are constants taken from DATA statements.

The momentum-exchange coefficients are evaluated as in the NOPHASE option.

Following the determination of interfacial areas and heat-transfer coefficients, the heat- and mass-transfer operations are the same as in the KQQM2 option described in Sec. V.B.2. Of course, because interfacial area is not convected using the simplified modeling, no convectible interfacial areas need to be updated.

2. The Standard Model. This section provides an overview of the KQQM2 models. The organizational structure follows the path of the calculation outlined in Sec. V.A.

a. Topologies and Flow Regimes. After an EOS call, the intracell transfer calculations in AFDM are started by defining the geometrical configuration of fluids in a computational cell called the topology. Once selected, topologies are not changed during a time step. The influence of the surrounding walls of the pool on the topology selection is neglected. Therefore, we use the notation topology, rather than flow regime. Twelve topologies are generated to model the various combinations of the three velocity fields. The physical parameters governing the choice are the number of existing velocity fields, the dominant liquid within the two liquid velocity fields, and the dominant phase. Particles that form the solid phase of velocity field 1 are assumed to possess a constant representative radius. The

subdivision into 12 topologies helps to set up an efficient logic in the vectorized code. The topologies used by AFDM are shown in Fig. 3.

The dominant liquid is chosen as a function of the liquid and particle volume fractions existing in a computational cell. The dominant or continuous phase is determined by taking average values for the liquid phase and comparing them to those of the vapor phase. A levitation criterion is used to evaluate whether liquid spheres of a size governed by a Weber number can be levitated in a vapor flow driven by the local pressure gradient. The criterion is limited by input vapor-volume fractions. For large vapor-volume fractions, vapor is always continuous, regardless of the levitation criterion. For large liquid-volume fractions, the same is true for the liquid-continuous phase.

With the present set-up of topologies, some distinction among a limited number of flow regimes has already been made. By choosing vapor as the continuous phase, the droplet flow regime is defined. Within liquid-continuous flows, we distinguish between four regimes: bubbly nucleating, bubbly, churn, and cellular. The bubbly nucleating regime prevails for small bubble radii and small vapor-volume fractions. It is characterized by bubbles being too small to coalesce or split from mechanical forces. Bubbles can grow as a consequence of liquid leaving the cell or vaporizing; otherwise, only a nucleation model updates the interfacial areas. All processes contributing to SA_{f} are active outside the bubbly nucleating regime. Bubbly flow is modeled up to vapor-volume fractions of about 0.3. For higher void fractions, churn flow is indicated that has an explicit effect on the calculation of the drag coefficient. All other effects with respect to surface areas and drag coefficients are implicitly taken care of by the use of a representative bubble size. For void fractions higher than about 0.5, with liquid-continuous flow still prevailing, the liquid tends to form bridges between the bubbles, and the momentum exchange between the phases becomes large. This is the cellular flow regime prevailing until a criterion to enter vapor-continuous flow is satisfied.

b. Calculation of Convectible Surface Areas. There are three "convectible" surface areas possible between the two discontinuous phases and the continuous phase. Bubbles and droplets form the discontinuous phases in the pool geometry. Models are restricted to evaluate spherical droplets or bubbles, called fluid spheres. However, the increase in surface areas beyond spherical shape is taken into account by either multipliers or a model

modification to describe the change of surface areas. The source and sink terms in Eq. (14) describe the splitting, coalescence, production, or loss of the fluid spheres. We will discuss the interfacial area source term resulting from dynamic forces as a representative example and add limited information about other processes.

To set up a model for the surface area source term, two physical quantities have to be known. First, one needs to assess the equilibrium size of the fluid sphere under the conditions existing in the cell. Second, the rate with which equilibrium is achieved has to be known. The equilibrium radius r_e can be described by a modified Weber criterion ¹⁷ with

$$r_e = \frac{We_{\sigma_{cd}}}{4\rho_c \Delta v^2} + \left[\left(\frac{We_{\sigma_{cd}}}{4\rho_c \Delta v^2} \right)^2 + C \frac{\mu_d^2}{\rho_d \rho_c \Delta v^2} \right]^{1/2}, \quad (24)$$

where We is the Weber number, which may be different for bubbles and droplets, c and d are indexes indicating the continuous and discontinuous phases, σ is the surface tension, μ is the dynamic viscosity, and Δv is the absolute value of the velocity difference between phases.

The second term of the square root accounts for the effects of viscous flow fields, with a constant, C , to be a user-defined input. The radius is related to the interfacial area by $a_e = 3\alpha_d/r_e$. A single-relaxation-time model is used to define the fluid sphere surface area a_d , using

$$\frac{d}{dt} a_d = \max \left(\frac{a_e - a_d}{\tau}, 0 \right), \quad (25)$$

where the dispersed phase volume fraction is presumed constant and the time constant τ is defined using¹⁸

$$\tau = \frac{C' r_d}{\Delta v} \left(\frac{\rho_d}{\rho_c} \right)^{1/2}, \quad (26)$$

Fig. 3.
The 12 topologies used in AFDM.

where $r_d = 3\alpha_d/a_d$ and C' is another user-defined constant. Equation (25) is integrated over a time step Δt , using limiters on the time constant to prevent overshooting.

The different source terms are assumed to be independent of each other and, therefore, can be added. Equally independent is the sink term described by the coalescence of fluid spheres. The rate of decrease in interfacial area resulting from coalescence is

$$\frac{d}{dt} a_d = -a_d^2 C_a \quad , \quad (27)$$

where C_a is a coalescence probability that is determined by modeling the statistical frequency of hypothesized collisions resulting from random velocity fluctuations as in SIMMER-11.³

In the above discussion, the convectible surface areas were functions of the volume fractions and the sphere radii. However, in describing nucleation of bubbles in a continuous liquid, the surface areas are given by

$$a_d = 4\pi r_d^2 n = \left[36\pi n \alpha_d^2 \right]^{1/2} \quad , \quad (28)$$

where n is the number density of nucleating bubbles. The change in number density is a function of a dimensionless superheat to model delays in nucleation during rapid evaporation.¹⁹

There are three different regimes with unique sets of source and sink terms. First, at low vapor-volume fractions and small bubble radii, the bubbles are treated as rigid spheres incapable of coalescence or splitting processes. The only source term is that of nucleation. Second, for the remaining liquid-continuous regimes, a turbulence breakup model²⁰ is introduced in addition to the dynamic forces, nucleation, and coalescence models. Turbulence is assumed to cause bubble fragmentation if the frequency of forces originating from turbulent eddies corresponds to a bubble eigenfrequency. Third, for vapor-continuous regimes, a flashing model exists. The internal overpressure of the droplets at the bulk temperature is compared to the pressure that can be accommodated by surface tension to determine the maximum droplet size that can escape fragmentation.

c. Determination of Instantaneous Interfacial Areas. Once the convectible surface areas are updated, they have to be subdivided in case a given topology has more than one discontinuous component and/or structure. Step 1 calculates up to 10 instantaneous surface areas between the 5 possible energy components given in a cell. The required algebraic models are described in Vol. II. These models include relationships to represent liquid 1-particle contact based on melting-freezing criteria; two-phase, two-liquid contact at zero velocity difference based only on surface tension criteria; contact of two discontinuous components due to random collision at finite velocity difference; and a combination of the latter two processes. Additionally, weighing factors are introduced to redirect bubble surfaces to the liquid that undergoes nucleation.

For example, for two-phase, two-liquid contact at zero velocity differences, a model becomes necessary because the two liquids may co-exist in a given cell. Based on surface tension observations,²¹ three configurations are possible in AFDM, as shown in Fig. 4. Here, c and d denote the continuous and the discontinuous liquid, respectively, and g, the vapor phase. The model is not necessary for continuous vapor topologies because droplet-droplet interaction is modeled by random collision. In Fig. 4, the three configurations depend on two surface-tension parameters,

$$\begin{aligned}\sigma_1 &= \sigma_{cg} - \sigma_{dg} - \sigma_{cd} \quad , \quad \text{and} \\ \sigma_2 &= \sigma_{dg} - \sigma_{cg} - \sigma_{cd} \quad ,\end{aligned}\tag{29}$$

where the three surface tensions between vapor and continuous liquid, σ_{cg} , vapor and discontinuous liquid, σ_{dg} , and between both liquids, σ_{cd} , have to be known. For configurations 1 and 3, observation predicts a very limited contact between vapor bubbles and one of the liquid phases. However, to restrict the exclusiveness of this observation, a user-defined residual surface area, a_r , is introduced.

The increased contact between discontinuous vapor and discontinuous liquid spheres in case that film-boiling criteria are met is only taken into account by changing the heat-transfer coefficients.

d. Heat-Transfer Coefficients. After having evaluated the instantaneous interfacial surface areas, the standard AFDM modeling calculates heat-transfer coefficients so as to be consistent with the areas. Between

liquid, structure, and particle component pairs, the heat-transfer coefficient is based on bulk temperatures and steady-state profiles. Between the vapor field and the liquid components, the interface temperature is assumed to be the saturation temperature of the corresponding vapor. Heat-transfer processes considered are conduction, convection, and radiation. In general, a convective correlation of the Nusselt number is used in the continuous phase.²² For the discontinuous phases, convective heat-transfer correlations are used if the droplet is in the nonrigid mode. For the rigid mode a conductive heat-transfer coefficient is assumed. For example, if either liquid 1 or liquid 2 is the continuous fluid, the conductive/convective part of the heat-transfer coefficient between liquid 1 and liquid 2 is given by

$$h_{L1L2} = \frac{1}{d_d} \left[\frac{1}{k_c Nu_c} + \frac{1}{k_d Nu_d} \right]^{-1}, \quad (30)$$

where d is the fluid sphere diameter,

k is the thermal conductivity,

Nu is the Nusselt number, and

subscripts c and d indicate continuous and discontinuous phases, respectively.

The Nusselt numbers depend on the Prandtl number (Pr) of the continuous phase and the Reynolds number (Re) for the fluid spheres in the continuous phase. For $Re < 50$,

Configuration 1

Configuration 2

Configuration 3

Fig. 4.

Two-phase, two-liquid configurations in AFDM.

$$\begin{aligned}
Nu_d &= 2/C_d \quad , \\
Nu_c &= 2 + 0.55 Re^{1/2} Pr^{1/3} \quad , \quad Pr < 1 \quad , \\
Nu_c &= 2 + 0.95 Re^{1/2} Pr^{1/3} \quad , \quad Pr \geq 1 \quad ,
\end{aligned} \tag{31a}$$

where C_d is an input constant depending on the identity of the discontinuous liquid.

For $Re > 50$,

$$\begin{aligned}
Nu_d &= \frac{2}{C_d} + 0.00375 Pe_d \left(1 + \frac{\mu_d}{\mu_c}\right) \quad , \quad \text{and} \\
Nu_c &= 2 + 1.13 Pe_c^{1/2} \left| 1 - 1.43/Re^{1/2} \right| \quad ,
\end{aligned} \tag{31b}$$

where $Pe = \frac{|\vec{v}_c - \vec{v}_d| d_d}{\zeta}$, the Peclet number,

μ is the viscosity, and

ζ is the thermal diffusivity.

A special case is given for particles and continuous liquid 1 where additional turbulent heat transfer is taken into account. Both components are in the same velocity field, but do not have the same turbulent velocity fluctuations. Another special case occurs between liquid droplets when the vapor is in the continuous phase. Both liquid droplets exchange heat by direct contact during collision and by radiation. A third special case corresponds to film boiling. In case of the contact of two liquids, a stable film exists if the difference between the interface temperature and the liquid 2 saturation temperature is above the Leidenfrost point. The heat-transfer coefficient is then based on a combination of the convective and radiative Nusselt number inside the vapor film.²³ Heat transfer coefficients are calculated explicitly and are not changed during the heat- and mass-transfer calculations.

e. Momentum-Exchange Functions. The standard AFDM modeling uses Eq. (22) as the form for the momentum-exchange coefficients. The quantity $a_{qq'}$ represents a laminar term, and $b_{qq'}$ is part of a turbulent term. The laminar term is only a function of the viscosity, the interfacial area, and the fluid-sphere radius of the discontinuous phase. The turbulent term is more complex and includes a drag coefficient. In case of the drag between the discontinuous and the continuous fields, $b_{qq'}$ is calculated using a drag similarity hypothesis.²⁴ Hereby, a model is implemented that uses fluid spheres similarly to the model for the surface area source and sink terms. For modest velocity differences, the model calculates a mixture viscosity using data from both the continuous and discontinuous phases. The Reynolds number of the fluid spheres is based on this viscosity. The influence of distortion of the spheres and of the volume fraction on the drag coefficient is accounted for by introducing terms that compare surface tension forces to gravity forces and those that are functions of the volume fractions.

The momentum-exchange coefficients between two discontinuous components or a discontinuous component and the structure do not possess a laminar term, and their drag coefficient is assumed to be constant. However, if film boiling is indicated, the momentum-exchange coefficient between the vapor and the discontinuous liquid is increased to model at least a part of the vapor phase existing as a blanket around the liquid spheres.

f. Intracell Updates for Heat and Mass Transfer. Mass transfer between components is evaluated using a two-step algorithm in AFDM. First, the multicomponent vaporization and condensation rates are determined. For two-phase situations, these rates are calculated simultaneously with the intracell liquid and vapor heat-transfer rates. Second, melting and freezing rates are determined based on the departure from equilibrium resulting from the heat-transfer calculation.

Two different models are used depending on the presence or absence of vapor in a cell. For a two-phase cell, interfaces exist between liquid and vapor, and a total heat flux balance can be calculated at the interfaces. In the present code, mass transfer is only driven thermally, and no limitations exist because of diffusion processes. Mass-transfer rates are determined by summing the liquid and vapor energy equations and then using the fact that overall energy conservation can be maintained if all the heat- and

mass-transfer sources are summed to zero for each material (including both liquid and vapor components). This gives a mass-transfer rate of the form

$$\dot{r}_{GLm} = \frac{\phi_{Lm} + \phi_{Gm} + \phi_{S,Gm} + \phi_{P,Gm} + \phi_{homo,m}}{H(\dot{r}_{GLm})(i_{Gm} - i_{Con,Gm}) + H(-\dot{r}_{GLm})(i_{Vap,Gm} - i_{Lm})} \quad (32)$$

where

$$\begin{aligned} \phi_{Lm} &= h_{Lm} a_{GLm} (T_{Sat,Gm} - T_{Lm}) \quad , \\ \phi_{Gm} &= h_{GLm} a_{GLm} (T_{Sat,Gm} - T_G) \quad , \\ \phi_{S,Gm} &= Y_{Gm} a_{GS} (h_{SG} + h_{GS}) H(T_{Sat,Gm} - T_S^l) (T_{Sat,Gm} - T_S) \quad , \\ \phi_{P,Gm} &= Y_{Gm} a_{GP} (h_{PG} + h_{GP}) H(T_{Sat,Gm} - T_P^l) (T_{Sat,Gm} - T_P) \quad , \text{ and} \\ \phi_{homo,m} &= A_m^{min} (T_{Sat,Gm} - T_G, \Delta T_h) (T_{Sat,Gm} - T_G) H(T_{Sat,Gm} - T_G) \quad . \end{aligned}$$

In Eq. (32), the difference between the interfacial enthalpy and the bulk enthalpy is included in the effective heat of vaporization. The mass-transfer rate is then back-substituted into the energy conservation equations. The equations are solved by identifying two types of variables: sensitive and less sensitive. The sensitive variables are T_{L1} , T_{L2} , T_G , $\bar{p}_{G1}/\bar{p}_{L1}$, and $\bar{p}_{G2}/\bar{p}_{L2}$. The less sensitive variables are T_S and T_P . The sensitive variables are updated implicitly with a multivariate Newton-Raphson procedure. The less sensitive variables are updated explicitly with limiters on the heat-transfer coefficient to avoid overshoots. The main difficulty with this procedure is the apparent tendency of the Jacobian matrix in the Newton-Raphson iteration to become singular when the products of the heat-transfer coefficients times the interfacial areas are much larger than the liquid thermal inertia. At these points, which component vaporizes and which component condenses appear to become indeterminate. These situations are resolved by limiting those interfacial areas that can be anticipated to yield unrealistic transfer rates.

