60
8-14-95 JS ②

BNL- 52473
FZKA 5591
Formal Report

ASSESSMENT OF THE IVA3 CODE FOR MULTIFIELD FLOW SIMULATION

H. B. STEWART

JULY 1995

DEPARTMENT OF APPLIED SCIENCE

BROOKHAVEN NATIONAL LABORATORY
UPTON, LONG ISLAND, NEW YORK 11973

DISCLAIMER

BNL-52473
UC-405
FZKA 5591

Assessment of the IVA3 Code for Multifield Flow Simulation

H.B. STEWART

July 1995

Department of Applied Science

Brookhaven National Laboratory
Associated Universities, Inc.
Upton, Long Island, New York 11973

Research sponsored by
Forschungszentrum Karlsruhe
Karlsruhe, Germany

under Contract No. DE-AC02-76CH00016 with the
Office of Scientific Computing
United States Department of Energy
Washington, D.C.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Assessment of the IVA3 Code for Multifield Flow Simulation

H. Bruce Stewart
Department of Applied Science
Building 490-D
Brookhaven National Laboratory
Upton, New York 11973

Abstract

This report presents an assessment of the IVA3 computer code for multifield flow simulation, as applied to the premixing phase of a hypothetical steam explosion in a water-cooled power reactor.

The first section of this report reviews the derivation of the basic partial differential equations of multifield modeling, with reference to standard practices in the multiphase flow literature. Basic underlying assumptions and approximations are highlighted, and comparison is made between IVA3 and other codes in current use. Although Kolev's derivation of these equations is outside the mainstream of the multiphase literature, the basic partial differential equations are in fact nearly equivalent to those in other codes.

In the second section, the assumptions and approximations required to pass from generic differential equations to a specific working form are detailed. Some modest improvements to the IVA3 model are suggested.

In Section 3, the finite difference approximations to the differential equations are described. The discretization strategy is discussed with reference to numerical stability, accuracy, and the role of various physical phenomena — material convection, sonic propagation, viscous stress, and interfacial exchanges — in the choice of discrete approximations. Comparing this strategy with the salient features of

typical premixing simulations suggests that a more efficient strategy for this application might be to treat convection explicitly and at least some of the heat and mass transfer terms implicitly. There is also cause for concern about the approximations of time evolution in some heat transfer terms, which might be adversely affecting numerical accuracy.

The fourth section documents the numerical solution method used in IVA3. An explanation for erratic behavior sometimes observed in the first outer iteration is suggested, along with possible remedies. Also the subtle relations between stability, accuracy, and the automatic time step selection algorithm are discussed; specific analyses for further assessment of the overall numerical strategy are proposed.

Finally, six recommendations for future assessment and improvement of the IVA3 model and code are made. Briefly, they are: (1) improve code efficiency in the numerical treatment of material convection; (2) improve code efficiency (and perhaps accuracy) in numerical treatment of heat and mass transfer; (3) implement a more consistent representation of virtual mass and drag forces; (4) investigate the model sensitivity to the magnitude of viscous stresses; (5) develop improved visualization techniques to identify numerical stability and accuracy problems which may be masked by automatic time step size selection; and (6) apply state-of-the-art software tools to further improve code documentation.

Contents

1 Basic Equations of Multifield Flow

1.1 Introduction

The physical basis for an assessment of the IVA3 multifield model should begin with an understanding of the basic partial differential equations for multifield approximations of interpenetrating multifluid flow. The existing documentation (KFK 4948, 4949, 4950) of IVA3 by Kolev includes an extensive discussion of the derivation of multifield flow equations. However, that discussion involves idiosyncratic approaches which are not in the mainstream of multiphase flow literature. This makes it difficult to compare the IVA3 approach with other multifluid models. In fact, the equations ultimately used in the code are very close to those of other models; therefore it should be useful to provide a derivation of the IVA3 equations based on standard practices and concepts in the multiphase flow literature. This will make it possible to understand the similarity with other approaches, and to clarify the relatively minor differences. It will also provide a sound basis for any possible new code development.

The most striking departure from standard practice in Kolev's derivation of multifield flow equations is his representation of what he labels the local instantaneous equations. Normal practice is to begin with single-phase flow equations describing the local flow within a very small region occupied by a single phase of the multiphase mixture. (For the moment, we shall use the terms phase and field interchangeably, temporarily ignoring the fact that the specific application intended for IVA3 involves multicomponent fields.) Since the goal of multifield modeling is to avoid detailed description of the partitioning of space into regions occupied by a single phase, these local instantaneous equations are averaged in such a way as to filter out much of this fine-scale description.

One obvious way to do this would be to average over spatial control volumes large enough that each control volume contains more than one phase. This spatial averaging emphasizes the spatially interpenetrating nature of the phases to be modeled. Another possibility is to average over time intervals long enough that more than one phase occupies any given spatial location during the averaging interval. A third possibility is to average over a statistical ensemble of flow realizations such that at any given point in space and time, different realizations have different phases present on the fine scale. All these averaging approaches have been used, often in combination. Their purpose is the same: to pass from fine scale flow description with phases occupying mutually exclusive space-time locations, toward a multifield approximation in which the interpenetrating nature of the multiphase flow is exploited to simplify the model. This simplification is achieved by what might seem a complication: extending the velocity fields for each phase to be defined everywhere in space and time. The resulting multifield flow equations will be weighted by a new quantity, the average volume fraction of each field; this may be thought of as the average amount (by volume) of each phase present in a control volume whose size is larger than the fine scale of the phase distributions.

The essential point to be made at this juncture is that one begins with local instant flow equations which are just single-phase flow equations. The volume fractions, denoted α_ℓ for each field ℓ, do not appear in these local equations; they arise as a result of the averaging procedure used to pass to multifield equations.

In view of the well-established literature on deriving multifield equations by various forms of averaging, it would serve little purpose to repeat those derivations here in detail. In spite of the several different approaches in the multiphase flow literature, there is almost complete agreement on the proper form of the multifield equations and the approximations involved in reaching them. We propose to summarize those derivations, identifying the most important assumptions and approximations involved. This is important because the multifield equations are unlike the basic equations of mathematical physics, in that they do involve approximations of a much more serious nature than those involved in the equations for single-phase flow. The slow process of confronting multifield models with experimental data, then rethinking and improving the models, will require an understanding of the assumptions upon which the models are based. We may take encouragement from some of the successes already scored by multifield flow models, including understanding of some subtle, inherently dynamical phenomena such as flow regime changes (Lahey et al. 1992).

Before proceeding, let us state that only one version of IVA3 is being assessed here, namely the version intended for analysis of hypothetical core melt down and steam explosion in a pressurized water reactor. In this application, the multifield model describes three material fields, each moving with its own velocity field. Field 1 is a gas composed of a mixture of steam and air. Field 2 is a liquid consisting of water, potentially mixed with inert solid particles of reactor core material, or corium. The corium particles in field 2 are of the same substance as field 3, but are supposed to be finely fragmented and hence in mechanical and thermodynamic equilibrium with the nearby liquid water. Field 3 consists of reactor core material in a molten or partially melted state. We use the term "field" to refer both to any one of the three vector velocity fields describing the motion, and also to the composite material carried by each velocity field.

The multiphase flow literature contains many thorough discussions of the derivation of multifield equations by averaging. The following summary is drawn from the book by Ishii (1975), work of Nigmatulin (1979), review articles by Bouré and Delhaye (1981) and by Lahey and Drew (1989), and the thesis of Arnold (1988). The forms of the averaged equations used here can be found in Lahey and Drew (1989).

1.2 Local instantaneous equations

We begin by stating the local instantaneous equations describing the fluid flow on the microscopic scale, in very small regions occupied by one phase or field only. There are three such partial differential equations. The first is the equation of continuity, or conservation of mass:

$$\frac{\partial \rho_\ell}{\partial t} + \nabla \cdot (\rho_\ell \mathbf{V}_\ell) = 0. \tag{1}$$

Next is the equation of conservation of momentum:

$$\frac{\partial}{\partial t}(\rho_\ell \mathbf{V}_\ell) + \nabla \cdot (\rho_\ell \mathbf{V}_\ell \mathbf{V}_\ell) = \rho_\ell \mathbf{g} + \nabla \cdot \mathbf{T}_\ell. \tag{2}$$

And finally, the equation expressing the conservation of total energy, including both the internal thermodynamic energy e_ℓ and the kinetic energy of fluid motion described by the velocity field $\mathbf{V}_\ell$:

$$\begin{gathered}\frac{\partial}{\partial t}[\rho_\ell(e_\ell + \tfrac{1}{2}V_\ell^2)] + \nabla \cdot [\rho_\ell(e_\ell + \tfrac{1}{2}V_\ell^2)\mathbf{V}_\ell] = \\ -\rho_\ell \mathbf{g} \cdot \mathbf{V}_\ell + \nabla \cdot (\mathbf{T}_\ell \cdot \mathbf{V}_\ell) - \nabla \cdot \mathbf{q}_\ell'' + q_\ell'''\end{gathered} \tag{3}$$

In these equations we use the following notation:

$\rho_\ell =$ local instant density of field ℓ
$\mathbf{V}_\ell =$ local instant velocity of field ℓ; $V_\ell^2 = \mathbf{V}_\ell \cdot \mathbf{V}_\ell$
$\mathbf{g} =$ gravitational body force
$\mathbf{T}_\ell =$ stress tensor $= -P_\ell \mathbf{I} + \boldsymbol{\tau}_\ell$
$P_\ell =$ local instant pressure in field ℓ
$\boldsymbol{\tau}_\ell =$ viscous stress tensor
$e_\ell =$ specific internal energy of field ℓ
$\mathbf{q}_\ell'' =$ heat flux of thermal diffusion
$q_\ell''' =$ volumetric heat source for field ℓ

The energy equation can be expressed equivalently in terms of enthalpy h_ℓ, or in terms of the entropy s_ℓ.