The method is different for a single-phase cell where no liquid-vapor interfacial heat flux can be calculated. In such a case, the heat-transfer rates between the two liquid components, the particle field, and the structure are calculated implicitly by solving a 4 x 4 system of linear equations. Mass transfer is then only required to initialize a fictitious vapor volume used for numerical convenience. This is determined by using the departure from saturation conditions resulting from the heat-transfer calculation as a driving source in the energy conservation equations.

The rate of melting/freezing is obtained by an equilibrium model. Using the updated intracell energies, the freezing rate is proportional to the difference between the liquidus energy and the energy of liquid 1. The melting rate is proportional to the difference between the particle energy and the solidus energy. In case of freezing, the remaining liquid 1 internal energy assumes the liquidus energy, and the particle energy is calculated to ensure energy conservation inside the liquid 1-particle system. Similarly, in case of melting, the remaining particles have the solidus energy.

g. Update of Velocities and Interfacial Areas Based on Mass Transfer.

The heat- and mass-transfer models solve the conservation equations coupled with the EOS, as necessary. The final results are the densities and internal energies for the cell components. To maintain consistency with the temperatures, an inverse EOS call is made at this point.

Next, the axial and radial velocities are updated, as were the densities and internal energies by equating the time rate of change in momentum to the right side of the momentum equations. In other words, we solve

$$\frac{\partial(\bar{\rho}_q \vec{v}_q)}{\partial t} = - \sum_q \Gamma_{qq'} \left[H(\Gamma_{qq'}) \vec{v}_q + H(-\Gamma_{qq'}) \vec{v}_{q'} \right] ,$$

where the two net Γ s are given by

$$\Gamma_{31} = -\Gamma_{13} = (\tilde{\bar{\rho}}_p^n + \tilde{\bar{\rho}}_{L1}^n - \bar{\rho}_p^n - \bar{\rho}_{L1}^n)/\Delta t , \quad \text{and}$$

$$\Gamma_{32} = -\Gamma_{23} = (\tilde{\bar{\rho}}_{L2}^n - \bar{\rho}_{L2}^n)/\Delta t , \quad \text{and}$$

with the three momentum densities defined by

$$\bar{\rho}_1 = \bar{\rho}_p + \bar{\rho}_{L1} ,$$

$$\bar{\rho}_2 = \bar{\rho}_{L2} , \quad \text{and}$$

$$\bar{\rho}_3 = \bar{\rho}_{G1} + \bar{\rho}_{G2} + \bar{\rho}_{G3} .$$

Finally, the mass-transfer rates provide the data to update the convectible interfacial areas a second time. All surface areas are functions of the volume fractions. Therefore, the change in volume fractions has to be accounted for in the area updates. If new volume fractions are generated by phase transitions, initial surface areas and initial momentum coupling coefficients are associated with them.

C. Step 2: Estimation of End-of-Time-Step Values

This step is an integration of the differential equations with the right sides set to zero, the convective terms treated explicitly, and the interfacial heating terms ignored. The objective is to initialize the pressure iteration (Step 3) with end-of-time-step estimates for all the field variables. For example, each mass conservation equation is evaluated using

$$\begin{aligned} \bar{\rho}_{m,ij}^{n+1} = & \bar{\rho}_{m,ij}^n - \Delta t \left\{ \left[\langle \bar{\rho}_m \tilde{v}_q \rangle_{\theta+} - \langle \bar{\rho}_m \tilde{v}_q \rangle_{\theta-} \right] / \Delta z_j \right. \\ & \left. + \left[\langle \bar{\rho}_m \tilde{r} \tilde{u}_q \rangle_{\lambda+} - \langle \bar{\rho}_m \tilde{r} \tilde{u}_q \rangle_{\lambda-} \right] / r_i \Delta r_i \right\} , \end{aligned} \quad (34)$$

where $\theta+ = i, j + \frac{1}{2}$, $\theta- = i, j - \frac{1}{2}$,
 $\lambda+ = i + \frac{1}{2}, j$, $\lambda- = i - \frac{1}{2}, j$,
 i is the radial mesh index, and
 j is the axial mesh index.

The axial and radial velocity components are denoted by v and u , respectively. The $\langle \rangle$ notation indicates a variation of donor-cell differencing. In the axial direction, the defining expressions to convect a quantity, ψ , by a velocity, v , at the cell boundary, $\theta+$, are

$$\begin{aligned} \langle \psi v \rangle_{\theta+} = & \left[\psi_{ij} + \frac{\Delta z_j}{2} \left(\frac{\partial \psi}{\partial z} \right)_{ij} \right] v_{\theta+} - \frac{1}{2} \left(\frac{\partial \psi}{\partial z} \right)_{ij} v_{\theta+}^2 \Delta t , \quad v_{\theta+} \geq 0 , \quad \text{and} \\ \langle \psi v \rangle_{\theta+} = & \left[\psi_{i,j+1} - \frac{\Delta z_{j+1}}{2} \left(\frac{\partial \psi}{\partial z} \right)_{i,j+1} \right] v_{\theta+} - \frac{1}{2} \left(\frac{\partial \psi}{\partial z} \right)_{i,j+1} v_{\theta+}^2 \Delta t , \quad v_{\theta+} < 0 . \end{aligned} \quad (35)$$

The slopes $\partial\psi/\partial z$ are defined as either the minimum of three expressions or as zero according to

$$\left(\frac{\partial\psi}{\partial z}\right)_{ij} = \text{sign}\left(\frac{\partial\psi}{\partial z}\right)_{1,ij} \min\left\{\left|\left(\frac{\partial\psi}{\partial z}\right)_{1,ij}\right|, \left|\left(\frac{\partial\psi}{\partial z}\right)_{2,ij}\right|, \left|\left(\frac{\partial\psi}{\partial z}\right)_{3,ij}\right|\right\} ,$$

if $\text{sign}\left(\frac{\partial\psi}{\partial z}\right)_{2,ij} = \text{sign}\left(\frac{\partial\psi}{\partial z}\right)_{3,ij}$, and

$$\left(\frac{\partial\psi}{\partial z}\right)_{ij} = 0, \quad \text{if } \text{sign}\left(\frac{\partial\psi}{\partial z}\right)_{2,ij} \neq \text{sign}\left(\frac{\partial\psi}{\partial z}\right)_{3,ij} , \quad (36)$$

$$\text{where } \left(\frac{\partial\psi}{\partial z}\right)_{1,ij} = \frac{\psi_{i,j+1} - \psi_{ij}}{\Delta z_{j+1} + \Delta z_j} + \frac{\psi_{ij} - \psi_{i,j-1}}{\Delta z_j + \Delta z_{j-1}} ,$$

$$\left(\frac{\partial\psi}{\partial z}\right)_{2,ij} = \frac{2(\psi_{i,j+1} - \psi_{ij})}{\Delta z_j} , \quad \left(\frac{\partial\psi}{\partial z}\right)_{3,ij} = \frac{2(\psi_{ij} - \psi_{i,j-1})}{\Delta z_j} .$$

This method of differencing has second-order accuracy (at least for equally spaced cells in one dimension) when the slopes are given by $(\partial\psi/\partial z)_{1,ij}$. The limiters $(\partial\psi/\partial z)_{2,ij}$ and $(\partial\psi/\partial z)_{3,ij}$ prevent oscillations and overshoots when the gradients become too steep. At extrema, when $\partial\psi/\partial z$ is zero, Eq. (35) reduces to a first-order donor-cell approach. A first-order donor-cell approximation can also be obtained with the donor compiler option. The radial terms in Eq. (34) are evaluated similarly with ru replacing v and with a radial area coordinate replacing z in Eq. (35).

Three observations are required on the integration of the energy equations. First, terms involving $(\partial\alpha/\partial t)$ are evaluated using $\bar{\rho}_m^{n+1}$ obtained from Eq. (34). Second, terms such as $\langle \bar{\rho}_m e_r v_q \rangle_{\theta+}$ are evaluated assuming

$$\langle \bar{\rho}_m e_r v_q \rangle_{\theta+} = \langle \bar{\rho}_m v_q \rangle_{\theta+} \langle e_r \rangle_{\theta+} . \quad (37)$$

The first term on the right side of Eq. (37) is evaluated as in the mass conservation equation. A term such as $\langle \psi \rangle_{\theta+}$ is determined from

$$\langle \psi \rangle_{\theta+} = \langle \psi v \rangle_{\theta+} / v_{\theta+} . \quad (38)$$

Essentially, one of the velocities is factored out of Eq. (35). The prescription of Eq. (37) allows the nonlinearities affecting mass transport to appear in the energy transport terms. Third, in the liquid-energy equations, the convection of volume fractions is handled similarly to the convection of energy. A typical term is

$$\langle \alpha_m v_q \rangle_{\theta+} = \langle \bar{\rho}_m v_q \rangle_{\theta+} \langle \frac{1}{\rho_m} \rangle_{\theta+} \quad (39)$$

After obtaining the temperatures from an EOS inversion, the remaining Step 2 task is the evaluation of the momentum equation. Because of the space required, a complete discussion is in Vol. V. Five topics that seem important enough to mention here are the treatment of convection, momentum cell averaging, the virtual mass term, interfield drag, and the procedure to calculate estimated velocities.

The evaluation of the convective terms in the momentum equation follows the same philosophy used in the internal energy equations. The momentum terms $\langle \bar{\rho} v \rangle$ or $\langle \bar{\rho} u \rangle$ are evaluated as in Eq. (34), summed over the momentum field, and then multiplied by a donor-cell velocity. For example, the convective term in the axial momentum equation is differenced according to

$$\begin{aligned} \frac{1}{r} \frac{\partial}{\partial r} (\bar{\rho}_q v_q r u_q) + \frac{\partial}{\partial z} (\bar{\rho}_q v_q^2) = & \frac{1}{r_i \Delta r_i} \left[\langle \tilde{\rho}_q^n r \tilde{u}_q^n \rangle_{i+\frac{1}{2}, j+\frac{1}{2}} \langle \tilde{v}_q^n \rangle_{i+\frac{1}{2}, j+\frac{1}{2}} \right. \\ & - \left. \langle \tilde{\rho}_q^n r \tilde{u}_q^n \rangle_{i-\frac{1}{2}, j+\frac{1}{2}} \langle \tilde{v}_q^n \rangle_{i-\frac{1}{2}, j+\frac{1}{2}} \right] + \frac{1}{\Delta z_{j+\frac{1}{2}}} \left[\langle \tilde{\rho}_q^n \tilde{v}_q^n \rangle_{i, j+1} \langle \tilde{v}_q^n \rangle_{i, j+1} \right. \\ & - \left. \langle \tilde{\rho}_q^n \tilde{v}_q^n \rangle_{i, j} \langle \tilde{v}_q^n \rangle_{i, j} \right] \end{aligned} \quad (40)$$

As the subscripts in Eq. (40) indicate, averaging considerations are required to evaluate the momentum equation because of the staggered mesh. The following logic is used. All the terms in Eq. (34) are placed on the left side of the equations, and the result is equated to $D_{m,ij}$. Similar terms are defined for the momentum cells. In the axial direction,

$$\begin{aligned}
D_{m,\theta+} = & \bar{\rho}_{m,\theta+}^{n+1} - \bar{\rho}_{m,\theta+}^n + \frac{\Delta t}{r_i \Delta r_i} \left[\langle \bar{\rho}_m^n \tilde{r} \tilde{u}_q^n \rangle_{i+\frac{1}{2},j+\frac{1}{2}} - \langle \bar{\rho}_m^n \tilde{r} \tilde{u}_q^n \rangle_{i-\frac{1}{2},j+\frac{1}{2}} \right] \\
& + \frac{\Delta t}{\Delta z_{j+\frac{1}{2}}} \left[\langle \bar{\rho}_m^n \tilde{v}_q^n \rangle_{i,j+1} - \langle \bar{\rho}_m^n \tilde{v}_q^n \rangle_{i,j} \right] .
\end{aligned} \tag{41}$$

Because $D_{m,\theta+}$ should be zero, the objective is to equate $D_{m,\theta+}$ to a combination of $D_{m,i,j}$ and $D_{m,i,j+1}$ by defining appropriate averages. The most important result is that a cell-centered quantity, ψ_{ij} , should be averaged according to

$$\psi_{\theta+} = (\psi_{ij} V_{ij} + \psi_{i,j+1} V_{i,j+1}) / 2V_{\theta+} , \text{ in the axial direction, and} \tag{42}$$

$$\psi_{\lambda+} = (\psi_{ij} V_{ij} + \psi_{i+1,j} V_{i+1,j}) / 2V_{\lambda+} , \text{ in the radial direction,} \tag{43}$$

where V is a cell volume, and the momentum cell volumes, $V_{\theta+}$ and $V_{\lambda+}$, are obtained from the distance between cell centers.

The virtual mass terms were given in Eqs. (6) and (7). The coefficient C_G is defined for a momentum cell by

$$\begin{aligned}
C_G &= 0 \quad \text{for single-phase liquid flow, or } \alpha_{G,f} < 0 , \\
C_G &= \frac{1}{2} \frac{1 + 2\alpha_{G,f}}{1 - \alpha_{G,f}} \quad \text{for bubbly flow, or } 0 \leq \alpha_{G,f} < \alpha_{BFR} , \\
C_G &= 3.3 \quad \text{for nonbubbly liquid-continuous flow, or } \alpha_{BFR} \leq \alpha_{G,f} < \alpha_{CC} , \\
C_G &= 3.3 \left[\frac{\alpha_{CD} - \alpha_{G,f}}{\alpha_{CD} - \alpha_{CC}} \right]^2 \quad \text{for a transition regime, or } \alpha_{CC} \leq \alpha_{G,f} < \alpha_{CD} , \text{ and} \\
C_G &= 0 \quad \text{for vapor-continuous flow, or } \alpha_{CD} \leq \alpha_{G,f} \leq 1.0 ,
\end{aligned} \tag{44}$$

where $\alpha_{G,f} = \alpha_G / (1 - \alpha_S)$,

α_{BFR} = the cutoff for bubbly flow,

α_{CC} = the lower limit for cellular flow, and

α_{CD} = the upper limit for cellular flow.

In the KQOM1 model, $\alpha_{BFR} = 0.3$, $\alpha_{CC} = 0.5$, and $\alpha_{CD} = 0.7$. In the KQOM2 model, these are calculated and/or input parameters. The volume fractions used in Eq. (44) are those obtained using $\bar{\rho}_m^{n+1}$.

The treatment of the velocities in interfield drag deserves mention. If the SIMMER-II prescription is followed, these terms should be evaluated using

$$K_{qq'} \vec{v}_{qq'} = [a_{qq'} + b_{qq'} |\vec{v}_{q'}^n - \vec{v}_q^n|] (\vec{v}_{q'}^{n+1} - \vec{v}_q^{n+1}) \quad (45)$$

This will result in potential problems if $\vec{v}_{q'}^n \approx \vec{v}_q^n$. In Step 2 of AFDM, a second expression is evaluated using

$$K_{qq'} \vec{v}_{qq'} = [a_{qq'} + b_{qq'} |\vec{v}_{qq'}|] \vec{v}_{qq'} \quad (46)$$

where $\vec{v}_{qq'} = (\vec{v}_{q'}^{n+1} + \vec{v}_{q'}^n - \vec{v}_q^{n+1} - \vec{v}_q^n)/2$.

Equation (46) requires an iteration to estimate end-of-time-step velocities but is more stable under discontinuities in drag caused by changing topologies. Because Eq. (46) gives problems if $b_{qq'}^{n+1} \gg b_{qq'}^n$, Eq. (45) or (46) is used, depending on which expression gives the largest diagonal coefficient to the vapor equation in the set of three equations required to solve for the velocity at each interface.

Calculation of velocities and velocity derivatives with respect to pressure is the final operation in Step 2. For this calculation, all cell-centered coefficients must be space-averaged and, when desirable, updated based on estimated convection of mass. For example, we assume

$$\bar{b}_{qq'}^n = b_{qq'}^n \left(\frac{\bar{\rho}_q^{n+1} \bar{\rho}_{q'}^{n+1}}{\bar{\rho}_q^n \bar{\rho}_{q'}^n} \right) \quad (47)$$

Then, because Eq. (46) means the equations are nonlinear, a multivariate Newton-Raphson iteration is set up. Convergence of this iteration gives the velocities. Finally, because the coefficient matrix in this iteration consists of velocity derivatives, the required $\partial \vec{v}_q / \partial p$ can be obtained by simply changing the right side of the equation set.

D. Step 3: The Pressure Iteration

The pressure iteration in the SIMMER-II code attempted to obtain consistent velocities and pressures that reduced the error to near zero in the overall liquid continuity equation (for single-phase cells) or the overall vapor continuity equation (for two-phase cells) assuming that derivatives in density with respect to pressure were constant. This approach resulted in inaccuracies in some situations requiring both short time steps and pseudo-single-phase compressibilities for some two-phase cells, as well as giving spurious pressure spikes and problems in vapor convection at two-phase/single-phase boundaries.

The AFDM approach is designed to eliminate these problems by forcing consistency between end-of-time-step pressures and the EOS. A cost/benefit tradeoff does exist, however, between variables that are extrapolated at the beginning of the pressure iteration and then reevaluated using converged velocities and pressures, compared to variables whose errors in their associated conservation equations are reduced to near zero by converging with the pressure and velocity evaluation.

The conservation relationships chosen to be reduced to zero are those describing $(\bar{\rho}_p + \bar{\rho}_{L1})$, $\bar{\rho}_{L2}$, $\bar{\rho}_G$, and e_G . The reasons for the selection of these relationships are as follows:

(a) The overall vapor density, $\bar{\rho}_G = \bar{\rho}_{g1} + \bar{\rho}_{g2} + \bar{\rho}_{g3}$, is crucial to the EOS and is known to affect the pressure iteration results.

(b) The overall liquid density plays a similar role. However, because the properties of material 1 may significantly differ from those of material 2, obtaining the change in liquid composition also is important to the final pressure. The SIMMER-II code had significant problems with fuel flowing into an all-sodium cell or vice versa. These two liquid densities are consequently converged independently.

(c) The pressure-volume work term in the vapor internal energy equation was identified as leading to instability in SIMMER-II. The AFDM approach is to converge a modified vapor energy equation that includes the work term, but maintains energy convection as computed in Step 2.

(e) Apparently, the change in vapor composition was adequately treated in SIMMER-II by evaluations that are external to the pressure iteration. This is also the assumption made in AFDM.

In addition, when SESAME is operational, the liquid internal energy has a density dependence. Numerical tests demonstrated that a reasonable approach was to assume that the Step 2 estimate of the internal energy did not change and to accommodate the EOS by adjusting the liquid temperature. Consequently, the mathematical expressions providing residual errors that are to be reduced to zero in the AFDM pressure iteration are

(a) the error in pressure given by

$$\epsilon_{ij} = f(\alpha_{S,ij}, \tilde{\rho}_{2,ij}^{n+1}, \dots, \tilde{\rho}_{7,ij}^{n+1}, \tilde{T}_{2,ij}^{n+1}, \dots, \tilde{T}_{5,ij}^{n+1}) - \tilde{p}_{ij}^{n+1} \quad (48)$$

(b) the error in mass conservation for each momentum field given by

$$\begin{aligned} D_{q,ij} = & [\tilde{\rho}_{q,ij}^{n+1} - \tilde{\rho}_{q,ij}^n] / \Delta t + [\langle \tilde{\rho}_q^{n+1} \tilde{v}_q^{n+1} \rangle_{\theta+} - \langle \tilde{\rho}_q^n \tilde{v}_q^n \rangle_{\theta-}] / \Delta z_j \\ & + [\langle \tilde{\rho}_q^n \tilde{u}_q^{n+1} \rangle_{\lambda+} - \langle \tilde{\rho}_q^n \tilde{u}_q^{n+1} \rangle_{\lambda-}] / r_i \Delta r_i \quad (49) \end{aligned}$$

(c) the error in the vapor internal energy given by

$$\begin{aligned} D_{eG,ij} = & \frac{(\tilde{\rho}_{G,ij}^{n+1})_o \tilde{e}_{G,ij}^{n+1} - \tilde{\rho}_{G,ij}^n \tilde{e}_{G,ij}^n}{\Delta t} + \frac{\langle \tilde{\rho}_G^{n+1} \tilde{e}_G^{n+1} \tilde{v}_G^{n+1} \rangle_{\theta+} - \langle \tilde{\rho}_G^n \tilde{e}_G^n \tilde{v}_G^n \rangle_{\theta-}}{\Delta z_j} \\ & + (\langle \tilde{\rho}_G^n \tilde{e}_G^n \tilde{u}_G^{n+1} \rangle_{\lambda+} - \langle \tilde{\rho}_G^n \tilde{e}_G^n \tilde{u}_G^{n+1} \rangle_{\lambda-}) / r_i \Delta r_i \\ & + \tilde{p}_{ij}^{n+1} (\tilde{\alpha}_{G,ij}^{n+1} - \tilde{\alpha}_{G,ij}^n) / \Delta t + \tilde{p}_{ij}^{n+1} [\langle \tilde{\alpha}_G^{n+1} \tilde{v}_G^{n+1} \rangle_{\theta+} - \langle \tilde{\alpha}_G^n \tilde{v}_G^n \rangle_{\theta-}] / \Delta z_j \quad (50) \\ & + \tilde{p}_{ij}^{n+1} [\langle \tilde{\alpha}_G^n \tilde{u}_G^{n+1} \rangle_{\lambda+} - \langle \tilde{\alpha}_G^n \tilde{u}_G^{n+1} \rangle_{\lambda-}] / r_i \Delta r_i \quad , \quad \text{and} \end{aligned}$$

(d) the relationship for constant liquid/particle internal energies,

$$D_{e_r,ij} = \tilde{e}_{r,ij}^{n+1} - (\tilde{e}_{r,ij}^{n+1})_o \quad (51)$$

In Eqs. (48) - (51), the numerical subscripts indicate components in order of appearance in Table II. The variables superscripted by $n+1$ change during the iteration, except where an "o" subscript exists implying usage of Step 2 estimates. The $\tilde{e}_{G,ij}^{n+1}$ and $\tilde{e}_{r,ij}^{n+1}$ terms are obtained from the EOS call necessary to evaluate Eq. (48). The EOS call is implied by the "f" function notation.

The objective of the pressure iteration is to reduce each error expressed by Eqs. (48) - (51) to less than a small input value. To accomplish this objective, Eqs. (48) - (51) are each expanded in a Taylor series with the macroscopic densities, the temperatures, and the cell pressure being the independent variables. The resulting expressions are

(a) the expansion of the EOS,

$$\epsilon_{ij} + \frac{\partial \epsilon_{ij}}{\partial p_{ij}} \Delta p_{ij} + \sum_{q=1}^3 \frac{\partial \epsilon_{ij}}{\partial \bar{\rho}_{q,ij}} \Delta \bar{\rho}_{q,ij} + \sum_{r=2}^5 \frac{\partial \epsilon_{ij}}{\partial T_{r,ij}} \Delta T_{r,ij} = 0 \quad , \quad (52)$$

(b) the expansion of the mass conservation relationships,

$$\begin{aligned} D_{q,ij} + \frac{\partial D_{q,ij}}{\partial \bar{\rho}_{q,ij}} \Delta \bar{\rho}_{q,ij} + \frac{\partial D_{q,ij}}{\partial p_{ij}} \Delta p_{ij} + \frac{\partial D_{q,ij}}{\partial p_{i+1,j}} \Delta p_{i+1,j} \\ + \frac{\partial D_{q,ij}}{\partial p_{i-1,j}} \Delta p_{i-1,j} + \frac{\partial D_{q,ij}}{\partial p_{i,j+1}} \Delta p_{i,j+1} + \frac{\partial D_{q,ij}}{\partial p_{i,j-1}} \Delta p_{i,j-1} = 0 \quad , \end{aligned} \quad (53)$$

(c) the expansion of the vapor energy equation,

$$\begin{aligned} D_{eG,ij} + \frac{\partial D_{eG,ij}}{\partial e_{G,ij}} \left[\sum_{q=1}^3 \frac{\partial e_{G,ij}}{\partial \bar{\rho}_{q,ij}} \Delta \bar{\rho}_{q,ij} + \sum_{r=2}^5 \frac{\partial e_{G,ij}}{\partial T_{r,ij}} \Delta T_{r,ij} \right] + \sum_{r=2}^5 \frac{\partial D_{eG,ij}}{\partial T_{r,ij}} \Delta T_{r,ij} \\ + \sum_{q=1}^3 \frac{\partial D_{eG,ij}}{\partial \bar{\rho}_{q,ij}} \Delta \bar{\rho}_{q,ij} + \frac{\partial D_{eG,ij}}{\partial p_{ij}} \Delta p_{ij} + \frac{\partial D_{eG,ij}}{\partial p_{i+1,j}} \Delta p_{i+1,j} \\ + \frac{\partial D_{eG,ij}}{\partial p_{i-1,j}} \Delta p_{i-1,j} + \frac{\partial D_{eG,ij}}{\partial p_{i,j+1}} \Delta p_{i,j+1} + \frac{\partial D_{eG,ij}}{\partial p_{i,j-1}} \Delta p_{i,j-1} = 0 \quad , \end{aligned} \quad (54)$$

and (d) the expansion expressing that liquid and particle energies are constant (and neglecting the influence of vapor conditions),

$$D_{e,r,ij} + \sum_{q=1}^2 \frac{\partial D_{e,r,ij}}{\partial \bar{p}_{q,ij}} \Delta \bar{p}_{q,ij} + \sum_{r'=2}^4 \frac{\partial D_{e,r,ij}}{\partial T_{r',ij}} \Delta T_{r',ij} = 0 \quad (55)$$

Equations (52) - (55) are solved using the EOS derivatives, the derivatives from the higher-order differencing expressions, and the constraints that the macroscopic density ratios within a given momentum field are constant and that the velocities depend only on pressure using the velocity derivatives from Step 2. Algebraic manipulation allows Eqs. (52) - (55) to be placed in the form of a matrix equation. The equation is

$$\underline{A}_{ij} \vec{\Delta x}_{ij} = - \bar{B}_{1ij} \Delta p_{i-1,j} - \bar{B}_{2ij} \Delta p_{i+1,j} - \bar{B}_{3ij} \Delta p_{i,j-1} - \bar{B}_{4ij} \Delta p_{i,j+1} - \bar{S}_{ij}, \quad (56)$$

where vector $\vec{\Delta x}_{ij}$ represents $(\Delta p_{ij}, \Delta \bar{p}_{q,ij}, \Delta T_G)^T$. By multiplication of Eq. (56) by $\underline{A}_{ij}^{-1}$, the vector $\vec{\Delta x}_{ij}$ may be represented by five equations. The first equation is an implicit relationship between cell pressure variations and neighboring cell pressure variations. It is obtained using the first row of $\underline{A}_{ij}^{-1}$.

The equations describing pressure changes are solved based on the matrix solution algorithm picked by the user and the code optimization procedure. Once the changes in pressure are known, we can back-substitute into Eqs. (52) - (55) and use the constant density ratios (within a momentum field) to obtain changes in the remaining cell variables. Then new residual errors can be calculated by Eqs. (48) - (51) and another iteration started. This procedure continues until Eqs. (48) - (51) show sufficiently small residuals. When convergence is obtained, we possess the end-of-time-step pressures and estimated velocities to be used for convection in Step 4.

Expressions for the derivatives and other details of Step 3, including special cases and an underrelaxation option, are presented in Vol V.

E. Step 4: Final End-of-Time-Step Values

This step determines final end-of-time-step densities, energies, interfacial areas, and velocities. The mass and energy conservation equations are evaluated using the velocities from Step 3. Initially, the interfacial heating terms are ignored, and the equations are similar to Step 2. For example, the finite difference mass conservation equation now is

$$\begin{aligned} \bar{\rho}_{m,ij}^{n+1} = & \bar{\rho}_{m,ij}^n - \Delta t \left\{ \left[\langle \bar{\rho}_m \tilde{v}_q^{n+1} \rangle_{\theta+} - \langle \bar{\rho}_m \tilde{v}_q^{n+1} \rangle_{\theta-} \right] / \Delta z_j \right. \\ & \left. + \left[\langle \bar{\rho}_m r \tilde{u}_q^{n+1} \rangle_{\lambda+} - \langle \bar{\rho}_m r \tilde{u}_q^{n+1} \rangle_{\lambda-} \right] / r_i \Delta r_i \right\} . \end{aligned} \quad (57)$$

Because these are the final expressions for mass and energy convection, arrays are also updated to maintain totals for transport of mass and energy across cell boundaries.