The averaging procedure will involve the three conservation equations (1)-(3), together with associated jump conditions describing the transfer of mass, momentum, and energy across the interfaces common to any pair of phases or fields.

The jump condition for mass can be written as

$$\sum_\ell \rho_\ell (\mathbf{V}_\ell - \mathbf{V}_i) \cdot \mathbf{n}_\ell = 0, \tag{4}$$

where $\mathbf{n}_\ell$ is the unit normal to the interface, and $\mathbf{V}_i$ is the local velocity of the interface. The same equation is conveniently written as

$$\sum_\ell \dot{m}_\ell = 0$$

by defining the interfacial mass transfer flux

$$\dot{m}_\ell \equiv \rho_\ell (\mathbf{V}_\ell - \mathbf{V}_i) \cdot \mathbf{n}_\ell.$$

This is a superficial flux, to be multiplied by interfacial area, and is therefore sometimes denoted $\dot{m}_\ell''$.

The momentum jump condition is

$$\sum_\ell \dot{m}_\ell \mathbf{V}_\ell = \sum_\ell \mathbf{n}_\ell \cdot \mathbf{T}_\ell. \tag{5}$$

The jump condition for the total energy, internal plus kinetic, is

$$\sum_{\ell} \dot{m}_{\ell}(e_{\ell} + \frac{1}{2}V_{\ell}^{2}) + \sum_{\ell} \mathbf{q}_{\ell} \cdot \mathbf{n}_{\ell} = \sum_{\ell} (\mathbf{n}_{\ell} \cdot \mathbf{T}_{\ell}) \cdot \mathbf{V}_{\ell}. \tag{6}$$

In each case, since a local interface between two phases is being described, the summation is taken over those two phases. (This differs from the convention to be used later, that sums over ℓ are understood to taken over all fields unless otherwise indicated.) After averaging has been carried out, the contributions of the interfacial transfers will involve all fields present (in a macroscopic control volume, or in a statistical ensemble.)

1.3 Averaged multifield equations

1.3.1 General considerations

The local instantaneous partial differential equations (1)-(3) are applicable only within a region occupied by field ℓ, while the jump conditions (4)-(6) apply only at an interface between two fields. By taking averages, the local instantaneous equations are transformed to equations involving averaged quantities $\langle \rho_{\ell} \rangle$, $\langle e_{\ell} \rangle$, $\langle \mathbf{V}_{\ell} \rangle$ which will be taken as defined simultaneously for all fields at every point.The purpose of the averaging is to remove the need for a detailed description of the local distribution of the separate phases. Although the interface topology cannot be completely eliminated from the problem, it will ultimately appear only through certain assumptions needed to specify averaged interfacial terms which depend on flow regime.

The averaging operator has been considered in the multiphase flow literature in several different forms; $\langle \cdot \rangle$ may stand for volume average

$$\langle f \rangle = Vol^{-1} \iiint_{Vol} f(\mathbf{x}', t) d\mathbf{x}'$$

or for time average

$$\langle f \rangle = T \int_{t-T}^{t} f(\mathbf{x}, t') dt'$$

or a combination of time and volume averaging, or an ensemble average

$$\langle f \rangle = \int_{\mathcal{M}} f(\mathbf{x}, t, \mu) dm(\mu)$$

integrated over realizations μ occurring with probability $m(\mu)$ in a statistical ensemble $\mathcal{M}$.

Without repeating the details of the averaging procedure, we note some of the major considerations involved.

(1) Because the fields interpenetrate, averaging will include integration over the interfaces separating the phases one from another. The interfacial contributions may be expressed generally in the form $\langle \boldsymbol{\phi}_\ell \cdot \nabla \chi_\ell \rangle$, where $\boldsymbol{\phi}_\ell$ stands for a flux, and χ_ℓ is the field indicator function defined as

$$\chi_\ell(\mathbf{x}, t) = \begin{cases} 1 \text{ if field } \ell \text{ occupies location } \mathbf{x} \text{ at time } t = 0 \\ 0 \text{ otherwise.} \end{cases}$$

Since χ_ℓ is a step function, $\nabla \chi_\ell$ is a distribution.

In most cases, putting these interfacial average contributions in usable form will involve assumptions about the topology of the interface(s), determined by the specific flow regime.

(2) The many nonlinearities in the local instantaneous equations mean that, in order to obtain equations in which the averaged quantities such as $\langle \rho_\ell \rangle$, $\langle e_\ell \rangle$, $\langle \mathbf{V}_\ell \rangle$ appear as dependent variables, averages of products will need to be transformed to expressions involving products of averages. To some extent this difficulty can be finessed by defining appropriately weighted averages as the dependent variables; but in some crucial places, it will become necessary to simply neglect the covariance, that is, the difference between the average of a product and the product of averages. This means that serious approximations must be made before even the basic form of the multifield equations are written.

(3) A related problem is that one will also want, during the averaging derivation, to approximate the average of a quantity multiplied by an already averaged quantity, that is, to approximate $\langle f_\ell \langle g_\ell \rangle \rangle$ by $\langle f_\ell \rangle \langle g_\ell \rangle$. This can be justified for smoothly varying functions f_ℓ and g_ℓ provided that, in the case of volume averaging, the averaging control volume is sufficiently small compared to the length scale on which the averaged quantities vary; see Lahey and Drew (1989). In particular, this assumption would come into doubt in case one would attempt to model flows with large-scale interfaces between fields.

1.3.2 Mass and momentum equations

Let us now consider the averaged equation expressing the conservation of mass based on eqs. (1) and (4). This balance equation will involve in the time derivative the average $\langle \chi_\ell \rho_\ell \rangle$, which can be rewritten by introducing the definition of the field volume fraction

$$\alpha_\ell \equiv \langle \chi_\ell \rangle \tag{7}$$

and the weighted average

$$\langle f_\ell \rangle^\chi \equiv \langle \chi_\ell f_\ell \rangle / \alpha_\ell . \tag{8}$$

It then becomes possible to express the first term of the averaged mass conservation equation as

$$\partial(\alpha_\ell \langle \rho_\ell \rangle^\chi)/\partial t$$

This represents a reasonable definition of the averaged phase density which serves as a convenient dependent variable. It must be borne in mind that at the end of the day, the multifield equations will only be valid with this interpretation of $\langle \rho_\ell \rangle$.

Next, the divergence term of the phase mass conservation equation will generate a term $\langle \chi_\ell \rho_\ell \mathbf{V}_\ell \rangle$. Again a suitable weighted average can be defined as

$$\langle f_\ell \rangle^{\chi\rho} = \langle \chi_\ell \rho_\ell f_\ell \rangle / \alpha_\ell \langle \rho_\ell \rangle^\chi \tag{9}$$

Once again, this is a reasonable way to define the averaged phase velocity, and is convenient for obtaining usable equations, provided it be remembered that $\langle \mathbf{V}_\ell \rangle$ should always be interpreted as $\langle \mathbf{V}_\ell \rangle^{\chi\rho}$.

Finally, with the interfacial contribution associated with phase change included, the averaged mass conservation equation for field ℓ reads

$$\frac{\partial}{\partial t}(\alpha_\ell \langle \rho_\ell \rangle^\chi) + \nabla \cdot (\alpha_\ell \langle \rho_\ell \rangle^\chi \langle \mathbf{V}_\ell \rangle^{\chi\rho}) = \mu_\ell \tag{10}$$

where

$\mu_\ell =$ volumetric mass generation rate due to phase or field change

$$= -Vol^{-1} \textstyle\iint_{A_i} \dot{m}_\ell dA_i$$

The notation μ_ℓ of IVA3 is used here, although Γ_ℓ is common in the multiphase flow literature.

Next consider the averaged balance of momentum based on eqs. (2) and (5). The same definitions of $\langle\rho_\ell\rangle$ and $\langle\mathbf{V}_\ell\rangle$ serve equally well for transforming the time derivative term in the momentum equation. However, the spatial divergence term contains an additional factor $\mathbf{V}_\ell$; here there is no further possibility to define away the difficulty, and the present state of the art in multiphase flow modeling approximates the average of the product $\langle\mathbf{V}_\ell\mathbf{V}_\ell\rangle$ by the product of the averages $\langle\mathbf{V}_\ell\rangle$ and $\langle\mathbf{V}_\ell\rangle$, and simply discards the difference or covariance term $\langle\mathbf{V}_\ell\mathbf{V}_\ell\rangle - \langle\mathbf{V}_\ell\rangle\langle\mathbf{V}_\ell\rangle$. Equivalently, the same approximation may be expressed as supposing that the corresponding correlation tensor to be the unit tensor, as in Lahey and Drew (1989).

Similar approximations for averaged pipe flow equations were studied by Birkhoff in 1964. He observed that covariance terms can be large in cases where the density ratio is large and the ratio of velocities is large. Neglecting the covariance is a serious assumption; all multifield models are based on such assumptions, and the success of multifield modeling is some demanding applications shows that the neglected covariances do not necessarily cripple multifield models. However, it should be borne in mind that the basic multifield equations contain approximations more serious than those typical of the basic equations of mathematical physics.

Accepting this assumption and neglecting the covariance in the momentum divergence, and incorporating the interfacial momentum jump conditions, the averaged momentum conservation equation can be written in the form

$$\begin{aligned}&\frac{\partial}{\partial t}(\alpha_\ell\langle\rho_\ell\rangle^{\chi}\langle\mathbf{V}_\ell\rangle^{\chi\rho}) + \nabla\cdot(\alpha_\ell\langle\rho_\ell\rangle^{\chi}\langle\mathbf{V}_\ell\rangle^{\chi\rho}\langle\mathbf{V}_\ell\rangle^{\chi\rho}) = \\ &-\nabla(\alpha_\ell\langle P_\ell\rangle^{\chi}) + \nabla\cdot[\alpha_\ell(\langle\boldsymbol{\tau}_\ell\rangle^{\chi} + \mathbf{T}_\ell^{Re})] + \langle P_\ell\rangle_i\nabla\alpha_\ell \\ &+\alpha_\ell\langle\rho_\ell\rangle^{\chi}\mathbf{g} + \mathbf{F}_{\ell i} - \mathbf{F}_{\ell w} + \mu_\ell\mathbf{V}_{\ell i}\end{aligned} \tag{11}$$

where

$\mathbf{T}_\ell^{Re} =$ Reynolds stress tensor $\langle \chi_\ell \rho_\ell \mathbf{V}_\ell' \mathbf{V}_\ell' \rangle / \alpha_\ell$
$\langle \tau_\ell \rangle^\chi =$ average viscous stress
$\mathbf{V}_\ell' =$ velocity fluctuations $\mathbf{V}_\ell - \langle \mathbf{V}_\ell \rangle^{\chi\rho}$
$\langle P_\ell \rangle_i =$ pressure at interface
$\mathbf{g} =$ gravitational body force
$\mathbf{F}_{\ell i} =$ interfacial momentum source
$\mathbf{F}_{\ell w} =$ wall friction
$\mathbf{V}_{\ell i} =$ velocity at the interface

Note that here and below, terms of the form $\mu_\ell f_\ell$ are averages weighted by the interfacial mass transfer $\dot{m}_\ell$, that is,

$$\mu_\ell f_\ell \equiv \langle \rho_\ell f_\ell (\mathbf{V}_\ell - \mathbf{V}_i) \cdot \nabla \chi_\ell \rangle$$

In eq. (11) the pressure contribution $-\langle P_\ell \rangle_i \nabla \alpha_\ell$ to interfacial momentum transfer is written explicitly; the remaining contributions, in $\mathbf{F}_{\ell i}$, include drag, virtual mass, and lift forces. Assuming a single local pressure for all phases

$$P = \langle P_\ell \rangle^\chi = \langle P_\ell \rangle_i, \tag{12}$$

the two pressure terms may be combined:

$$-\nabla(\alpha_\ell \langle P_\ell \rangle^\chi) + \langle P_\ell \rangle_i \nabla \alpha_\ell = -\alpha_\ell \nabla P.$$

Wall friction $\mathbf{F}_{\ell w}$ includes frictional drag; other forces such as lateral lift may exist but are usually neglected except in special applications

1.3.3 Energy equation

Now consider the averaged energy equation based on (3) and (6). As usual in thermodynamics, there is more than one way to express the energy balance, according to whether one chooses the specific internal energy, the enthalpy, or the entropy as the primary dependent variable. Here we adapt Kolev's approach of beginning with an averaged energy equation expressed as a balance for the sum of the enthalpy plus the kinetic energy of the average motion. Following Lahey and Drew (1989),

$$\begin{aligned}
&\frac{\partial}{\partial t}[\alpha_\ell \langle \rho_\ell \rangle^\chi (\langle h_\ell \rangle^{\chi\rho} + \tfrac{1}{2}\langle \mathbf{V}_\ell \rangle^{\chi\rho} \cdot \langle \mathbf{V}_\ell \rangle^{\chi\rho} + e_\ell^{Re})] + \\
&\nabla \cdot [\alpha_\ell \langle \rho_\ell \rangle^\chi (\langle h_\ell \rangle^{\chi\rho} + \tfrac{1}{2}\langle \mathbf{V}_\ell \rangle^{\chi\rho} \cdot \langle \mathbf{V}_\ell \rangle^{\chi\rho} + e_\ell^{Re}) \langle \mathbf{V}_\ell \rangle^{\chi\rho}] = \\
&\alpha_\ell \frac{\partial P}{\partial t} - \nabla \cdot \alpha_\ell (\langle \mathbf{q}_\ell'' \rangle^\chi + \mathbf{q}_\ell^{Re}) + \nabla \cdot [\alpha_\ell (\langle \boldsymbol{\tau}_\ell \rangle^\chi + \mathbf{T}_\ell^{Re}) \cdot \langle \mathbf{V}_\ell \rangle^{\chi\rho}] \\
&+ \alpha_\ell \langle \rho_\ell \rangle^\chi \mathbf{g} \cdot \langle \mathbf{V}_\ell \rangle^{\chi\rho} + \mu_\ell [h_{\ell i} + \tfrac{1}{2}(\mathbf{V}_\ell \cdot \mathbf{V}_\ell)_i] + Q_\ell + \alpha_\ell q_\ell''' + \mathbf{F}_{\ell i} \cdot \mathbf{V}_{\ell i}
\end{aligned} \tag{13}$$

where

$e_\ell^{Re} =$ turbulent kinetic energy
$h_{\ell i} =$ enthalpy at the interface
$Q_\ell =$ interfacial heat source $\langle q_\ell'' \cdot \nabla \chi_\ell \rangle$
$\langle \mathbf{q}_\ell'' \rangle^\chi =$ average heat flux
$\mathbf{q}_\ell^{Re} =$ turbulent heat flux
$q_\ell''' =$ volumetric heat generation rate

Here again we assume a single local pressure for all phases $P = \langle P_\ell \rangle^\chi = \langle P_\ell \rangle_i$.

The energy e_ℓ^{Re} associated with the turbulent fluctuations is included in this balance. The treatment of e_ℓ^{Re} has caused some confusion in multifield modeling. Ishii (1975) incorporated the quantity e_ℓ^{Re} implicitly in the phase average internal energy when deriving the averaged energy equation. A number of multiphase flow models have been based on Ishii's equations, without noticing the incorporation of e_ℓ^{Re} into $\langle e_\ell \rangle$. This affects the manner in which interfacial energy transfer is constituted. Arnold (1988) has shown that with careful consideration of the interfacial energy sources it is correct to express the interfacial flux of energy due to mass transfer in terms of the enthalpy, when turbulent kinetic energy is included in the balance. However in the balance for average internal energy only, the interfacial energy flux should carry the internal energy, and not the enthalpy, according to Arnold.

Most multifield computer codes simply neglect the turbulent kinetic energy. Arnold shows that internal energy equations so derived may violate the second law of thermodynamics. However if the discrepancies are small, this may be tolerable. We now specifically choose to follow the common practice and simply drop e_ℓ^{Re} from the balance. As a consequence, the energy transferred with mass is retained in the form $\mu_\ell h_{\ell i}$, although Arnold recommends $\mu_\ell e_{\ell i}$, along with other correction terms. The resulting error should be small; furthermore, it will turn out that the approximations used in transforming to an entropy formulation partly compensate for the missing correction terms suggested by Arnold.

We now follow Kolev in transforming the above equation to express it in terms of the average entropy $\langle s_\ell \rangle^{\chi\rho}$. Of course it would be possible to carry out thermodynamic transformations on the local instantaneous energy equation (3) in its accepted form, and then average each variant form. However, it is very difficult to compare the results, because of the different forms appropriate for the interfacial contributions. An illustration of this difficulty is given by Arnold et al. (1990), p. 486.

In view of this complication, we prefer to transform the averaged equations. This means that thermodynamic relations used in the transformation of the equations will involve the average quantities $\langle h_\ell \rangle^{\chi\rho}$, $\langle e_\ell \rangle^{\chi\rho}$, $\langle s_\ell \rangle^{\chi\rho}$ and are therefore approximations, not thermodynamic identities.