Next, Step 4 convects the interfacial areas. Using the ARCV1 option, the interfacial areas calculated in Step 1 are each assigned to liquid 1, liquid 2, or the vapor and divided by the appropriate density. Then, the differential equation describing convection is

$$\frac{\partial (\bar{\rho}_q a_q^p)}{\partial t} + \sum_{m \in q} \nabla \cdot (\bar{\rho}_m a_q^p \vec{v}_q) = 0 , \quad (58)$$

where a_q^p is the interfacial area per unit mass for momentum field q , and $q = 1$ does not include particles.

Equation (58) is evaluated similarly to the internal energy updates using

$$(a_q^p)_{ij}^{n+1} = \frac{1}{\bar{\rho}_{q,ij}^{n+1}} \left\{ \bar{\rho}_{q,ij}^n (a_q^p)_{ij}^n - \sum_{m \in q} CA_m^{n+1} \right\} , \quad (59)$$

$$\begin{aligned} \text{where } CA_m^{n+1} = & \frac{\Delta t}{\Delta z_j} \left[\langle \bar{\rho}_m \tilde{v}_q^{n+1} \rangle_{\theta+} \langle \tilde{a}_q^p \rangle_{\theta+}^n - \langle \bar{\rho}_m \tilde{v}_q^{n+1} \rangle_{\theta-} \langle \tilde{a}_q^p \rangle_{\theta-}^n \right] \\ & + \frac{\Delta t}{r_i \Delta r_i} \left[\langle \bar{\rho}_m r \tilde{u}_q^{n+1} \rangle_{\lambda+} \langle \tilde{a}_q^p \rangle_{\lambda+}^n - \langle \bar{\rho}_m r \tilde{u}_q^{n+1} \rangle_{\lambda-} \langle \tilde{a}_q^p \rangle_{\lambda-}^n \right] , \end{aligned}$$

and the velocities in such terms as $\langle \tilde{a}_q^p \rangle_{\theta+}^n$ also are those from Step 3. In the ARCV2 option, the velocity associated with the discontinuous phase is used to convect the interfacial area, a_f^c , using a pure donor-cell approach. Because both the incoming and outgoing fluxes need to be specified for each cell interface, the formulas involved are too complex for a meaningful simple summary. A description of the formalism is in Vol. II.

The expressions for the convection of momentum are defined to use the bracketed expressions from Eq. (57). As an example, the convective term in the axial momentum equation is

$$\begin{aligned} \frac{1}{r} \frac{\partial}{\partial r} (\bar{\rho}_q v_q r u_q) + \frac{\partial}{\partial z} (\bar{\rho}_q v_q^2) = \frac{1}{r_i \Delta r_i} & \left[\langle \tilde{\rho}_q^n r \tilde{u}_q^{n+1} \rangle_{i+\frac{1}{2}, j+\frac{1}{2}} \langle \tilde{v}_q^n \rangle_{i+\frac{1}{2}, j+\frac{1}{2}} \right. \\ & - \langle \tilde{\rho}_q^n r \tilde{u}_q^{n+1} \rangle_{i-\frac{1}{2}, j+\frac{1}{2}} \langle \tilde{v}_q^n \rangle_{i-\frac{1}{2}, j+\frac{1}{2}} \left. \right] + \left[\langle \tilde{\rho}_q^n \tilde{v}_q^{n+1} \rangle_{i, j+1} \langle \tilde{v}_q^n \rangle_{i, j+1} \right. \\ & \left. - \langle \tilde{\rho}_q^n \tilde{v}_q^{n+1} \rangle_{i, j} \langle \tilde{v}_q^n \rangle_{i, j} \right] / \Delta z_{j+\frac{1}{2}} . \end{aligned} \quad (60)$$

The interfield drag term in the momentum equations is evaluated to be fully implicit in the velocity differences, removing the flow-regime effects of the previous time step. Thus, we have

$$K_{qq'} \vec{v}_{qq'} = [a_{qq'} + b_{qq'} |\vec{v}_{qq'}|] \vec{v}_{qq'} , \quad (61)$$

where $\vec{v}_{qq'} = \vec{v}_q^{n+1} - \vec{v}_{q'}^{n+1}$, and the momentum equations are solved by a multivariate Newton-Raphson iteration. In this evaluation, the volume fractions and other averages of cell-centered quantities use the updated densities from Eq. (57).

After final end-of-time-step velocities have been determined, the final internal energies are calculated by the addition of the interfacial energy production terms existing on the left side of Eqs. (8) – (12). For this purpose, interfacial velocities must be defined. These seem arbitrary; fortunately, their choice does not affect energy conservation. The velocity in the virtual mass term $\vec{v}_{GL}$ was believed to be best represented by some liquid velocity because of the inertia in the liquids. Because the virtual mass concept is based on component volumes, $\vec{v}_{GL}$ is defined by the volume-averaged velocity or

$$\vec{v}_{GL} = \frac{\alpha_P + \alpha_{L1}}{\alpha_P + \alpha_{L1} + \alpha_{L2}} \vec{v}_{L1} + \frac{\alpha_{L2}}{\alpha_P + \alpha_{L1} + \alpha_{L2}} \vec{v}_{L2} \quad (62)$$

In the cases of fluid/fluid and fluid/structure drag interactions, the choice was made to interpolate velocities based on momentum-field volume fractions because of the stability this approach gives. Interpolation means

$$\vec{v}_{qq'} = \frac{\alpha_q}{\alpha_q + \alpha_{q'}} \vec{v}_{q'} + \frac{\alpha_{q'}}{\alpha_q + \alpha_{q'}} \vec{v}_q \quad (63)$$

$$\vec{v}_{qS} = \frac{\alpha_S}{\alpha_q + \alpha_S} \vec{v}_q \quad (64)$$

The interfield heating terms are then evaluated on a per unit mass basis at each interface for each energy component. The cell-centered energies are updated by adding the four-cell boundary contributions and dividing by two.

The final operation in Step 4 is an inverse of the EOS to obtain the cell temperatures from the internal energies and smear densities.

F. Boundary Conditions and Time-Step Controls

AFDM cannot execute without initial conditions and boundary conditions. Initial conditions are described by the user through input. Appendix A contains an input description. Numerically, AFDM handles boundaries by boundary cells as in SIMMER-II. Boundary condition options are somewhat limited because of the attention in AFDM development given to the interior of the calculational domain.

In the radial direction, both boundaries are represented by a rigid, free-slip condition. This means the normal component of the velocity is zero, and the boundary cells reflect the scalar information from the first real cell such that gradients are zero. In addition, the gradients of the tangential velocity components are zero.

Several user-specified options are available in the axial direction. First, a rigid, free-slip possibility exists as in the radial direction. Second, a user input table can be used to specify boundary cell pressures as a function of time. Scalar quantities and tangential velocities are still

reflected into the boundary cell; however, normal velocities are computed. Third, either axial boundary can be specified to exist at constant composition. This option reflects scalar quantities into the boundary cells at the beginning of the problem. Thereafter, the cell-centered quantities in the boundary cells remain fixed. Normal velocities are calculated, and gradients in tangential velocities are zero. Fourth, a continuative outflow option exists. For this boundary condition, all gradients are set to zero at the beginning of each time step. The dynamics over a time step are then calculated by the standard algorithm. In particular, the pressure difference between the first real cell and the boundary cell that accumulates over a time step will change the normal velocities. Fifth, a user input table can be specified giving each velocity as a function of time. For the normal case (inflow), the boundary cell is assumed to exist at constant composition (the composition of the first real cell at the beginning of the problem). If outflow is specified for any velocity, the scalar quantities in the boundary cell reflect conditions in the first real cell. As with the other options, gradients in tangential velocities are zero.

The AFDM time-step size is selected based on the minimum of six criteria. First, a user-specified initial time step exists. This furnishes an upper limit on the time-step size for an input number of cycles. Second, no time step can be more than twice the size of the previous time step. Third, a velocity Courant condition controlled by user input exists similar to that in SIMMER-II. Fourth, an optimum number of pressure iterations can be selected to minimize the overall calculative effort. If the last time step, Δt^n , requires ITERA pressure iterations, the next time-step size will be permitted to be no larger than

$$\Delta t^{n+1} = \frac{\text{OPTPIT}}{\text{ITERA} + 1} \Delta t^n, \quad (65)$$

where OPTPIT is a user-defined input.

Fifth, the pressure change caused by Step 1 heat- and mass-transfer operations is multiplied by the Step 2 vapor velocity derivative to obtain an estimated vapor velocity. A time-step size is determined so that this estimated velocity is below an input multiple of the Courant condition (default of 10). Sixth, an input maximum time-step size exists valid for the entire problem execution.

Time-step controls based on output edits or the problem termination time were deliberately omitted so that these selections will not change problem reproducibility. Also, an input minimum time-step size exists. A Δt^n selected below this minimum will cause problem termination.

VI. OBSERVATIONS BASED ON AFDM DEVELOPMENT

Volume I of the AFDM documentation has provided a summary of the scope of the AFDM code, indicating the approaches taken to solve the equations for multiphase compressible flow in two dimensions with three velocity fields. Much of the AFDM approach was oriented towards severe LMFBR accidents. Indeed, the initial primary purpose of AFDM was to examine ideas to eliminate observed problems in the SIMMER-II code.

The improvements to SIMMER-II investigated in AFDM are shown in Table I. Although a further assessment program appears desirable to achieve definitive and/or quantitative conclusions, some preliminary observations can be made at this time. In order of the presentation in Table I, these observations are as follows.

1. The use of three velocity fields poses no apparent stability problems. There is significant cost both in terms of the extra constitutive relationships required and in solving the equations. However, the use of three velocity fields does significantly change some phenomena; consequently, the additional effort seems justified.

2. The interface to the SESAME EOS was made operational. However, using SESAME made code-running times increase by a factor of 8 or more compared to the SAEOS. Several changes could reduce this penalty. The use of densities and temperatures as the independent EOS variables resulted in the programming of a time-consuming mechanical equilibrium iteration to obtain cell pressures for the SESAME option. This type of iteration has to be eliminated to perform practical multiphase calculations because of the large number of EOS calls resulting from changing conditions.

3. The geometric topology information was represented to the extent permitted by the limited components available for pool flow. A closer approach to "truth" requires the convection of additional information. A problem with the existing code is the presence of abrupt topology shifts.

Development of an approach to smoothing transitions is desirable, possibly by addressing the question of the time scales involved.

4. The ARCV1 option of convecting interfacial areas seems to work satisfactorily when adjacent cells have the same topology. Abrupt changes in the continuous fluid pose difficulties. Insufficient experience exists on the use of the ARCV2 option.

5. Although a vast increase in modeling detail over SIMMER-II is present, improvements in representing fluid sphere breakup processes and heat-transfer mechanisms are still desirable. The modeling of such phenomena as flashing and film boiling could be given more attention. Also, current models have many input parameters. Additional experimental comparisons are needed.

6. The approach to higher-order differencing used in AFDM does work with multiphase flow. There is a significant computational penalty and some reduction on code robustness. (Programming of the DONOR option is not optimized.) However, calculation of the reactivity in a melting LMFBR code requires information on density and energy gradients near the core boundary that cannot be easily obtained with a first-order donor-cell approach.

7. The use of virtual mass tends to obscure the existence of other problems. However, the use of virtual mass is theoretically appropriate, and the increase in stability obtained with virtual mass in accelerating situations is highly beneficial.

8. The increase in computational effort on a given time step resulting from inclusion of EOS nonlinearities within the pressure iteration is amply justified. However, additional attention to the two-phase/single-phase transition is still required for some problems where large time steps are used.

9. Inclusion of the vapor pressure-volume work term within the pressure iteration appears to have eliminated the instability that this term caused in SIMMER-II.

10. Consistent convection as far as was possible with a staggered mesh eliminated the outstanding SIMMER-II problems in this area. Residual concerns with the staggered mesh exist and give results that are less than fully satisfactory for some idealized problems.

11. Some SIMMER-II problems were eliminated in the integrated AFDM V/C format. Others appeared with different characteristics. The treatment of rapid non-equilibrium simultaneous V/C of two or more materials possessing

significantly different saturation properties, such as boiling points, is a tough problem.

12. The attempt to use vector programming was successful. There is a computational penalty associated with the gather/scatter and vector-merge techniques used, as well as a storage penalty. As more knowledge is acquired, increased efficiency appears possible, particularly if close attention is paid to the characteristics of the algorithm.

In general, AFDM allows the assessment of the SIMMER-II deficiencies that it was designed to investigate. There are, of course, other aspects of the computation of severe LMFBR accidents that are uncertain, had to be ignored in AFDM, and/or still pose residual difficulties. Additional effort will continue to improve the knowledge base, but judgment decisions always will be required for what remains unknown.

REFERENCES

1. J. E. Boudreau, F. H. Harlow, W. H. Reed, and J. F. Barnes, "A Proposal for Computer Investigation of LMFBR Core Meltdown Accidents," Los Alamos Scientific Laboratory report LAUR-74-243 (1974).
2. C. R. Bell, P. B. Bleiweis, J. E. Boudreau, F. R. Parker, and L. L. Smith, "SIMMER-I: An S_n , Implicit, Multifield, Multicomponent, Eulerian, Recriticality Code for LMFBR Disrupted Core Analysis," Los Alamos Scientific Laboratory report LA-NUREG-6467-MS (January 1977).
3. L. L. Smith, Compiler, "SIMMER-II: A Computer Program for LMFBR Disrupted Core Analysis," Los Alamos National Laboratory report LA-7515-M, NUREG/CR-0453, Rev. 1 (1980).
4. M. Ishii, Thermo-fluid Dynamic Theory of Two-Phase Flow, Eyrolles, Paris (1975), Vol. 22.
5. F. Ruel, "AFDM Progress Report," draft, private communication, September 10, 1987.
6. N. I. Kolev, "Transient Three-Phase Three-Component Systems, Part 1: Formulation of the System of Differential Equations," Los Alamos National Laboratory report LA-TR-85-26, translated (from German) by Leo Kanner, Assoc., Redwood City, California (1985).
7. M. Ishii and K. Mishima, "Two-Fluid Model and Hydrodynamic Constitutive Relations," Nuclear Engineering and Design, 82, pp. 107-126 (1984).