We begin by subtracting the mechanical energy balance, which is the dot product of the averaged momentum equation (11) with the average field velocity $\langle \mathbf{V}_\ell \rangle^{\chi\rho}$. Making use of the mass conservation equation (10), we get

$$\begin{gathered}
\frac{\partial}{\partial t}(\alpha_\ell \langle \rho_\ell \rangle^{\chi} \langle h_\ell \rangle^{\chi\rho}) + \nabla \cdot [\alpha_\ell \langle \rho_\ell \rangle^{\chi} \langle h_\ell \rangle^{\chi\rho} \langle \mathbf{V}_\ell \rangle^{\chi\rho}] = \\
\alpha_\ell \frac{\partial P}{\partial t} + \alpha_\ell \nabla P \cdot \langle \mathbf{V}_\ell \rangle^{\chi\rho} - \nabla \cdot \alpha_\ell (\langle \mathbf{q}_\ell'' \rangle^{\chi} + \mathbf{q}_\ell^{Re}) \\
+\alpha_\ell (\langle \boldsymbol{\tau}_\ell \rangle^{\chi} + \mathbf{T}_\ell^{Re}) : \nabla \langle \mathbf{V}_\ell \rangle^{\chi\rho} + \mu_\ell h_{\ell i} + \tfrac{1}{2} \mu_\ell (\mathbf{V}_{\ell i} - \langle \mathbf{V}_\ell \rangle^{\chi\rho})^2 \\
+Q_\ell + \alpha_\ell q_\ell''' + \mathbf{F}_{\ell i} \cdot (\mathbf{V}_{\ell i} - \langle \mathbf{V}_\ell \rangle^{\chi\rho})
\end{gathered} \tag{14}$$

If we wish to express this in terms of specific internal energy instead of enthaply, we use the approximation $\langle h_\ell \rangle^{\chi\rho} \simeq \langle e_\ell \rangle^{\chi\rho} + P / \langle \rho_\ell \rangle^{\chi}$. Again we emphasize that this expression involving averaged quantities is an approximation, and not a thermodynamic identity. The approximation can be justified as in Arnold (1988). The result

$$
\begin{aligned}
&\frac{\partial}{\partial t}(\alpha_\ell \langle \rho_\ell \rangle^\chi \langle e_\ell \rangle^{\chi\rho}) + \nabla \cdot [\alpha_\ell \langle \rho_\ell \rangle^\chi \langle e_\ell \rangle^{\chi\rho} \langle \mathbf{V}_\ell \rangle^{\chi\rho}] = \\
&-P\frac{\partial \alpha_\ell}{\partial t} - P\nabla \cdot (\alpha_\ell \langle \mathbf{V}_\ell \rangle^{\chi\rho}) - \underbrace{\nabla \cdot \alpha_\ell(\langle \mathbf{q}_\ell^{''} \rangle^\chi + \mathbf{q}_\ell^{Re})}_{A} \\
&+ \underbrace{\alpha_\ell(\langle \boldsymbol{\tau}_\ell \rangle^\chi + \mathbf{T}_\ell^{Re}) : \nabla \langle \mathbf{V}_\ell \rangle^{\chi\rho}}_{B} + \mu_\ell h_{\ell i} + \underbrace{\frac{1}{2}\mu_\ell(\mathbf{V}_{\ell i} - \langle \mathbf{V}_\ell \rangle^{\chi\rho})^2}_{C} \\
&+ Q_\ell + \alpha_\ell q_\ell^{'''} + \underbrace{\mathbf{F}_{\ell i} \cdot (\mathbf{V}_{\ell i} - \langle \mathbf{V}_\ell \rangle^{\chi\rho})}_{D}
\end{aligned}
\tag{15}
$$

is the form of the energy equation used by Amarasooriya and Theofanous (1991). We observe that they neglect the average and turbulent heat flux divergences (A), the energy dissipated by the average $\langle \boldsymbol{\tau}_\ell \rangle^\chi$ and turbulent stress $\mathbf{T}_\ell^{Re}$ (B), the kinetic energy dissipation associated with phase change (C), and the work associated with interfacial momentum transfer (D).

Now let us return to equation (14) and make another transformation of the enthalpy form to express the balance in terms of the average entropy $\langle s_\ell \rangle^{\chi\rho}$. This involves two substitutions. First we subtract $\langle h_\ell \rangle^{\chi\rho}$ times the mass balance equation (10) to rewrite eq. (14) in terms of the material derivative

$$D\langle h_\ell \rangle^{\chi\rho}/Dt \equiv \frac{\partial}{\partial t}\langle h_\ell \rangle^{\chi\rho} + \langle \mathbf{V}_\ell \rangle^{\chi\rho} \cdot \nabla \langle h_\ell \rangle^{\chi\rho}.$$

As a result, the energy carried with mass becomes $\mu_\ell(h_{\ell i} - \langle h_\ell \rangle^{\chi\rho})$; this can be rewritten using the relation

$$\mu_\ell(h_{\ell i} - \langle h_\ell \rangle^{\chi\rho}) \simeq \mu_\ell T_\ell(s_{\ell i} - \langle s_\ell \rangle^{\chi\rho}) + \mu_\ell(P_i - \langle P \rangle^\chi)/\langle \rho_\ell \rangle^\chi$$

which can be justified using arguments similar to those in Arnold (1988), pp. 96-97. Under the assumption of a single pressure, the pressure difference term in the above expression vanishes.

Next, we use the approximation

$$\langle\rho_\ell\rangle^X D\langle h_\ell\rangle^{X\rho}/Dt \simeq \langle\rho_\ell\rangle^X\langle T_\ell\rangle^{X\rho}D\langle s_\ell\rangle^{X\rho}/Dt + DP/Dt \tag{16}$$

which can again be justified as in Arnold (1988); cf. pp. 92 and 96. The result is

$$\begin{aligned}\alpha_\ell\langle\rho_\ell\rangle^X\langle T_\ell\rangle^{X\rho}D\langle s_\ell\rangle^{X\rho}/Dt = &-\underbrace{\nabla\cdot\alpha_\ell(\langle\mathbf{q}_\ell''\rangle^X + \mathbf{q}_\ell^{Re})}_{A}\\ &+\underbrace{\alpha_\ell(\langle\boldsymbol{\tau}_\ell\rangle^X + \mathbf{T}_\ell^{Re}) : \nabla\langle\mathbf{V}_\ell\rangle^{X\rho}}_{B} + \mu_\ell T_\ell(s_{\ell i} - \langle s_\ell\rangle^{X\rho})\\ &+\underbrace{\frac{1}{2}\mu_\ell(\mathbf{V}_{\ell i} - \langle\mathbf{V}_\ell\rangle^{X\rho})^2}_{C} + Q_\ell + \alpha_\ell q_\ell''' + \underbrace{\mathbf{F}_{\ell i}\cdot(\mathbf{V}_{\ell i} - \langle\mathbf{V}_\ell\rangle^{X\rho})}_{D}\end{aligned} \tag{17}$$

Comparing this with equation (2.4.5.7) of Kolev, we see that again the turbulent dissipation associated with $\mathbf{T}_\ell^{Re}$ (B), and the energy dissipated by interfacial drag (D) are neglected. The average heat flux $\langle\mathbf{q}_\ell''\rangle^X$ is initially constituted by Kolev as proportional to $\nabla\langle T_\ell\rangle$, but is later neglected. The energy source associated with kinetic energy of mass transfer (C) does appear in Kolev's entropy balance equation. The dissipation from average viscous stress $\langle\boldsymbol{\tau}_\ell\rangle^X$ is optional in IVA3, and can be omitted in premixing problems.

The neglected turbulent fluctuation terms involving $\mathbf{T}_\ell^{Re}$, and $\mathbf{q}_\ell^{Re}$ are commonly omitted in multiphase flow modeling, as little is known about them. Thus the whole of term (A) is neglected. The other neglected terms in IVA3 — the divergence of average heat flux $\langle\mathbf{q}_\ell''\rangle^X$ and the energy dissipated by drag (D) — are dominated by the terms retained.

Again comparing eq. (17) with eq. (15), we see that IVA3 retains the kinetic energy dissipation associated with phase change (C), whereas Amarasooriya and Theofanous (1991) omit it. It is worth noting that because the transformation from eq. (15) to eq. (17) involves approximations such as eq. (16), we could not expect the two models to give identical results even if the treatment of the kinetic energy dissipation associated with phase change (C) were the same in both codes. Thus the entropy formulation eq. (17) has the disadvantage of making precise inter-code comparison of benchmark problems difficult. Kolev claims that the entropy formulation has the advantage of a simple form, without terms involving derivatives of pressure or volume fraction, as in eq. (15) or eq. (14). This claimed advantage is not very persuasive, as the computational effort involved in evaluating the extra terms in a numerical solution scheme is a relatively small fraction of the overall computation. There is however one theoretical advantage to the entropy formulation in IVA3: it can be more readily checked that $D\langle s_\ell\rangle^{X\rho}/Dt \geq 0$, in agreement with the second law of thermodynamics. Arnold et al. (1990) have noted that the second law is not always satisfied for other formulations such as eq. (15), and have recommended corrections to the average internal energy equation used in other codes, to insure that the second law holds. Deviations from the second law may be small in magnitude, and do not necessarily represent a significant error in the energy balance; but in any event, agreement with the second law is of course reassuring.

In sum, the entropy formulation of the energy balance has a slight advantage over the more usual formulation in terms of internal energy. If precise inter-code comparison were important, the advantage of the entropy formulation would be less compelling; however, precise comparisons are not very practical in view of the many different equations of state in different codes.

2 Working Form of Multifield Equations

We are now ready to put the averaged balance equations in working form. This involves dropping terms which are neglected, and constituting the interfacial transfer terms. We also derive a porous medium formulation, and introduce additional balance equations which describe the multicomponent fields.

Every aspect of the present description has been validated by close reading of the relevant parts of the Fortran source listing of IVA3, in the version used for premixing analysis.

2.1 Partial differential equations

Let us restate the three balance equations (10), (11), and (17) with only those terms which are actually treated in IVA3. We also transform the momentum equations to material derivative form, by subtracting the corresponding mass equation times the velocity. The finite difference momentum equations are more conveniently understood with reference to the material derivative form of the differential equations.

The partial differential equations express the balance of mass for each field

$$\frac{\partial}{\partial t}(\alpha_\ell \rho_\ell) + \nabla \cdot (\alpha_\ell \rho_\ell \mathbf{V}_\ell) = \mu_\ell \tag{18}$$

the balance of momentum for each field

$$\begin{gathered} \alpha_\ell \rho_\ell D\mathbf{V}_\ell / Dt + \alpha_\ell \nabla P = \\ \nabla \cdot (\alpha_\ell \boldsymbol{\tau}_\ell) + \alpha_\ell \rho_\ell \mathbf{g} + \mathbf{F}_{\ell i} - \mathbf{F}_{\ell w} + \mu_\ell (\mathbf{V}_{\ell i} - \mathbf{V}_\ell) \end{gathered} \tag{19}$$

and the balance of entropy for each field

$$\begin{gathered} \alpha_\ell \rho_\ell T_\ell D s_\ell / Dt = \\ + \tfrac{1}{2} \mu_\ell (\mathbf{V}_{\ell i} - \mathbf{V}_\ell)^2 + \mu_\ell T_\ell (s_{\ell i} - s_\ell) + Q_\ell + \alpha_\ell q_\ell^{'''} \end{gathered} \tag{20}$$

where

$\mu_\ell =$ volumetric mass generation rate
$\boldsymbol{\tau}_\ell =$ average viscous stress
$\mathbf{g} =$ gravitational body force
$\mathbf{F}_{\ell i} =$ interfacial momentum source
$\mathbf{F}_{\ell w} =$ wall friction
$\mathbf{V}_{\ell i} =$ velocity at the interface
$s_{\ell i} =$ entropy at the interface
$Q_\ell =$ interfacial heat transfer without mass transfer
$q_\ell^{'''} =$ volumetric heat generation rate

Recall again that terms of the form $\mu_\ell f_\ell$ are averages weighted by the interfacial mass transfer $\dot{m}_\ell$, that is,

$$\mu_\ell f_\ell \equiv \langle \rho_\ell f_\ell (\mathbf{V}_\ell - \mathbf{V}_i) \cdot \nabla \chi_\ell \rangle$$

In particular, such terms can include contributions from interfaces with more than one other field, as specified below.

2.2 Porous body formulation

Multifield flow models can be formulated for flow through a porous medium. In the thermohydraulics of intact cores, the fuel rod arrays are conveniently treated as an anisotropic porous medium. For premixing analysis, engineering structures within the vessel might be modeled as a porous medium.

A simple method of deriving a porous medium formulation is to consider a multifield model with $\ell = 1, \ldots L$ fields augmented by a field $L+1$ representing the porous medium. Its volume fraction $\tilde{\alpha}_{L+1}$ in an $(L+1)$-field formulation with

$$\sum_{\ell=1}^{L+1} \tilde{\alpha}_\ell = 1$$

is related to the volume porosity γ of the medium by

$$1 - \tilde{\alpha}_{L+1}(\mathbf{x}) = \gamma(\mathbf{x}).$$

The momentum equation for field $L+1$ is ignored under the assumption that $\mathbf{V}_{L+1} = 0$, and the energy equation is ignored also. The effect of the porous medium on the momenta of fields $1, \ldots L$ may be modeled in $\mathbf{F}_{\ell w}$. The $(L+1)$-field formulation reduces to an L-field model in which

$$\sum_{\ell=1}^{L} \alpha_\ell = 1$$

by defining α_ℓ to satisfy

$$\gamma \alpha_\ell = \tilde{\alpha}_\ell.$$

That is, the porous medium formulation of the multifield equations is obtained by writing $\gamma \alpha_\ell$ wherever α_ℓ appears in equations (18), (19), (20).

In some cases it might be possible to argue directly on physical grounds for a different treatment of engineering structures displacing flow volume. The formulation just derived is consistent with treating the structures in a porous medium formulation.

The numerical implementation of porosity factors will be discussed in section 3 below.

2.3 Multicomponent fields

IVA3 treats fields 1 and 2 as multicomponent fields. In fact, the code internally allows field 3 to have two material components also; however, this appears to be an artifact of a version of IVA3 which was designed to model the annular flow regime of an intact core using field 3 to represent water droplets. Since this modeling option is not intended for the premixing application, we ignore the multicomponent option for field 3, and discuss only fields 1 and 2. Note that the dispersal of corium particles into field 2 lacks a model for the dispersal rate in the present version; but since a two-component treatment of field 2 is foreseen, and the supporting code infrastructure is in place, we shall discuss it.

Field 1 consists of a mixture of air and saturated steam. The equation of state for this two-component mixture is

$$\rho_1 = \rho_{air} + \rho_{vapor}.$$

This composition of the mixture is described by introducing a concentration

$$c_1 \equiv \rho_{air}/\rho_1, \tag{21}$$

from which it follows that

$$1 - c_1 = \rho_{vapor}/\rho_1.$$

The density of each component is evaluated at its partial pressure. In solving the model numerically, it will be necessary to find ρ_1 given P, T_1, and c_1. This is done by finding the partial pressures which satisfy

$$\begin{aligned} P &= P_{air} + P_{vapor} \\ \rho_{air} &= P_{air}/(R_{air}T_1) \\ \rho_{vapor} &= \rho_{vapor}(T_1, P_{vapor}) \end{aligned}$$

by eliminating P_{air} in favor of P_{vapor}

$$\begin{aligned} P_{vapor} &= P - R_{air}T_1\rho_{air} \\ &= P - \frac{c_1}{1-c_1}R_{air}T_1\rho_{vapor}(T_1, P_{vapor}). \end{aligned}$$

This equation is then solved for P_{vapor} using a Newton iteration; the formulae used are equations (3.2.3) to (3.2.5) in KFK 4948. Further details on computing the mixture equation of state and its partial derivatives can be found in Kolev (1991a).

The purpose of defining the concentration as a density ratio in eq. (21) was to make $\alpha_1\rho_1 c_1$ the conserved quantity in the mass balance for air. The evolution of the concentration c_1 of air in field 1 is therefore described by the conservation equation

$$\frac{\partial}{\partial t}(\alpha_1\rho_1 c_1) + \nabla\cdot(\alpha_1\rho_1 c_1 \mathbf{V}_1) = \mu_{air}.$$

Normally μ_{air} is zero, although IVA3 does in principle allow for air introduced from an external source at a prescribed rate $\mu_{air} = c_1^{ext}\mu_1^{ext}$. The same balance can be rewritten in terms of the material derivative by subtracting c_1 times the mass balance eq. (18) of field 1 to obtain

$$\alpha_1\rho_1 Dc_1/Dt = \mu_{air} - c_1\mu_1.$$

Notice that μ_1^{ext} will also appear in μ_1, so the net source of air in the material derivative form of the concentration equation will be $(c_1^{ext} - c_1)\mu_1^{ext}$.

Field 2 consists of a mixture of liquid water and corium particles in thermal equilibrium. Again one wishes that $\alpha_2\rho_2 c_2$ be the conserved quantity in the mass balance for the corium component of field 2. Thus one defines

$$c_2 \equiv \alpha_{2,corium}\rho_{corium}/\alpha_2\rho_2 \tag{22}$$

where $\alpha_{2,corium}$ is the volume fraction of the corium assigned to field 2. In contrast to field 1, where each gas component occupies the full volume fraction α_1, here we have $\alpha_{2,corium} < \alpha_2$. In consequence, the composite equation of state is

$$1/\rho_2 = c_2/\rho_{corium} + (1 - c_2)/\rho_{water}.$$

The evaluation of ρ_2 is nevertheless straightforward, since the component equations of state involve only the system pressure P and temperature T_2:

$$\begin{aligned}\rho_{corium} &= \rho_{corium}(T_2, P)\\ \rho_{water} &= \rho_{water}(T_2, P).\end{aligned}$$

The concentration c_2 then evolves according to the conservation equation

$$\frac{\partial}{\partial t}(\alpha_2\rho_2c_2) + \nabla\cdot(\alpha_2\rho_2c_2\mathbf{V}_2) = \mu_{dispersal},$$

where $\mu_{dispersal}$ describes the dispersal of corium particles from field 3 into field 2. Expressed in material derivatives, this gives

$$\alpha_2\rho_2 Dc_2/Dt = \mu_{dispersal} - c_2\mu_2.$$

Notice that $\mu_{dispersal}$ will also appear as a term in μ_2, so the net contribution of dispersal to the material derivative form of the c_2 concentration equation will be $(1-c_2)\mu_{dispersal}$; this will vanish if $c_2 = 1$, insuring that c_2 never exceeds 1.