8. D. Malnes, "Critical Two-Phase Flow Based on Nonequilibrium Effects," Proceedings of the ASME Winter Annual Meeting, ASME, New York, pp. 11-17 (November-December 1975).
9. H. Bruce Stewart, "Two-Phase Flow: Models and Methods," Journal of Computational Physics, 56, pp. 363-409 (1984).
10. D. R. Liles and W. H. Reed, "A Semi-Implicit Method for Two-Phase Fluid Dynamics," Journal of Computational Physics, 26, pp. 390-407 (1978).
11. Safety Code Development Group, Energy Division, "TRAC-PF1/MOD1: An Advanced Best-Estimate Computer Program for Pressurized Water Thermal-Hydraulic Analysis," Los Alamos National Laboratory report LA-10157-MS, NUREG/CR-3858 (July 1986).
12. J. Michael McGlaun, "Improvements in CSQII: An Improved Numerical Convection Algorithm," Sandia National Laboratories report SAND82-0051 (1982).
13. Bram van Leer, "Towards the Ultimate Conservative Difference Scheme. IV. A New Approach to Numerical Convection," Journal of Computational Physics, 23, pp. 276-299 (1977).
14. E. A. Fischer, personal communication, Kernforschungszentrum Karlsruhe, January 14, 1986.
15. K. S. Holian, Editor, "T-4 Handbook of Material Properties Data Bases, Vol. 1c: Equations of State," Los Alamos National Laboratory report LA-10160-MS (November 1984).
16. A. A. Amsden, T. D. Butler, and F. H. Harlow, "Numerical Study of Downcomer Flow Dynamics," Los Alamos Scientific Laboratory report LA-NUREG-6797-SR (May 1977), pp. 6-14.
17. G. Kocamustafaogullari, I. Y. Chen, and M. Ishii, "Unified Theory for Predicting Maximum Fluid Particle Size for Drops and Bubbles," Argonne National Laboratory report ANL-84-67, NUREG/CR-4028 (1984).
18. S. A. Krzeczowski, "Measurement of Liquid Droplet Disintegration Mechanisms," Int. J. Multiphase Flow, 6, pp. 227-239 (1980).
19. N. Abuaf, B. J. C. Wu, G. A. Zimmer, and P. Saha, "A Study of Nonequilibrium Flashing of Water in a Converging-Diverging Nozzle," Brookhaven National Laboratory report BNL-NUREG-51317, NUREG/CR-1864, Vol. 2 (1984).
20. M. Sevik and S. H. Park, "The Splitting of Drops and Bubbles by Turbulent Fluid Flow," J. Fluid Engng., 95, pp. 53-60 (1973).
21. Y. H. Mori, "Configuration of Gas-Liquid Two-Phase Bubbles in Immiscible Liquid Media," Int. J. Multiphase Flow, 4, pp. 383-396 (1978).

22. S. Sideman, "Direct Contact Heat Transfer Between Immiscible Liquids," in Advances in Chemical Engineering, T. B. Drew et al., Eds. (Academic Press, New York, 1966).
23. F. S. Gunnerson and A. W. Cronenberg, "Film Boiling and Vapor Explosion Phenomena," Nuclear Technology, 49, pp. 380-391 (1980).
24. M. Ishii and N. Zuber, "Drag Coefficient and Relative Velocity in Bubbly, Droplet, or Particulate Flows," AIChE Journal, 25, No. 5, pp. 843-855 (1979).

APPENDIX A

AFDM INPUT DESCRIPTION

The input for AFDM is in a free-format style. The input variables have been divided into classes. Each class has been given an identifier, and each variable in a class has been given a variable identifier. All variables with the exception of the mesh-cell variables have been given a default value.

If CLASS is used as the class identifier, VAR_i is used as the variable identifier, and v_i is used as the value of the variable, then the card format would be

CLASS $VAR_1 v_1, VAR_2 v_2, \dots, VAR_n v_n$

When an ampersand, &, is the last symbol on a card, the card is continued to the next card. The ampersand may not appear between a variable and its value. When VAR_i is an array, the slash, /, is used to terminate the array input. There are three types of array input.

1. $VAR v_1 v_2 \dots v_n /$,
2. $VAR i_1 v_1 i_2 v_2 \dots i_n v_n /$, and
3. $VAR v_1 m_1 v_2 m_2 \dots v_n m_n /$.

Type 1 array input stores each value of the variable into contiguous storages. If not enough values are given to fill the array, only the first n values will be stored.

Type 2 array input stores each value in a specified element. If the value $i_j v_j$ is given, the value v_j will be stored into the i_j element of the array. If any $i_j = 0$, then the i_{j+k} , $k > 0$ are not given, and the values v_{j+l} , $l = 0, 1, 2, \dots$, are stored contiguously following v_{j-1} .

Type 3 array input has two values associated with each value of the array. If the two values v_i and m_i are given, both will be associated with the i element of the array.

If the continuation card is needed for the array type input, the ampersand may be put after any value. For the Type 3 array input, the associated values must not be separated by an ampersand.

I. THE FIRST CARD OF THE INPUT DECK

The first card of the input deck is a START or a RESTART. This card has 80 characters at most and is the title line on film output. On the RESTART card, the last field is N_{DMP} (the number of the dump to use for the restart). If $N_{DMP} > 0$, restart from dump N_{DMP} . If $N_{DMP} \leq 0$, restart from the last dump on the file. The first field is either START (starting a problem) or RESTART (restarting a problem from a dump). One of these cards must be given for every run. All input data may be changed when restarting from a dump. This can be extremely dangerous because the mesh variables are not reinitialized and could lead to some inconsistent relationships between variables.

FORMAT:

- a. START An AFDM problem started from a new set of input
- b. RESTART AFDM is restarted from the last dump (-1).

II. MISCELLANEOUS INPUT

Card ID: MISCELLANEOUS

<u>Variable ID</u>	<u>Description</u>
COURTN	The fraction of the velocity Courant condition used as a time-step control.
GRAVITY	Acceleration constant of gravity in the axial direction acting on vapor and liquid. (+/- = upward/downward acceleration) (m/s^2) (suggested value: -9.8).
MVIT	The maximum number of velocity iterations for which the acceleration of convergence is applied.
MITMAX	The maximum number of matrix solution iterations in subroutine MATSOL (suggested value: 200).
MITERP	The maximum number of pressure iterations for each time step.
OPTPIT	The optimum number of pressure iterations.
ISVITP	Defines the turning point of iteration programming in the routine VITERP. Until this number of iterations has been executed, the iteration is executed over all cells including

<u>Variable ID</u>	<u>Description</u>
--------------------	--------------------

converged cells except for the case where all cells have converged. After this number of iterations has been executed, the iteration is executed only over the cells that have not converged. Thus, by correctly choosing this number, the CPU time of this routine can be reduced. [Default value: 5.]

UNLS3	An array of four underrelaxation constants. Defaults for the SESAME EOS option are 0.4, 0.6, 0.8, 1.0 and for the analytical EOS are 1.0, 1.0, 1.0, 1.0.
-------	--

ISVIT	Same definition as ISVITP except for VITER. [Default value: 5.]
-------	---

The NITSRU and MITCRC input is needed only if the PSOL1 option is selected.

NITSRU	The number of matrix solution iterations in subroutine MATSOL between matrix spectral radius and omega relaxation parameter updates. (Suggested value: 5.)
--------	--

MITCRC	The maximum number of matrix solution iterations in subroutine MATSOL before both row and line inversion solutions are evaluated to determine the line inversion direction that results in the fastest rate of convergence. (Suggested values: 50-500.)
--------	---

IPRCND, NINTV, IPWMTH, and IADPTC input is needed only if the option PSOL2 is selected.

IPRCND	Preconditioning method selection option used in the Conjugate Residual Method and Chebyshev Polynomial Iteration Method. [Default value: 3] = 1, SSOR (symmetric SOR) = 2, SIC (shifted incomplete Crout factorization) = 3, MIC (modified incomplete Crout factorization) = 4, SMIC (shifted modified incomplete factorization) MIC gave the best result in the test case. The differences in the efficiencies of these methods were within about a factor of 2.5. SMIC is equivalent to MIC in its method. SMIC takes more CPU time than MIC to factor the matrix, but it has a potential to reduce the number of iterations if an appropriate weight parameter is used. (Modification of function W is required to modify the weight parameter.)
--------	--

NINTVL	Interval of speed measurement (cycles per time step). After the first cycle, after every NINTVL cycle, and so on, the program checks the speed of each solver. The matrix solver to be used for the next NINTVL cycles then is chosen. The Banded Matrix-Direct Solution Method, Conjugate Residual Method, and Chebyshev Polynomial Iteration Method are the choices of solvers. [Default value: 30 cycles.]
--------	---

Variable ID	Description
-------------	-------------

IPWMTH	<p>The option for the method to estimate the eigenvalue in the Chebyshev Polynomial Iteration Method. The estimated eigenvalue is used to accelerate the iteration process by improving the Chebyshev parameters.</p> <p>= 1, the power method on A (coefficient matrix). The most expensive but most stable method.</p> <p>= 2, the power method on S, where the matrix S is asymptotically related to A. This is the least expensive method, but the estimations are not guaranteed to be correct.</p> <p>= 3, the power method on $\tilde{A}$, where $\tilde{A}$ is asymptotically related to A. The efficiency is lower than option 2, but the method is more stable than 2. The estimate may not be correct when the coefficient matrix is nearly symmetric or skew-symmetric until after a large number of Chebyshev iterations. [Default value: 3.]</p>
--------	--

IADPTC	<p>The interval of evaluation of the Chebyshev parameter during the Chebyshev iteration. As described in IPWMTH option, if IPWMTH = 3 is selected, it is better to choose a large value of IADPTC (that is, > 10) when the coefficient matrix is nearly symmetric or skew-symmetric. [Default value: 20.]</p>
--------	--

Note: IPWMTH and IADPTC influence the efficiency of the Chebyshev Method.

FORMAT: MISCELLANEOUS GRAVITY g COURTN c MITCRC m &
 MITMAX $m_{\max}$ NITSRU n &
 MITERP n_p MVIT m_v OPTPIT n_{opt} &
 UNSL3 1 v_1 2 v_2 3 v_3 4 v_4 /

III. MOMENTUM EXCHANGE FUNCTION INPUT FOR OPTION KQOM1

Card ID: MXC

Variable ID	Description
-------------	-------------

FRICF	Friction factor. Default is 0.005
-------	-----------------------------------

ALPSID	α_S for infinite drag. Default is 0.9
--------	--

CDK(MNVEL + 1)	<p>CDK(1) = $C_{D,L1,L2}$ Liquid 1/liquid 2 drag coefficient</p> <p>CDK(2) = $C_{D,L1,G}$ Liquid 1/vapor drag coefficient</p> <p>CDK(3) = $C_{D,L2,G}$ Liquid 2/vapor drag coefficient</p> <p>CDK(4) = ξ_t Churn-turbulent multiplier</p> <p>Defaults are (0.44, 1.0, 1.0, 0.0)</p>
----------------	---

KLS(MNVEL,3)	Momentum coupling length scales (m). Defaults are
--------------	---

$$\begin{bmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{bmatrix} = \begin{bmatrix} .003 & 1.4 \times 10^{-5} & 2.6 \times 10^{-3} \\ .003 & 1.4 \times 10^{-5} & 2.6 \times 10^{-3} \\ .0003 & 1.4 \times 10^{-5} & 10.00 \end{bmatrix}$$

<u>Variable ID</u>	<u>Description</u>
--------------------	--------------------

XMU(MNMAT)	Viscosities (kg/m-s). Defaults are $(4.3 \times 10^{-3}, 5.3 \times 10^{-3}, 2.0 \times 10^{-5})$.
------------	--

```

FORMAT:  MXC FRIC f ALPSID  $\alpha_S$ , ID &
          CDK 1  $C_{D,L1,L2}$  2  $C_{D,L1,G}$  3  $C_{D,L2,G}$  4  $\xi_t$  / &
          KLS 1  $R_1$  2  $R_2$  3  $R_3$  . . . 9  $R_9$  / &
          XMU 1  $\mu_1$  2  $\mu_2$  3  $\mu_3$  /
  
```

Note: $r_1 = r_{L1} = KLS(1,1)$ = Single-phase/bubbly value
 $r_2 = r_{L2} = KLS(2,1)$ = Single-phase/bubbly value
 $r_3 = r_G = KLS(3,1)$ = Single-phase/bubbly value
 $r_4 = r_{L1} = KLS(1,2)$ = Churn-turbulent value
 $r_5 = r_{L2} = KLS(2,2)$ = Churn-turbulent value
 •
 •
 •
 $r_9 = r_G = KLS(3,3)$ = Dispersed flow value

Alternatively, lines containing CDK and KLS can be omitted, and best-estimate defaults for a fuel-steel pool will be obtained.

IV. MOMENTUM-EXCHANGE COEFFICIENTS INPUT FOR OPTION KQOM2

Card ID: MXC

<u>Variable ID</u>	<u>Default</u>	<u>Description</u>
ALPCC	0.50	The vapor-volume fraction at the transition between churn and cellular flow.
ALPCD	0.65	The vapor-volume fraction at the transition between droplet and cellular flow.
ALPDM	0.8	The maximum volume fraction for bubbles or droplets used to assess the mixture viscosity for the drag, similar to the Reynolds number.
ALPLMP	0.01	The volume fraction of liquid 1 or particles at which C_{PCP} or C_{LCP} start to decrease linearly to zero.
ALPMP	0.95	The volume fraction of particles compared with the sum of particles and liquid, at which the continuous liquid 1 viscosity becomes high.
ALPNC	0.1	The maximum vapor-volume fraction for the noncoalescing bubbly regime.

<u>Variable ID</u>	<u>Default</u>	<u>Description</u>
ALPNF	0.95	The no-flow volume fraction.
ALPPF	0.7	A volume fraction multiplier defining the influence of ALPHAP on the continuous liquid definition.
ALPTC	0.005	The droplet volume fraction below which the momentum coupling to the vapor is increased.
CAM	0.0	The multiplier of the linear variation of the surface area multiplied with the vapor-volume fraction.
CBC	0.2	The multiplier of the particle volume fraction to assess the maximum vapor-volume fraction for bubbly flow.
CCD	1.0	A multiplier on the drag coefficient between the continuous and discontinuous phase.
CCLG	0.2	The minimum fraction of the contact area between continuous liquid and vapor.
CCOB	2.0	A multiplier for the coalescence rate of bubbles.
CCOD	0.01	A multiplier for the coalescence rate of droplets.
CCS	1.0	The multiplier of the velocity term of the momentum-coupling coefficient between the structure and the continuous phase.
CCSM	10^4	The maximum momentum-coupling coefficient between the continuous phase and the wall ($\text{N}\cdot\text{s}/\text{m}^4$).
CDD	1.0	The multiplier of the momentum-exchange coefficient between two discontinuous velocity fields.
CDL	0.44	The drag coefficient of droplets in fully turbulent flow (not used in the current code).
CDLG	0.2	The minimum fraction of the contact area between discontinuous liquid and vapor.
CDS	1.0	The multiplier of the momentum-coupling coefficient between structure and the discontinuous phase.
CFB	5.0	The maximum film-boiling multiplier for the momentum exchange between bubbles and droplets.

<u>Variable ID</u>	<u>Default</u>	<u>Description</u>
CFD	0.5	A multiplier of the equilibrium radius reached by fragmentation of droplets by dynamic forces.
CFL	1.0	A multiplier of the time constant of the droplet radius during flashing.
CFM	0.0	A multiplier of the exponent for the drag coefficient correction factor in cellular flow.
CFS	1.0	A multiplier of the time constant for fragmentation of droplets by dynamic forces.
CFT	1.0	A multiplier of the time constant for fragmentation of bubbles by dynamic forces.
CFV	1.0	A multiplier of the viscosity term for fragmentation by dynamic forces.
CL1P	0.5	The fraction of the common surface of the liquid 1-particle system at $l_{LPC} = 0$, which represents the surface area between liquid 1 and particles.
CLCP	0.2	The fraction of liquid 1 droplet surface that always remains without a solid crust.
CMT	1.0	A multiplier of the liquid 1 melting temperature to define the melting/freezing threshold.
CNC	10.0	A factor to define the gas volume fraction at which the nucleation model fades out.
CNL	0.1	A multiplier of the square of the threshold bubble radius for the noncoalescing bubbly regime.
CNU	0.9	The maximum value of the weight factor defining the influence of nucleation on the bubble surface area.
CPCP	0.2	The fraction of the particle surface area that always remains without a liquid 1 film.
CPL1	0.3	The multiplier for the effective contact between liquid 1 and particles at $l_{LPC} = 1$, i.e., random collision.
CPM	5.0	The ratio of the particle and liquid 1 volume fractions at which droplet size becomes zero.
CPP	0.3	A multiplier of the effective contact area between discontinuous components at random collision.
CPV	1.0	A multiplier of the linear dependence of the weight factor for the combination of persisting and collision contact.