In addition to the inert component concentrations c_1 and c_2, an additional property, the particle number density n_ℓ evolves with each field. This quantity applies whenever a field is dispersed, for example bubbles, droplets, or solid particles, and gives the number of such particles per unit of volume. If the dispersed field particles are of uniform size, then the particle number density n_ℓ together with the volume fraction α_ℓ determine the diameter D_ℓ of an individual particle, from which the interfacial surface area per unit volume can be computed. This interfacial area is a key parameter in constituting interfacial transfer terms, particularly heat transfer.

The particle number density for a dispersed field ℓ evolves according to

$$\partial n_\ell/\partial t + \nabla\cdot(n_\ell\mathbf{V}_\ell) = N_\ell$$

where N_ℓ is the particle production rate; this typically describes a relaxation toward some equilibrium value n_ℓ^* with characteristic time τ_b.

2.4 Constitutive relations

We now begin a description of how the interfacial transfers of mass, momentum, and energy are constituted. IVA3 provides a very flexible framework for treating a variety of different flow and heat transfer regimes. At this stage of IVA3 assessment, the detailed consideration of every correlation used in every regime considered is less pressing than an overview of the general manner in which these terms are handled. In particular, we shall have some important comments to make in the next two sections regarding the treatment of heat, mass, and momentum transfer in the numerical solution procedure. With this in mind, we shall here give a limited but representative sample of the constitutive relations in IVA3, sufficient to illustrate all the difficulties which will confront us in assessing the numerical solution procedure.

2.4.1 Mass transfer

Mass transfer among the fields is constituted within the following general categories. For field 1, water vapor is created by evaporation, and removed by condensation; including the external mass source (which exists as an input option in IVA3) gives

$$\mu_1 = \mu_{evap} - \mu_{cond} + \mu_1^{ext}$$

For field 2, liquid water can be created by condensation, and removed by evaporation. The inert component corium enters field 2 by dispersal from field 3. Including a possible external mass source gives

$$\mu_2 = \mu_{cond} - \mu_{evap} + \mu_{dispersal} + \mu_2^{ext}$$

For field 3, corium is removed by dispersal to field 2, so

$$\mu_3 = -\mu_{dispersal} + \mu_3^{ext}$$

To illustrate the salient features of the mass transfer relations, we shall consider the contribution to phase change μ_{evap} due to the presence of field 3, particles of very hot corium. Note that the expressions given below are only these *contributions* to phase change; in a typical flow regime, the full expression for μ_{evap} would include other terms as well. The transfer of mass by phase change involves heat transfer as well, and in what follows, the contributions to μ_{evap} and to Q_ℓ are both given.

In order to accurately describe the constitution of heat and mass transfer, it is necessary to give not only the correlations used, but also the logic of flow regime and heat transfer regime identification. In the case of heat and mass transfer associated with particles of field 3, the expressions to be given below are used in either of two flow regimes: (i) continuous field 2 and dispersed field 3 with no field 1, or (ii) continuous field 2 with dispersed field 3 and field 1 as bubbles. If either of these flow regimes is identified (based on criteria involving mainly the volume fractions α_ℓ), then one of the following four heat transfer regimes will be selected: (1) convective heat transfer only; (2) subcooled nucleate boiling with partly compensating convective heat transfer; (3) nucleate boiling; (4) film boiling with radiative and convective heat transfer.

The first step in heat transfer regime identification is to compute the field 3 temperature threshold T_{3b} for the onset of nucleate boiling

$$T_{3b} = T_{sat} + \left[\frac{\alpha_c}{\alpha_b}(T_{sat} - T_2)\right]^{1/2}$$

where α_b is an empirical function of pressure, and α_c is a convective heat transfer coefficient, given as an empirical function of the corium particle size D_3 (determined from the field 3 particle number density n_3), the thermal conductivity of field 2, and the Peclet number for field 3 corium particles moving through continuous liquid field 2.

If $T_3 < T_{3b}$, then heat transfer is by convection from field 3 to field 2 with no phase change, case (1):

$$\begin{gathered} \mu_{evap} = 0 \\ Q_3 = -Q_2 = Q_{conv} = (\frac{6\alpha_3}{D_3})\alpha_c(T_2 - T_3) \end{gathered} \tag{23}$$

If on the other hand $T_3 > T_{3b}$, then further identification of the regime requires computing empirical expressions for a minimum stable film boiling temperature T_{3FB}, a critical heat flux Q_{32cr}, and a postulated nucleate boiling heat flux Q_{NB}. If either $T_3 > T_{3FB}$ or $Q_{NB} > Q_{32cr}$, the heat transfer regime is film boiling with radiative and convective heat transfer, case (4):

$$\begin{gathered} \mu_{evap} = (Q_{RAD} + Q_{FB})/(h_{vapor,sat} - h_{water}) \\ Q_3 = -Q_{RAD} - Q_{FB} - Q_{CONV} \\ Q_2 = Q_{CONV}. \end{gathered} \tag{24}$$

If neither the critical heat flux nor the film boiling temperature are exceeded, then it remains only to compare T_2 against the saturation temperature $T_{sat}(P)$. If $T_2 > T_{sat}$, there is nucleate boiling, case (3):

$$\begin{gathered} \mu_{evap} = Q_{NB}/(h_{vapor,sat} - h_{water}) \\ Q_3 = -Q_{NB} \end{gathered} \tag{25}$$

If on the other hand $T_2 < T_{sat}$, there is subcooled nucleate boiling with compensating convective heat transfer, case (2):

$$\begin{gathered}\mu_{evap} = (Q_{NB} - Q_{conv})/(h_{vapor,sat} - h_{water}) \\ Q_3 = -Q_{NB} \\ Q_2 = Q_{conv}\end{gathered} \tag{26}$$

The main features which will be important in discussing the numerical solution procedure are (1) the heat fluxes appear as source terms both in the mass and in the entropy equations; (2) the heat fluxes depend strongly on temperature differences, either between the phases, or relative to the saturation temperature; and (3) where the saturation temperature appears, there is a strong dependence on the pressure.

2.4.2 Momentum transfer

The terms in the field momentum equations which need to be constituted are the average stress tensor, the phase change contribution, and the interfacial forces composed of drag, added or virtual mass, and lift forces. The wall friction term is present in IVA3 only for cells in the spatial discretization for which the porosity factor γ is less than one, i.e. regions of intact reactor core or other engineering structures which displace a significant amount of the volume available to flow.

Average stress The pressure stress tensor has already been considered; we are here concerned with the remaining shear stress contribution to the total stress. Let us begin with the average stress tensor. In IVA3, this is constituted as the single-phase laminar viscous stress in its simplest form:

$$\nabla \cdot (\alpha_\ell \tau_\ell) = \alpha_\ell \rho_\ell \nu_\ell \nabla^2 \mathbf{V}_\ell \tag{27}$$

where ν_ℓ is the single-field kinematic viscosity; for multicomponent fields, this is computed by the composite rules of Kolev (1991a).

This expression could be strictly justified only for laminar flow of the continuous field. (By continuous field, we mean as usual the field which occupies a microscopically connected subregion of the volume open to flow, e.g. the liquid field in the flow regime of gas bubbles and solid particles flowing through connected liquid.). In turbulent flow, one would expect the average shear stress to be much larger, and not necessarily in the simple form above. Using the assumption of Reynolds that turbulent stresses take the same mathematical form as viscous stress, the effective viscosity coefficient would be much larger. For turbulent two-phase flow, the average shear stress might be greater still. Furthermore, in turbulent two-phase flow, one could imagine that a shear stress term might be appropriate for the dispersed phases as well as the continuous phase.

Not much is known about stresses in turbulent multiphase flow, although there are carefully derived recommendations for bubble flow (Nigmatulin 1979; Biesheuvel and van Wijngaarden 1984). The shear stress terms used in IVA3 surely underestimate the real stresses. In light of the incomplete state of knowledge of these effects, it would be prudent to regard the shear stress terms used in IVA3 as a starting point to explore the sensitivity of simulations to the modeling of shear stresses. Sensitivity studies could be performed with an artificially increased viscosity coefficient (already foreseen in the Fortran source), or with reference to the known expressions for bubble flow. There will be a limit to the magnitude of viscosity which can be computed stably under the IVA3 numerical scheme, as discussed below; however this limit will be several orders of magnitude larger than the viscosity coefficients currently used, so meaningful sensitivity tests are quite feasible.

Phase change contribution Constituting the phase change contribution to momentum transfer requires a specification of $\mathbf{V}_{\ell i}$, the velocity with which mass arrives in field ℓ by phase change. IVA3 follows a common practice of choosing this velocity to be the velocity of the field *from which* the mass comes. For example, for field 1, the velocity is

$$\mathbf{V}_{1i} = \begin{cases} \mathbf{V}_2 \text{ for evaporation} \\ \mathbf{V}_1 \text{ for condensation} \end{cases}$$

so the contribution to momentum transfer is

$$\mu_1(\mathbf{V}_{1i} - \mathbf{V}_1) = \mu_{evap}(\mathbf{V}_2 - \mathbf{V}_1).$$

By examining the momentum balance expressed in material derivative form (cf. equations (31-33) below), it can be seen that this assumption implies that condensation will not exert a decelerating force on the remaining gas, while vapor added to the gas by evaporation will need some force to accelerate it from the velocity $\mathbf{V}_2$ to velocity $\mathbf{V}_1$.

This assumption can be referred to as a donor field approximation. Sometimes in the literature one sees this described as a donor cell approximation, but that is a serious abuse of terminology: donor cell refers to spatial discretization of flow terms, whereas here we are choosing a field to associate with $\mathbf{V}_{\ell i}$, with the spatial location playing no role at this stage.

Donor field is not the only assumption which might be made for $\mathbf{V}_{\ell i}$. Some models use a compliance factor to set $\mathbf{V}_{\ell i}$ to some value between the velocities of the donor field and the accepting field. In some applications the value of the compliance factor might have an important effect, but for premixing analysis this is not a major consideration, or at least other modeling concerns are much more important.

Drag, virtual mass, and lift The principal interfacial force in most flow regimes is usually taken as a frictional drag force, generally constituted as some drag coefficient times the velocity of the dispersed field relative to the continuous field.

In flow regimes where the continuous phase is much more dense than the dispersed phase, one must also consider a virtual mass or added mass effect. This arises because a bubble moving through a liquid medium must accelerate not only its own mass, but also the mass of the liquid it displaces, which is of course much larger. This displaced mass is called the added mass, and the mass of the bubble plus the added mass is the virtual mass of the bubble. These terms are sometimes used loosely, so that one speaks of virtual mass when referring to what is, strictly speaking, the added mass term. The virtual mass effect also exists in droplet flow, but is clearly of no significance when the continuous phase is much less dense than the continuous phase. It would be significant for the gas field in bubble flow, and for the gas and liquid fields if there should arise a situation in which the corium is (locally) the continuous phase.

Associated with the added mass term is a lift force also acting on the dispersed field (Drew and Lahey 1987; Park 1992). Considering the motion of the gas, field 1, a general form for bubble flow would be

$$\mathbf{F}_{1i} = C_{21}^{d}(\mathbf{V}_2 - \mathbf{V}_1) + C_{21}^{vm}[\underbrace{D_1\mathbf{V}_1/Dt - D_2\mathbf{V}_2/Dt}_{\textit{added mass}} + \underbrace{(\mathbf{V}_2 - \mathbf{V}_1) \times \nabla \times \mathbf{V}_2}_{\textit{lift}}]$$

where

$$D_\ell \mathbf{V}_\ell / Dt \equiv \partial \mathbf{V}_\ell / \partial t + \mathbf{V}_\ell \cdot \nabla \mathbf{V}_\ell$$

Combining the added mass and lift terms is attractive from a theoretical viewpoint because, taken together, the two terms comprise a force which satisfies the criterion of *objectivity*: constitutive equations should retain their form under a change of coordinates from one non-inertial frame of reference to another. Applying this criterion can require great care, and the literature includes some debate as to whether, in a given situation, objectivity is a strict principle or just a good approximation. In multiphase flow, even greater care is required. Arnold (1988) includes a discussion of these issues.

The precise form of the drag force varies according to the Reynolds number for relative motion through the continuous phase, e.g.

$$Re_{21} = D_1(1-\alpha_1)\rho_2 \left|\mathbf{V}_2 - \mathbf{V}_1\right| / \eta_2$$

and also according to the bubble diameter D_1 derived from the bubble number density n_1. Typically, unless this Reynolds number is very low, C^d_{21} depends on $|\mathbf{V}_2 - \mathbf{V}_1|$; for example, in the case of cap bubbles,

$$C^d_{21} = \alpha_1 \frac{\rho_2}{D_1} c^d_{21} \left|\mathbf{V}_2 - \mathbf{V}_1\right|$$

where $c^d_{21} = 2(1-\alpha_{21})^2$ and $\alpha_{21} = \alpha_1/(\alpha_1+\alpha_2)$ is a modification of the usual two-phase formulation to allow for the volume displaced by the third field.

It should be noted that although the correct form for the drag force is

$$\mathbf{F}_{1i} = \alpha_1 \frac{\rho_2}{D_1} c^d_{21} \left|\mathbf{V}_2 - \mathbf{V}_1\right| (\mathbf{V}_2 - \mathbf{V}_1)$$

the IVA3 code actually uses the absolute values of the components of the relative velocity $(\mathbf{V}_2 - \mathbf{V}_1)$ rather than $|\mathbf{V}_2 - \mathbf{V}_1|$. Denoting $\mathbf{V} = (u, v, w)$ and $\mathbf{F}_{1i} = (F_{1i,x}, F_{1i,y}, F_{1i,z})$,

$$F_{1i,x} = \alpha_1 \frac{\rho_2}{D_1} c^d_{21} \left|u_2 - u_1\right| (u_2 - u_1)$$

and so on.

The added mass coefficient used in IVA3 for bubble flow is

$$C_{21}^{vm} = \tfrac{1}{2}\alpha_1\rho_2\frac{1+2\alpha_{21}}{1-\alpha_{21}}$$

The most important fact to note about this expression is the appearance of ρ_2; comparison with the differential equation shows that this increases the inertia of the gas field by the large factor ρ_2/ρ_1. Typically the gas inertia would be negligible next to the balance of ∇P and the drag force; but the virtual inertia could be important for treating the gas field correctly, especially in situations of strong acceleration.

In IVA3, the lift term is neglected completely, and the spatial derivatives in the virtual mass terms are also omitted. Incorporating these terms in the numerical solution procedure would pose a problem if convection were to be treated implicitly in the momentum equations; however, in a semi-implicit scheme, there is no obstacle to including the full virtual mass and lift terms, treated with explicit (old time level) finite differences. Although IVA3 claims to use a fully implicit scheme, it is not necessary for premixing analysis, and probably inefficient; this will be discussed in detail below.

Complete description of the interfacial momentum transfer expressions in IVA3 involves a number of different (mechanical) flow regimes, identified by logical decisions different from, and independent of, the heat transfer regime selection. To avoid unnecessary and confusing generality, we shall give a description for the specific mechanical regime of gas bubbles and corium particles in continuous liquid field 2. The interfacial forces consist of the liquid force $\mathbf{F}_{21}$ on bubbles just described, and the liquid force $\mathbf{F}_{23}$ on corium particles in field 3, appearing as

$$\begin{aligned}\mathbf{F}_{1i} &= \mathbf{F}_{21}\\ \mathbf{F}_{2i} &= -\mathbf{F}_{21}-\mathbf{F}_{23}\\ \mathbf{F}_{3i} &= \mathbf{F}_{23}\end{aligned}$$

where

$$\mathbf{F}_{23} = C_{23}^{d}(\mathbf{V}_2-\mathbf{V}_3) + C_{23}^{vm}[\underbrace{D_3\mathbf{V}_3/Dt - D_2\mathbf{V}_2/Dt}_{added\ mass} + \underbrace{(\mathbf{V}_2-\mathbf{V}_3)\times\nabla\times\mathbf{V}_2}_{lift}]$$

and C_{23}^{d} again depends on a (modified) Reynolds number. The added mass of the fuel particles in liquid field 2 could almost certainly be neglected, because corium is much more dense than water.

2.4.3 Entropy transfer

The most important interfacial term in the entropy balance is Q_ℓ; as explained above, the determination of Q_ℓ is made in conjunction with the evaluation of mass transfer. The example given above will suffice for this assessment.

It remains to constitute $\mathbf{V}_{\ell i}$ and $s_{\ell i}$. The choice of $\mathbf{V}_{\ell i}$ in IVA3 is the same as the donor field approximation used for the momentum equation:

$$\mathbf{V}_{1i} = \begin{cases} \mathbf{V}_2 \text{ for evaporation} \\ \mathbf{V}_1 \text{ for condensation} \end{cases}$$

Thus for example

$$\frac{1}{2}\mu_1(\mathbf{V}_{1i} - \mathbf{V}_1)^2 = \frac{1}{2}\mu_{evap}(\mathbf{V}_2 - \mathbf{V}_1)^2$$

with a null contribution for condensation (due to the material derivative form of the equation; cf. Sec. 2.4.2 above).

The interfacial entropy $s_{\ell i}$ is constituted in similar fashion, e.g.

$$s_{1i} = \begin{cases} s_2 \text{ for evaporation} \\ s_1 \text{ for condensation} \end{cases}$$

In constituting $\mu_\ell T_\ell(s_{\ell i} - s_\ell)$, the entropy transfer due to phase change is subtracted, and simultaneously the corresponding heat flux is left out of Q_ℓ. For example, in eqs. (25), the heat flux Q_{NB} is drawn from field 3 and directed entirely to production of vapor, but Q_{NB} is not added to the balance of entropy for field 1. So $\mu_{evap}T_1(s_{1i} - s_1)$ is adjusted by the same amount to give

$$\begin{gathered} \mu_{evap}T_1(s_2 - s_1) + \mu_{evap}(h_{vapor,sat} - h_{water}) = \\ \mu_{evap}T_1(s_2 - s_{1,sat}) + \mu_{evap}T_1(s_{1,sat} - s_1) + \mu_{evap}(h_{vapor,sat} - h_{water}) \\ = \mu_{evap}T_1(s_{1,sat} - s_1) \end{gathered}$$

This has the advantage of removing from the balance a dominating term which is both added and subtracted, improving the precision of the remaining balance computation.