<u>Variable ID</u>	<u>Default</u>	<u>Description</u>
CPVM	0.2	The lower limit of the weight factor for the combination of persisting and collision contact between discontinuous components.
CRG	1.0	A multiplier of the equilibrium surface area reached by turbulence fragmentation.
CRTB	8.0	A multiplier of the exponent of the probability for the coalescence of bubbles.
CRTD	1.0	A multiplier of the exponent of the probability for the coalescence of droplets.
CTHETA	1.0^{+5}	A multiplier of the exponent to assess the number of nucleating bubbles.
CTT	1.0	A multiplier of the time constant for the fragmentation by turbulence.
DROHY	100.0	The density differences to define the limits of the linearized hysteresis at the cellular-droplet regime's transaction (kg/m^3).
DROMIN	10.0	The minimum density difference between continuous and discontinuous components (kg/m^3).
DVRT	0.2	The reference velocity difference for the fragmentation of bubbles by dynamic forces (m/s).
ILPC	0	The indicator for whether the liquid 1-particle contact is based on a collision model, $I_{LPC} = 1$, or on permanent contact, $I_{LPC} = 0$, for continuous vapor cells.
NDROP	1.0^{+7}	The number of newly created droplets at condensation inception per unit of fluid volume (m^{-3}).
NMAX	1.0^{+11}	The maximum number of nucleating bubbles per fluid volume (m^{-3}).
NMIN	1.0^{+5}	The minimum number of nucleating bubbles per fluid volume (m^{-3}).
RMB	1.0^{-6}	The minimum vapor bubble radius (m).
RMD	1.0^{-6}	The minimum droplet radius (m).
RXB	0.1	The maximum bubble radius (m).
RXD	0.1	The maximum droplet radius (m).

<u>Variable ID</u>	<u>Default</u>	<u>Description</u>
TCNUC	1.0 ⁻⁴	Time constant for the nucleation source term of the convectible bubble surface area (s).
THETA0	2.0 ⁻³	Threshold value for the nondimensional temperature difference that defines the departure from saturation.
WECRIT	22.0	The critical Weber number at the onset of droplet flow.
WEFB	10.0	The critical Weber number for the fragmentation of bubbles.
WEFD	13.0	The critical Weber number for the fragmentation of droplets.

FORMAT: All variables are read in with the form VAR_i v_i, where VAR_i is one of the variables and v_i is the value.

V. HEAT-TRANSFER COEFFICIENT INPUT FOR OPTION KQQM1

Card ID: HTC

<u>Variable ID</u>	<u>Description</u>
XICC	Contact coefficient. Default is 10.
HLS(MM MAT)	Droplet/bubble radius for heat transfer in L1, L2, and G, respectively (m). Defaults are 0.001, 0.0001, and 0.0025.

FORMAT: HTC XICC ξ_t HLS 1 r_{L1} 2 r_{L2} 3 r_G /

VI. HEAT-TRANSFER INPUT FOR OPTION KQQM2

Card ID: HTC

<u>Variable ID</u>	<u>Default</u>	<u>Definition</u>
WP	0.2	Thermal boundary-layer coefficient for particles.
WL1	1.0	Conduction boundary-layer coefficient inside L1 when L1 is continuous.
WL1D	0.2	Thermal boundary-layer coefficient for L1 particles.

<u>Variable ID</u>	<u>Default</u>	<u>Definition</u>
WL2D	1.0	Thermal boundary-layer coefficient for L2 droplets.
WG	0.2	Thermal boundary-layer coefficient for vapor bubbles.
SH	0.5	Coefficient that defines an artificial radius around a particle where turbulence affects the heat transfer from the particle.
HS	2.0+4	Default value for heat-transfer coefficient to the structure ($\text{W/m}^2\text{-K}$).
EMISS	0.5	Emissivity of liquid 2.
EMISSP	0.9	Emissivity of vapor.
CSH	0.05	Ratio of the departure from nucleate boiling and the Leidenfrost point. $\text{CSH} = \Delta T_{\text{DNB}} / \Delta T_{\text{min}}$.
EPSIP	0.78	Coefficient used to define the first guess for the Nusselt number in the film-boiling model.
EPSNUT	0.8	Convergence criterion for the total Nusselt number in the film-boiling model.
STEBOL	5.68 ⁻⁸	Stefan-Boltzmann constant ($\text{W/m}^2\text{-K}^4$).
WL2	1.0	Conduction boundary-layer coefficient inside L2 when L2 is continuous.
CMF	0.5	First coefficient defining the Leidenfrost point as a function of the critical temperature of liquid 2.
CMS	0.62	Second coefficient defining the Leidenfrost point as a function of the critical temperature of liquid 2.
CCFB	0.05	Limiter for α^* (when the film-boiling model is turned on).
CLT	0.1	Multiplier on the turbulent equivalent conductivity between L1 and P if L1 is the continuous phase.
CRL	1.0	Multiplier on the radiation heat transfer coefficient between discontinuous L1 and discontinuous L2.

VII. MASS-TRANSFER INPUT

Card ID: MTC

<u>Variable ID</u>	<u>Default</u>	<u>Definition</u>
AM	1.0+3, 1.0+3	Homogeneous condensation coefficient (W/m^3-K^2).
EPSRO	0.1	Convergence parameter for the mass-transfer rate (kg/m^3-s).
EPSTEM	1000.0	Convergence parameter for the energy-transfer rate (J/m^3-s).
LAMCUT	1.0+5	Threshold limiting mass-transfer (V/C) rate (kg/m^3-s).
FRGM	0.5	Fraction of vapor mass that can condense in one iteration.
FTLM	0.9	Fractional change in liquid temperature in one iteration.
FTG	0.5	Fractional change in vapor temperature in one iteration.
DTMPM	10.0	A multiplier for the mass-transfer time-step control.
UNDERL	0.4, 0.6, 0.8, 1.0	An array of four underrelaxation constants.

VIII. HEAT SOURCE INPUT

Card ID: HEATSO

<u>Variable ID</u>	<u>Description</u>
DPOW	Time distribution of power. DPOW is input as N pairs of numbers. The first number of a pair is the power fraction; the second number is the corresponding time.
DAX	Axial distribution of power. DAX is input as M pairs of numbers. The first number of a pair is the power fraction; the second number of the pair is the number of the last axial cell associated with this power fraction.
DRAD	Radial distribution of power. DAX is input as M pairs of numbers. The first number of a pair is the power fraction; the second number of the pair is the number of the last radial cell associated with this power fraction.

<u>Variable ID</u>	<u>Description</u>
F RTP	Component distribution power. F RTP is an array of four numbers. F RTP(1)--distribution of power for the structure F RTP(2)--distribution of power for fluid 1 (particle + liquid 1 + vapor 1) F RTP(3)--distribution of power for the fluid 2 (liquid 2 + vapor 2) F RTP(4)--distribution of power for noncondensable vapor
POW	Total power (W).

FORMAT: HEATSO DPOW dP₁ T₁ dP₂ T₂.....dP_n T_n / &
 DAX dA₁ J₁ dA₂ J₂.....dA_m J_m / &
 DRAD dR₁ l₁ dR₂ l₂.....dR_L l_L / &
 F RTP 0 f₁ f₂ f₃ f₄ / &
 POW P

IX. PLOTTING INPUT

Card ID: PLOT

<u>Variable ID</u>	<u>Description</u>
R	The radius of the viewpoint (m).
HA	The horizontal angle. The origin is the center of the box. $0 \leq HA \leq 360^\circ$ rotated counterclockwise from the positive x-axis. The default is 225° .
VA	The vertical angle. $ VA \leq 90^\circ$ VA < 0 The perspective is viewed from below the origin. VA > 0 The perspective is viewed from above the origin. Default is 15° .
RZA	The ratio of the axial length to the radial length. The default is $RZA = Z_{\max}/r_{\max}$.
RFA	The ratio of the variable being plotted and the radial length. The default is $RFA = V_{\max}/r_{\max}$.
COLOR	The colors to be used in plotting. Colors are not available on microfiche. Color (1) - The color of the side bars. Default is 0.5 (red). Color (2) - The color of the box. Default is 1.5 (yellow). Color (3) - The color of the top of the surface. Default is 2.0 (green). Color (4) - The color of the underside of the surface. Default is 3.5 (magenta).

FORMAT: PLOT R r HA α VA β RZA ρ RFA f COLOR C₁ C₂ C₃ C₄ /

X. PROBLEM NAME INPUT

Card ID: PROBLEM

<u>Variable ID</u>	<u>Description</u>
.	"Name" a 40-character name of the problem

FORMAT: PROBLEM "name"

XI. EDIT INPUT

Card ID: EDIT

<u>Variable ID</u>	<u>Description</u>
PRT	The where-to-print flag. Default is 1. PRT = 1, print only on paper. 2, print only on film. 3, print on film and on paper.
PRTC	The number of cycles between prints. Default is 100.
PPFC	The number of cycles between postprocessor dumps. Default is 100.
DMPC	The number of cycles between dumps. The default is 100.

FORMAT: EDIT PRT i PRTC i_{PRT} PPFC i_{pp} DMPC i_{DMP}

XII. TIME INPUT

Card ID: TIME

<u>Variable ID</u>	<u>Description</u>
TSTART	The real time to be used for the first time step (s).
DTSTART	Δt - the first time-step increment (s).
DTMIN	The minimum time step (s).

<u>Variable ID</u>	<u>Description</u>
DTMAX	The maximum time step (s).
TWFIN	The last (largest) real time for the current run (s).
NDTO	The number of time steps when the time step is kept less than or equal DTSTART.

FORMAT: TIME TSTART t_1 DTSTART Δt_1 DTMIN $\Delta t_{\min}$ DTMAX $\Delta t_{\max}$ TWFIN t_{last} NDTO n

XIII. MESH INPUT

Card ID: MESH

<u>Variable ID</u>	<u>Description</u>
DR	The radial mesh width (m).
DZ	The axial mesh height (m).

FORMAT: MESH DR Δr_1 n_1 Δr_2 n_2 . . . Δr_j n_j / DZ Δz_1 m_1 Δz_2 m_2 . . . Δz_j m_j /

(1) The term n_j is the number of contiguous radial cells dimensioned Δr_j .
 $IB = \sum n_j$.

(2) The term m_j is in the number of contiguous axial cells dimensioned Δz_j .
 $JB = \sum m_j$.

XIV. CELL INPUT

Card ID: CELL

<u>Variable ID</u>	<u>Description</u>
REGION	Definition of the region of cells for the other variables.
ALPHA(m)	Trial values of the volume fractions for component m.
T (r)	Temperature for energy component r (K).
u (q)	Radial velocity for velocity component q (m/s).
v (q)	Axial velocity for velocity component q (m/s).
ASTR	Interfacial area of structure (m^2/m^3).

<u>Variable ID</u>	<u>Description</u>
FAIL	Structure failure flag.
RADL1	Radius of liquid 1 droplets (m).
RADL2	Radius of liquid 2 droplets (m).
RADG	Radius of vapor bubbles (m).
RADP	Radius of the particle (m).
DH	The hydraulic diameter (m).
REGFL	The flow-regime flag. When cellular or dispersed flow is possible, REGFL < 0.5 signals initialization of a liquid-continuous topology.
RHOS	The microscopic density of structure (kg/m^3).
PC	The single-phase cell pressure (Pa).
PG3	The noncondensable vapor pressure (Pa).
HSG	Structure heat-transfer coefficients ($\text{W/m}^2\text{-K}$).
	(m), (r), and (q) are not part of the ID. These indicate that the variables are arrays. <u>REGION</u> must be first.
	m = 1, 4 : m = 1, Structure
	2, Fuel particles
	3, Liquid fuel
	4, Coolant/steel liquid
	r = 1, 5 : r = 1, Structure
	2, Fuel particle 2
	3, Fuel liquid
	4, Coolant/steel liquid
	5, Vapor
	q = 1, 3 : q = 1, Liquid 1 (fuel particle and liquid)
	2, Liquid 2 (coolant/steel)
	3, Vapor

FORMAT: CELL REGION i_l i_u j_l j_u &

ALPHA 1 α_S^i 2 α_P^i 3 α_{L1}^i 4 α_{L2}^i / &

T 1 T_1 2 T_2 . . . 5 T_5 / &

U 1 u_1 2 u_2 3 u_3 / &

V 1 v_1 2 v_2 3 v_3 / &

RADL1 r_{L1} RADL2 r_{L2} RADG r_G RADP r_P ASTR a_S FAIL f

XV. EPSILON INPUT

Card ID: EPSILON

Variable ID	Description
-------------	-------------

MAT	Convergence parameter, ϵ_{MAT} , used for the solvers of the equations to obtain the pressure changes. In MATSOL, ϵ_{MAT} is compared to the Euclidean norm of the pressure changes divided by the Euclidean norm of the pressures. In the Conjugate Residual and Chebyshev Polynomial Iteration methods, the pressure equations can be expressed as $A x = q$, and the convergence criteria as $ B(q - A x) / B q < \epsilon_{MAT}$, where B is the preconditioner. Here, accuracy of the solution depends on both MAT and the condition number of the coefficient matrix. Because the equation is preconditioned, the condition number not only depends on the coefficient matrix but also on the preconditioning method. MAT influences directly the efficiency of the iterative methods. The factor to be considered is that if the solutions of the pressure equations have low accuracy, more pressure iterations are required to converge the pressure iteration. Probably three digits of accuracy is desirable.
-----	---

V	ϵ_V for the u-v velocity iteration
P	ϵ_P for the pressure iteration (Pa).
E	ϵ_E for the pressure iteration (W/m^3).
G	ϵ_G for the pressure iteration ($kg/m^3 \cdot s$).
L1	ϵ_{L1} for the pressure iteration ($kg/m^3 \cdot s$).
L2	ϵ_{L2} for the pressure iteration ($kg/m^3 \cdot s$).
T1	For the KQOM1 option T_1 is the vapor temperature convergence criterion (K).

FORMAT: EPSILON MAT ϵ_{MAT} V ϵ_V P ϵ_P E ϵ_E G ϵ_G L1 ϵ_{L1} L2 ϵ_{L2}

XVI. EOS INPUT

Card ID: EOS

<u>Variable ID</u>	<u>Description</u>
ALPHA0	A vapor volume fraction below which single-phase calculations are performed.
EPSTG	ϵ for the temperature iteration.
CG(m)	Heat capacity of vapor at constant volume (J/kg-K).
CL(m)	Heat capacity of liquid (J/kg-K).
CS(m)	Heat capacity of solid (J/kg-K).
ECRIT(m)	Base energy for noncondensable gases (J/kg).
PSTAR(m)	P^* (Pa).
RHO(r)	Microscopic density (kg/m ³). Four values are required for the structure, particles, and the two liquids.
R(m)	Gas constant of material m (J/kg-K).
TCRIT(m)	Temperature corresponding to ECRIT (K).
TSOL(m)	The solidus temperature (K).
TLIQ(m)	The liquidus temperature (K).
TSTAR(m)	T^* (K).
HFUS(m)	Heat of fusion (J/kg).
CVL(m)	Sonic velocity of liquid (m/s).
WMOLE(m)	The molecular weight.
TSUPM(m)	The superheat for material m (K).
RCGAS	Universal gas constant [default: 8315 (m ³ -Pa)/(kg mole-K)].
EPSQK(m)	Lennard-Jones parameter ϵ/κ (K).
SIGLJ(m)	Lennard-Jones parameter σ (Å).
NATOM(m)	Number of atoms per molecule.
SESFTYP	The type of file containing the SESAME DATA. = 0, direct access 1, sequential

<u>Variable ID</u>	<u>Description</u>
MATERIAL	A table of the SESAME material ID numbers.
SESNMAT	The number of materials requested by MATERIAL.
SESPR	The SESAME material table input print. = yes, print the SESAME tables no, do not print
SESTRP	The type of interpolation to be used on the SESAME tables. = 1, bilinear 2, biquadratic 3, birational
NRTAB	A table linking the seven AFDM densities to the SESAME materials.
SPNDMF	A flag to request the Spinodale calculation from the SESAME material tables. = yes, do the calculation no, do not do the calculation
SESNAM	Name of the input file containing the SESAME data.
NISOT	The number of density points on an isotherm.
UNLPEQ	An array of four underrelaxation constants [defaults: 0.4, 0.6, 0.8, and 1.0].
FORMAT:	EOS ALPHA0 α_0 EPSTG ϵ_{TG} RCGAS R^* & CG 1 CG1 2 CG2 3 CG3 / & CL 1 CL1 2 CL2 3 CL3 / & CS 1 CS1 2 CL2 3 CS3 / & ECRIT 1 eCrit,1 2 eCrit,2 3 eCrit,3 / & PSTAR 1 P_1^* 2 P_2^* 3 P_3^* / & RHO 1 ρ_S 2 ρ_P 3 ρ_{L1} 4 ρ_{L2} / & R 1 R1 2 R2 3 R3 / & TCRIT 1 TCrit,1 2 TCrit,2 3 TCrit,3 / & TSOL 1 TSol,1 2 TSol,2 3 TSol,3 / &

<u>Variable ID</u>	<u>Description</u>
--------------------	--------------------

TLIQ 1 $T_{\text{Liq},1}$ 2 $T_{\text{Liq},2}$ 3 $T_{\text{Liq},3}$ / &

TSTAR 1 T_1^* 2 T_2^* 3 T_3^* / &

HFUS 1 $e_{f,1}$ 2 $e_{f,2}$ 3 $e_{f,3}$ / &

CVL 1 c_1 2 c_2 3 c_3 / &

WMOLE 1 M_1 2 M_2 3 M_3 / &

TSUPM 1 $T_{\text{Sup},1}$ 2 $T_{\text{Sup},2}$ 3 $T_{\text{Sup},3}$ / &

EPSQK 1 $(\epsilon/k)_1$ 2 $(\epsilon/k)_2$ 3 $(\epsilon/k)_3$ / &

SIGLJ 1 σ_1 2 σ_2 3 σ_3 / &

NATOM 1 $n_{A,1}$ 2 $n_{A,2}$ 3 $n_{A,3}$ / &

UNLPEQ 1 v_1 2 v_2 3 v_3 4 v_4 /

The sample problems, Vol. VI, and Appendix H of Vol. VII should be consulted on preparation of input for the SESAME EOS.

XVII. THERMAL PROPERTY INPUT FOR OPTION KQQM1

Card ID: TPPROP

<u>Variable ID</u>	<u>Description</u>
--------------------	--------------------

KPS The thermal conductivity for particles (W/m-K).

KPL1 The thermal conductivity for liquid 1 (W/m-K).

KPL2 The thermal conductivity for liquid 2 (W/m-K).

KPG The thermal conductivity for vapor (W/m-K).

FORMAT: TPPROPKPS k_S KPL1 k_{L1} KPL2 k_{L2} KPG k_G

XVIII. THERMAL PROPERTY INPUT FOR OPTION KQQM2

Card ID: TPPROP

<u>Variable ID</u>	<u>Description</u>
SLNL1] SLFLL1] SLFEL1]- SLEXL1] TCRL1] TSLCL1]	The coefficients for the equation for the surface tension for liquid vapor for liquid 1.
SLNL2] SLFLL2] SLFEL2]- SLEXL2] TCRL2] TSLCL2]	The coefficients for the equation for the surface tension for liquid vapor for liquid 2.
SLLIN] SLLIF]- TSLIR]	<p>The coefficients for the equation for the surface tension for liquid 1-liquid 2.</p> <p>(See Vol. VI, Sec. IV.A, for the equations and units involved in surface tension relationships.)</p>
CKA(n)	<p>The CKA coefficients for the equation $k = C_{KA} + C_{KB}T$ for the thermal conductivity (W/m-K).</p> <p>n = 1, the structure n = 2, the particle n = 3, liquid 1 n = 4, liquid 2 n is not part of the variable ID.</p>
CKB(n)	The CKB coefficients for the equation $k = C_{KA} + C_{KB}T$ for the thermal conductivity (W/m-K ²). See the definition of CKA for the definition of n.
CMUA(n)	The CMA coefficients (kg/m-s) for the viscosity equation $\mu = C_{MA} \exp[C_{MB}/(\max(T_{Liq}, T_L))]$. The "n" represents liquids 1 and 2, respectively.
CMUB(n)	The CMB coefficients for the viscosity equation (K). See the description of CMUA.
CKAG(n)] CKBG(n)] CKCG(n)]	Coefficients to represent the gas thermal conductivity by the equation $k = C_{KAG} + C_{KBT} + C_{KCG}T^2$. The default values are zero. Zero signals a use of the Chapman-Enskog theory for thermal conductivity. The "n" represents fuel vapor, coolant vapor, and noncondensable gas, respectively.

FORMAT: SLNL1 σ_{LN} SLFLL1 σ_{LFL} SLFEL1 σ_{LFE} &
 SLEXL1 σ_{LEX} TCRL1 T_{Crit} TSLCL1 $T_{\sigma LC}$ &
 SLNL2 σ_{LN} SLFLL2 σ_{LFL} SLFEL2 σ_{LFE} &
 SLEXL2 σ_{LEX} TCRL2 T_{Crit} TSLCL2 $T_{\sigma LC}$ &
 SLLIN σ_{IN} SLLIF σ_{IF} TSLIIR $T_{\sigma IR}$ &
 CKA 1 CKAS 2 CKAP 3 CKAL1 4 CKAL2 / &
 CKB 1 CKBS 2 CKBP 3 CKBL1 4 CKBL2 / &
 CMUA 1 CMAL1 2 CMAL2 / &
 CMUB 1 CMBL1 2 CMBL2 / &
 CKAG 1 CKAG1 2 CKAG2 3 CKAG3 / &
 CKBG 1 CKBG1 2 CKBG2 3 CKBG3 / &
 CKCG 1 CKCG1 2 CKCG2 3 CKCG3 /

XIX. BOUNDARY INPUT

Card ID: BOUNDARY

Variable ID	Description
IBOT	Bottom boundary description flag.
ITOP	Top boundary description flag.
	IBOT/ITOP ≤ -2 , pressure vs time $= -1$, constant composition $= 0$, rigid wall $= +1$, continuous outflow $= +2$, velocity vs time
BVAR	Pressure/velocity vs time table

FORMAT: BOUNDARY ITOP i_T BVAR IVF BV_{T1} BT_{T1} BV_{T2} BT_{T2} . . . BV_{Tn} BT_{Tn} / &
 IBOT i_B BVAR IVF BV_{B1} BT_{B1} BV_{B2} BT_{B2} . . . BV_{Bn} BT_{Bn} /

NOTE: BVAR is needed only if ITOP/IBOT = +/- 2. If BVAR is needed, it must immediately follow i_T or i_B . IVF is used only if ITOP/IBOT = 2. If ITOP/IBOT = 2, then a BVAR variable must be given for each velocity field and IVF = 1 for the liquid 1 velocity field, 2 for the liquid 2 velocity field, and 3 for the vapor velocity field. Default is ITOP/IBOT = 0, BVAR = $-\infty$. SI units are used for pressure, velocity, and time.

APPENDIX B

NOMENCLATURE

This is a summary of the nomenclature used for the AFDM program. It includes the nomenclature for Vol. I and the terms for the remaining AFDM volumes. Usages adopted by other AFDM principal authors have been included as much as possible. However, the AFDM effort does involve an international "partnership." Therefore, some of the AFDM volumes can be expected to adopt additional/modified nomenclature.

Variable	Definition
a	Interfacial surface area per unit volume [m^2/m^3]
a^p	Convectible interfacial surface area per unit mass [m^2/kg]
a	Viscous component of the interfield momentum-exchange coefficient [$\text{N-s}/\text{m}^4$]
a	Liquid/vapor velocity ratio [dimensionless]
$[a]$	Three-by-three matrix representing the coefficients used to update the velocities based on mass-transfer results [$\text{kg}/\text{m}^3\text{-s}$]
a_r	Residual surface area in three-phase contact [m^2/m^3]
A	Homogeneous condensation coefficient [$\text{W}/\text{m}^3\text{-K}^2$]
A	Cell radial area [m^2]
$\underline{A}$	Matrix of Jacobian derivatives used in the pressure iteration [variable dimensions]

$\vec{b}$	Right-side vector in the equations to update the velocities based on mass transfer [$\text{kg/m}^2\text{-s}^2$]
b	Turbulent component of the interfield momentum-exchange coefficient [$\text{N-s}^2/\text{m}^5$]
$[B]$	Five-by-five Jacobian matrix used in the "two-phase" heat- and mass-transfer algorithm [variable dimensions]
$[B_S]$	Five-by-five Jacobian matrix used in the "single-phase" heat- and mass-transfer algorithm [variable dimensions]
$\vec{B}_1, \vec{B}_2, \vec{B}_3, \text{ and } \vec{B}_4$	Vectors containing the pressure derivatives of the four conservation relationships used Step 3 of the AFDM algorithm [variable dimensions]
C	User-defined nondimensional or dimensional constant
C'	User-defined nondimensional or dimensional constant
$\vec{C}$	Vector column representing the right sides of the equations used in the "two-phase" heat- and mass-transfer algorithm [variable dimensions]
$\vec{c}$	Right side of the relationship to maintain constant liquid/particle internal energies in Step 3 [J/kg]
c_A	Total molar density [kmol/m^3]
C_D	Drag coefficient [dimensionless]
C_G	Flow-regime-dependent part of the virtual mass coefficient [dimensionless]
c_k	Molar density of vapor species k [kmol/m^3]

c_m	Velocity of sound for density component m [m/s]
c_p	Specific heat at constant pressure (heat capacity) [J/kg-K]
$\vec{c}_S$	Vector column representing the right sides of the equations used in the "single-phase" heat- and mass-transfer algorithm [variable dimensions]
C_t	Input fraction used for the Courant time-step control [dimensionless]
CT_r	Convective term for the internal energy equation [J/m ³]
CV_q	Convective term for the momentum equation [N/m ³]
c_v or c	Specific heat at constant volume (heat capacity) [J/kg-K] (c_v preferred, unless used with other subscripts)
d	Diameter [m]
D	Error in one of the four conservation equations to be eliminated during the pressure iteration [variable dimensions]
D	Diffusion coefficient [m ² /s]
D	Effective energy of vaporization/condensation [J/kg]
$\vec{D}$	Right-side vector used in solving the momentum equations [kg/m ² -s]
D_h or d_h	Hydraulic diameter [m] (D_h preferred)
e	Specific internal energy [J/kg]
E	A factor in the derivative of the homogeneous condensation term [K]
E	The results of an energy summation [J]

e_f	Internal energy change in fusion [J/kg]
e_{lg}	Energy of vaporization [J/kg]
f	Frequency [s^{-1}]
f	Friction factor [dimensionless]
F	View factor (shape factor) [dimensionless]
F	Viscosity function [dimensionless]
F_v	Virtual mass force per unit volume [N/m^3]
F_{12}	View factor between liquid 1 and liquid 2 [dimensionless]
$\bar{g}$	Acceleration of gravity [m/s^2]
G	General dependent variable function [arbitrary dimensions]
G	Invariant acceleration [$+ 9.80 \text{ m/s}^2$]
Gr	Grashof number [$8r_d^3 \rho_G (\rho_L - \rho_G) G / \mu_G^2$] [dimensionless]
h	Heat-transfer coefficient [W/m^2-K]
h'	Heat-transfer coefficient modified to treat transfers between bulk vapor and another energy component [W/m^2-K]
h^+	Heat-transfer coefficient corrected for mass transfer [W/m^2-K]

For the following heat-transfer coefficients, usage without the commas is preferred.

h_{GLm} or $h_{G,Lm}$	Heat-transfer coefficient between vapor and the liquid m/vapor interface [W/m ² -K]
h_{GP} or $h_{G,P}$	Vapor-side heat-transfer coefficient for the particle-vapor interface [W/m ² -K]
h_{GS} or $h_{G,S}$	Vapor-side heat-transfer coefficient for the structure-vapor interface [W/m ² -K]
h_{GP}	Net heat-transfer coefficient between the vapor and the particles [W/m ² -K]
h_{GS}	Net heat-transfer coefficient between the vapor and the structure [W/m ² -K]
h_{LmG} or $h_{Lm,G}$	Heat-transfer coefficient between liquid m and the liquid m/vapor interface [W/m ² -K]
h_{PG} or $h_{P,G}$	Particle-side heat-transfer coefficient for the particle-vapor interface [W/m ² -K]
h_{SG} or $h_{S,G}$	Structure-side heat-transfer coefficient for the structure-vapor interface [W/m ² -K]
h_{lg}	Heat of vaporization [J/kg]
H	Heaviside function [dimensionless]
H	Product of the interfacial area and the heat-transfer coefficient. Used with two energy component subscripts [W/m ³ -K]
$\bar{H}_i$	Derivatives of the vapor energy equation with the vapor mole fraction differentiated with respect to density [W/kg-K]

$\tilde{H}_i^{(m)}$	Component of the [B] matrix containing terms of liquid energy equation m differentiated with respect to independent variable x_i [variable dimensions]
H_i^*	Collection of derivatives of the vapor energy equation excluding the mole fraction derivatives [arbitrary dimensions]
i	The imaginary unit such that $i^2 = -1$
i	Specific enthalpy [J/kg]
I	Integer value [dimensionless]
IH	Interfacial energy production over a time step [J/kg]
IT	FORTTRAN iteration index [dimensionless]
$\bar{J}$	Molar diffusion flux relative to the average molar velocity [kmol/m ² -s]
Ja	Jacob number $(c_{pL}\Delta T_{pL})/(h_{lg}p_G)$ [dimensionless]
k	Thermal conductivity [W/m-K]
k	Boltzmann constant [J/K-molecule]
$\bar{k}$	Wave number [m ⁻¹]
K	Interfield momentum-exchange coefficient [N-s/m ⁴]
L	Length [m]
m or M	The results of a mass summation [kg]
M	Molecular weight [kg/kmol]

n	Number per unit volume [m^{-3}]
n^*	Number per unit volume and unit time [$\text{m}^{-3} \text{ s}^{-1}$]
N	Integer variable [dimensionless]
n_A	Number of gas atoms per molecule [dimensionless]
$\vec{N}_k$	Molar flux of species k relative to a stationary coordinate reference frame [$\text{kmol}/\text{m}^2\text{-s}$]
Nu	Nusselt number ($d_h h/k$ or $2r_d h/k$) [dimensionless]
p	Pressure [N/m^2]
p_{cell}	Cell pressure [N/m^2]
p_{GM}^* , p_{Gm} , or p_{gm}	Partial pressure of vapor material component M (or m) [N/m^2] (p_{GM} preferred)
p_M^*	Input coefficient in the vapor pressure-temperature relationship for material M [N/m^2]
p' , p^+ , and p^*	Absolute value of pressure spatial gradients [N/m^3]
$p_{1\phi}$	Single-phase equilibrium pressure [N/m^2]
$p_{2\phi}$	Two-phase equilibrium pressure [N/m^2]
Pe	Peclet number ($RePr = D_h \vec{v} \rho c_p / k$) [dimensionless]
Pr	Prandtl number ($c_p \mu / k$) [dimensionless]
p_{sf}	Single-phase component of the pressure in the AEOS option [N/m^2]

q	Heat flux [W/m^2]
Q	Volumetric energy source term [W/m^3]
r	Radius of bubble, droplet, or particle [m]
r	Radial coordinate [m]
R	Gas constant [$\text{J}/\text{kg}\text{-K}$]
$\vec{R}$	Right-side vector used in obtaining derivatives of the velocities with respect to pressure [s/m]
R^0	Universal gas constant [$\text{J}/\text{kmol}\text{-K}$]
Re	Reynolds number ($D_h \vec{v} \rho / \mu$) [dimensionless]
R_r	Intermediate term to maintain constant internal energies in Step 3 for energy component r [K]
Rt_{rj} and Rt_{zj}	Intermediate quantities for the Courant time-step control [s^{-1}]
s	Specific entropy [$\text{J}/(\text{kg}\text{-K})$]
S	Sum of surface tensions [kg/s^2]
S	Surface area source [$\text{m}^2/\text{m}^3\text{-s}$]
$\vec{S}$	Vector containing the residual errors driving the pressure iteration [variable dimensions]
$\underline{S}$	Three-by-three coefficient matrix used in solving the momentum equations [kg/m^3]
t	Time [s]

T	Temperature [K]
T_M^*	Input exponent in the vapor pressure-temperature relationship for material M [K]
T_P^I	Particle/vapor interface temperature with mass transfer absent [K]
T_S^I	Structure/vapor interface temperature with mass transfer absent [K]
u	Radial velocity component [m/s]
$\vec{v}$	Velocity [m/s]
v	Axial velocity component [m/s]
V	Representing either an axial or a radial velocity component [m/s]
V	Volume [m ³]
VC_G	Overall coefficient in the virtual mass equation [kg/m ³]
$\bar{VM}$	Virtual mass term [N/m ³]
$V_{L1,p}$	Volume around a particle affected by turbulence [m ³]
$V_{qq'}^*$	Velocity difference used in Step 2 for the turbulent interfield momentum coupling term [m/s]
w_m	Mass fraction of gas material component m [dimensionless]
W	Weighting factor [dimensionless]
W	Pressure-volume or gravity work term [J/m ³]
$\underline{W}$	Three-by-three coefficient matrix of energy derivatives with respect to temperature [J/kg-K]

We	Weber number $[\rho_{CP}(v_{CP} - v_D)^2 d_D / \sigma_{D,CP}]$ [dimensionless]
x	Vector component generally indicating a particular independent variable [variable dimensions]
x	Function argument [variable dimensions]
X	(1/0) for values implying (nominal case/total vaporization) [dimensionless]
Y_{Gm}	Mole fraction of vapor component m [dimensionless]
z	Axial coordinate [m]
α	Volume fraction [dimensionless]
$\tilde{\alpha}$	Minimum effective vapor-volume fraction [$\tilde{\alpha} = \alpha_0(1 - \alpha_S)$] [dimensionless]
α_0	Minimum input vapor-volume fraction [dimensionless]
$\alpha_{G,eff}$	Effective gas volume fraction [$\alpha_{G,eff} = \alpha_G + \alpha_0\alpha_L$] [dimensionless]
α_{ge}	Effective gas volume fraction for two-phase flow [$\alpha_{ge} = \max(\alpha_{G,eff}, \tilde{\alpha})$] [dimensionless]
α_{Lo}	The total liquid volume fraction at the single-phase/two-phase transition [dimensionless]
α_{mo}	Volume fraction for component m at the single-phase/two-phase transition [dimensionless]
$\alpha_{S,ID}$	Input volume fraction for infinite (large) structure drag [dimensionless]
β	Angle [dimensionless]

γ	Heat capacity ratio [dimensionless]
Γ	Mass-transfer rate per unit volume. When subscripted, the positive rate is from the component corresponding to the first subscript to the component representing the second subscript [$\text{kg}/\text{m}^3\text{-s}$]
Γ_C	Coalescence rate [m/s]
δ	Boundary-layer thickness [m]
δ	Minimum stable film of vapor on a liquid 2 (coolant) droplet [m]
δ	Variation of a physical quantity [dimensionless]
δ_{ij} or $\delta(i,j)$	Kronecker delta [dimensionless]
Δ	Difference [dimensionless]
Δr	Radial mesh spacing [m]
Δt	Time-step size [s]
ΔT_h	Temperature range over which the homogeneous condensation term is quadratic in the temperature difference [K]
ΔT_{Sup}	Superheat [K]
Δz	Axial mesh spacing [m]
ϵ	Turbulent dissipation rate [m^2/s^3]
ϵ	Emissivity [dimensionless]

ϵ	Error in the cell pressure as compared with the EOS [N/m ²]
ϵ	Characteristic energy of interaction between molecules (Lennard-Jones parameter) [J]
ϵ_p	Convergence criterion for the pressure calculation in the SESAME interface [N/m ²]
ϵ_v	Convergence criterion used in solving the momentum equations [dimensionless]
ϵ_T	Convergence criterion for the temperature calculation in the SESAME interface [dimensionless]
ζ	Thermal diffusivity [m ² /s]
θ	Nondimensional temperature [dimensionless]
λ	Virtual mass parameter based on Drew's objectivity principle [dimensionless]
λ	Matrix eigenvalue [W/m ³ -K]
λ	Wavelength [m]
λ_c	Critical wavelength [m]
Λ	Axial/radial discriminator being (1/0) for the (axial/radial) direction
Λ	Derivative in the Taylor expansion of the mass-transfer rates [variable dimensions]
Λ_{rq}	Intermediate matrix used to maintain constant internal energies in Step 3 for energy component r and momentum field q [K-m ³ /kg]

μ	Viscosity (dynamic) [kg/m-s]
μ	Chemical potential [J/kmol]
ν	Viscosity (kinematic) [m ² /s]
ξ	Surface area multiplier [dimensionless]
ξ	Area coordinate, πr^2 [m ²]
ξ_d	Input interfield momentum-exchange function multiplier [dimensionless]
π	Pi (3.1415926536 . . .)
ρ	Microscopic density [kg/m ³]
$\bar{\rho}$	$\alpha\rho$, Macroscopic (smear) density [kg/m ³]
$\rho_{L,eff}$	Virtual (effective) density [kg/m ³]
ρ_{Lmo} or ρ_{Lmo}	Microscopic density at the single-phase/two-phase transition [kg/m ³]
σ	Surface tension [kg/s ²]
σ	Stefan-Boltzmann constant [W/m ² -K ⁴]
σ	Molecular diameter (Lennard-Jones parameter) [Å]
σ_{LG}	Surface tension between liquid and gas [kg/s ²]
σ_{LL}	Surface tension between two liquids [kg/s ²]
τ	Time constant [s]

ϕ	Heat flux [W/m ²]
ψ	Flow specifier [dimensionless]
ψ	Arbitrary function [arbitrary dimensions]
ω	Probability [dimensionless]
ω	Time-mixing parameter [dimensionless]
Ω_μ	Collision integral for viscosity [dimensionless]
Ω_D	Collision integral for mass diffusivity [dimensionless]
$\langle \rangle$	Brackets to indicate a quantity evaluated for spatial differencing [dimensionless]

Subscript	Definition
a	Average or mixture
basic	Unmodified interfield momentum-exchange coefficients
b	Bubble
B0	Burnout
BFR	Bubbly flow regime
C or c	Continuous (no preference)
CC	Liquid-continuous churn flow

CD or cd	Continuous-discontinuous (no preference)
CL	Continuous liquid
CLDL	Between the continuous and discontinuous liquids
CM	Common for the liquid 1 solid particulate system
Con	Refers to condensate conditions at the local partial pressure of the vapor
CP	Continuous phase
CS	Continuous structure
Crt, Crit, or crit	Critical (Crt preferred)
D or d	Discontinuous sphere or droplet
dc	Direct contact
DD	Discontinuous-discontinuous
DL	Discontinuous liquid
DP	Discontinuous phase
DS	Discontinuous structure
e	Equilibrium
e	Internal energy
EC	Effective instantaneous contact
ECS	Equivalent common surface

eff	Effective
ext	External source
F	Fragmentation
FB	Film boiling
g,v	Gravity and velocity
g	A vapor property
G	Vapor energy or vapor momentum field
GCL	Between vapor and the continuous phase
GDL	Between vapor and the discontinuous phase

A comma is used to separate two energy component subscripts, whereas a slash is used to separate two momentum component subscripts. If no danger of confusion exists, the comma or slash may be omitted. When possible, omission of the separator is the preferred usage for reasons of economy.

G,Lm or GLm Between vapor and liquid energy component m

G/Lm or GLm Between vapor and liquid momentum component m

gm Vapor density component m

Gm or GM Vapor material component m (Gm preferred)

G,P or GP Between vapor and the particle component

G,S or GS Between vapor and the structure energy components

G/S or GS Between the vapor and structure momentum components

H	Heat transfer
i	Arbitrary species component
i	Energy component subscript
i	Radial spatial index
i	Interface subscript
IC	Instantaneous contact
j	Matrix index
j	Axial spatial index
k	A second density, energy, or material component
L	Liquid (generally referring to a mixture of all liquids present)
LE	Leidenfrost
Liq	Liquidus
ρ_m	Liquid density component m
Lm	Liquid energy/material m or liquid momentum field m
Lm,G or LmG	Between liquid energy component m and vapor
Lm/G or LmG	Between liquid momentum field m and vapor
Lm,Lm' or LmLm'	Between liquid energy field Lm and Lm'
Lm,P or LmP	Between liquid energy component m and structure

Lm,S or LmS Between liquid energy component m and structure

Lm/S or LmS Between liquid momentum component m and structure

LM Liquid mixture

LL Nonvapor flow

L1P Between liquid 1 and particulates

L1CP Between liquid 1 and the continuous phase

m When used alone, m refers to a density component or a summation index. In combination with other subscripts or independently defined symbols it also can refer to a energy or material component. [In the SESAME/AFDM interface theory, "m" refers to the particle and liquid components.]

M Material component

max Maximum

mb Minimum bubble

md Minimum droplet

Min or min Minimum

Mlt or melt Melting (Mlt preferred)

MF Melting-freezing

mx b Maximum bubble

mx d Maximum droplet

n Vapor components in the SESAME/AFDM interface theory

NL Noncoalescing

o The single-phase/two-phase transition point

p Particle density component

p Pressure

P Particle energy or density component

PCP Between solid particulate and the continuous phase

P,G or PG Between the particle and the vapor energy components

P,Lm or PLm Between the particles and the energy component for liquid m

P,S or PS Between the particle and structure components

q Arbitrary velocity component

q' A second velocity component

L1, L2, and G normally are used to identify momentum fields. However, when a possible confusion with energy components is possible, the following notation is used.

q = L1 or q1 Signifying momentum field 1

q = L2 or q2 Signifying momentum field 2

q3 Signifying momentum field 3

r Energy component

s Structure density component

s Spinodal value (see Spg and Spl)

S *Structure energy or density component*

Sat or sat Saturation based on vapor partial pressure [Sat,Gm indicates saturation conditions for vapor component m] (Sat is preferred)

S,G or SG Between the structure and vapor energy components

S/G or SG Between the structure and vapor momentum components

S,Lm or SLm Between the structure and liquid energy component m

S/Lm or SLm Between the structure and liquid momentum component m

Sld Referring to values of pressure and internal energy from the solid EOS table

Sol Solidus

S,P or SP Between the structure and particle components

Spg Vapor spinodal limit

Spl Liquid spinodal limit

SS Solid structure

Sub Sublimation

Sup or sup Superheat (Sup preferred)

Sus Solid side of the sublimation curve

T	Topology
T=0	Signifies absolute zero
TR	Threshold of levitation
TZ	Hysteresis transition
$\vec{v}$	Velocity
Van	Referring to values of pressure and internal energy from the SESAME 301 table
Vap	Referring to saturated vapor conditions at the local partial pressure of the vapor
x	A component subscript defined based on local needs
X,Y	Between X and Y
θ or θ_+	Spatial index, $(i, j + \frac{1}{2})$ (θ_+ is to be used when θ_- is possible)
θ_-	Spatial index, $(i, j - \frac{1}{2})$
λ or λ_+	Spatial index, $(i + \frac{1}{2}, j)$ (λ_+ is to be used when λ_- is possible)
λ_-	Spatial index, $(i - \frac{1}{2}, j)$
ξ	Spatial index representing either λ or θ
ρ	Thermodynamic density
ϕ	Phase

Superscript	Definition
a	Associated
c	Convection
FB	Film boiling
i	Input value
I	Interface
k	Iteration index
mol	Molar quantity
n	Beginning-of-time-step value
n+1	End-of-time-step value
P	Combination of persisting and collision contact
v	Collision contact
κ	Iteration index
ρ	Per unit mass
σ	Persisting contact
*	Single-phase pressure equilibrium condition (used for the SESAME EOS interface)
$\left. \begin{matrix} ' \\ + \\ * \end{matrix} \right\}$	Gradients or derivatives

Variable Modifiers (Over a Symbol)

Modifier	Definition
-	Indicating a cell-averaged value
~	Intermediate value
≈	Secondary intermediate value
-	Vector
Λ	Secondary (internal) index