For dispersal of fine corium particles from field 3 into field 2, there is no such compensating adjustments of the heat flux and mass transfer terms. The donor field rule is

$$s_{2i} = s_{3i} = s_3 \text{ for dispersal}$$

so the field 2 entropy balance equation should include a term

$$\mu_{dispersal} T_2 (s_{2i} - s_2) = \mu_{dispersal} T_2 (s_3 - s_2)$$

while in the field 3 entropy balance, the corresponding term is null because of the donor field rule.

Any volumetric heat sources $\alpha_\ell q_\ell'''$, including for example the radiative heat transfer Q_{RAD}, are treated as being included in Q_ℓ.

2.5 Final working form

We now repeat the working form of the averaged balance equations, with general forms of the transfer terms, and examples (in square brackets) constituted as described above. The example used for heat and mass transfer is nucleate boiling; for momentum transfer the example chosen is bubbles and corium particles in continuous liquid.

The balance of mass for field 1 is

$$\begin{gathered}\frac{\partial}{\partial t}(\alpha_1 \rho_1) + \nabla \cdot (\alpha_1 \rho_1 \mathbf{V}_1) = \mu_{evap} - \mu_{cond} + \mu_1^{ext} \\ \left[= \frac{Q_{NB}}{h_{vapor,sat} - h_{water}} = \left(\frac{6\alpha_3}{D_3}\right) \alpha_b \frac{(T_3 - T_{sat})^2}{h_{vapor,sat} - h_{water}} \right]\end{gathered} \tag{28}$$

The balance of mass for field 2 is

$$\begin{gathered}\frac{\partial}{\partial t}(\alpha_2 \rho_2) + \nabla \cdot (\alpha_2 \rho_2 \mathbf{V}_2) = \mu_{cond} - \mu_{evap} + \mu_{dispersal} + \mu_2^{ext} \\ \left[= \frac{-Q_{NB}}{h_{vapor,sat} - h_{water}} \right]\end{gathered} \tag{29}$$

The balance of mass for field 3 is

$$\frac{\partial}{\partial t}(\alpha_3\rho_3) + \nabla\cdot(\alpha_3\rho_3\mathbf{V}_3) = -\mu_{dispersal} + \mu_3^{ext} \qquad (30)$$

$$[=0]$$

The balance of momentum for field 1 is

$$\alpha_1\rho_1 D\mathbf{V}_1/Dt + \alpha_1\nabla P =$$

$$\alpha_1\rho_1\nu_1\nabla^2\mathbf{V}_1 + \alpha_1\rho_1\mathbf{g} + \mu_{evap}(\mathbf{V}_2 - \mathbf{V}_1) + \mathbf{F}_{1i} \qquad (31)$$

$$\left[\mathbf{F}_{1i} = \mathbf{F}_{21} = C_{21}^{d}(\mathbf{V}_2 - \mathbf{V}_1) + C_{21}^{vm}\frac{\partial}{\partial t}(\mathbf{V}_2 - \mathbf{V}_1)\right]$$

The balance of momentum for field 2 is

$$\alpha_2\rho_2 D\mathbf{V}_2/Dt + \alpha_2\nabla P =$$

$$\alpha_2\rho_2\nu_2\nabla^2\mathbf{V}_2 + \alpha_2\rho_2\mathbf{g} + \mu_{cond}(\mathbf{V}_1 - \mathbf{V}_2) + \mu_{dispersal}(\mathbf{V}_3 - \mathbf{V}_2) + \mathbf{F}_{2i} \qquad (32)$$

$$\left[\begin{array}{c} \mathbf{F}_{2i} = -\mathbf{F}_{21} - \mathbf{F}_{23} \\ = (C_{21}^{d} + C_{21}^{vm}\frac{\partial}{\partial t})(\mathbf{V}_1 - \mathbf{V}_2) + (C_{23}^{d} + C_{23}^{vm}\frac{\partial}{\partial t})(\mathbf{V}_3 - \mathbf{V}_2) \end{array}\right]$$

The balance of momentum for field 3 is

$$\alpha_3\rho_3 D\mathbf{V}_3/Dt + \alpha_3\nabla P =$$

$$\alpha_3\rho_3\nu_3\nabla^2\mathbf{V}_3 + \alpha_3\rho_3\mathbf{g} + \mathbf{F}_{3i} \qquad (33)$$

$$\left[\mathbf{F}_{3i} = \mathbf{F}_{23} = C_{23}^{d}(\mathbf{V}_2 - \mathbf{V}_3) + C_{23}^{vm}\frac{\partial}{\partial t}(\mathbf{V}_2 - \mathbf{V}_3)\right]$$

The balance of entropy for field 1 is

$$\alpha_1\rho_1T_1Ds_1/Dt =$$

$$\tfrac{1}{2}\mu_{evap}(\mathbf{V}_2-\mathbf{V}_1)^2+\mu_{evap}T_1(s_{1,sat}-s_1)+Q_1 \tag{34}$$

$$[Q_1=0]$$

The balance of entropy for field 2 is

$$\alpha_2\rho_2T_2Ds_2/Dt=\tfrac{1}{2}\mu_{cond}(\mathbf{V}_2-\mathbf{V}_1)^2+\tfrac{1}{2}\mu_{dispersal}(\mathbf{V}_2-\mathbf{V}_3)^2$$

$$+\mu_{cond}T_2(s_{2,sat}-s_2)+\mu_{dispersal}T_2(s_3-s_2)+Q_2 \tag{35}$$

$$[Q_2=0]$$

The balance of entropy for field 3 is

$$\alpha_3\rho_3T_3Ds_3/Dt=Q_3$$

$$\left[=-(\frac{6\alpha_3}{D_3})\alpha_b(T_3-T_{sat})^2\right] \tag{36}$$

These are the forms used in IVA3, with one exception: IVA3 includes modifications of the entropy transfer associated with phase change. These modifications are a term

$$\mu_{cond}c_1T_1(s_{air}-s_{vapor})$$

added to the right side of eq. (34), and a term

$$\mu_{evap}c_2T_2(s_{corium}-s_{water})$$

added to the right side of eq. (35). Such terms do not appear when a field consists of only one component. The term added to eq. (34) will be zero in case $c_1=0$, and also in case $c_1=1$ (because μ_{cond} would then necessarily be zero). These terms arise from the mass loss from each field (e.g. condensation from field 1 vapor). The donor field rule nullifies the mass loss term in the material derivative form of the entropy balance only when $s_1=s_{vapor}$, that is when $c_1=0$. Using the correct value s_{vapor} for the mass leaving field 1 when $c_1>0$ gives rise to the additional terms above.

3 Finite Difference Equations

3.1 Time scales and stability

In order to solve the multifield flow equations successfully, it is necessary to define a discrete approximation, and a procedure for advancing the solution of the appropriate initial-boundary value problem by one time step. IVA3 chooses a finite difference approximation, based on the usual staggered grid.

There are two principal considerations in defining the details of the finite difference approximation: first, the discrete solution should be accurate and remain numerically stable over time, and second, the computation of the solution should be efficient. The stability of finite difference approximations can be established by consideration of characteristic times associated with the various physical processes being described. In the case of multifield flow, the physical processes can be grouped as sonic propagation, interfacial coupling, fluid convection, and viscous stress. If one is content to solve the discrete equations for time step sizes smaller than all relevant characteristic times, one may use explicit finite differences, in which all terms other than time differences involve only variables at the current time level. There is no difficulty in advancing explicit difference equations by one time step. This approach is preferred if all evolutionary processes must be resolved in detail in the numerical scheme.

If on the other hand, some physical processes have very short characteristic times, and do not need to be resolved on their short time scales, the corresponding terms in the finite difference equations can be treated with implicit differences, using variables at the new time level. When done carefully, this yields a method which gives stable solutions using time steps larger than the related characteristic times. The price to be paid is that the procedure for advancing one time step becomes more difficult, involving simultaneous equations for the variables at the new time level.

Of course the stability sought is numerical stability; IVA3 is intended for simulation of highly transient behavior, and physical instabilities will be present and must be accurately simulated. The usual signature of numerical instability is growing oscillation with a period of two time steps, and is not difficult to recognize and distinguish from physical instability.

In multifield models such as IVA3, there are four groups of characteristic times. The interfacial exchange terms define characteristic times which may be viewed as relaxation times for the local temperature, pressure, or field velocity. The spatial derivative terms are implicated in sonic propagation, material convection, and viscous stress. The associated characteristic time for sonic propagation is the time for a pressure disturbance to travel the width of the smallest grid step; explicit differencing of sonic propagation would limit the time step size according to the Courant-Friedrichs-Lewy condition

$$\triangle t \leq \min(\triangle x, \triangle y, \triangle z)/c.$$

For convection, the characteristic time is the time for the fastest flowing material to move across the smallest grid step; explicit treatment of convection limits the time step size to

$$\triangle t \leq \min(\triangle x/u, \triangle y/v, \triangle z/w).$$

The characteristic time relating the viscosity to the grid size implies a time step limit for explicit treatment of viscous stress

$$\triangle t \leq \min(\triangle x^2, \triangle y^2, \triangle z^2)/2\nu.$$

The choice of strategy in IVA3 seems to be to treat convection, sonic propagation, viscous stress, and interfacial momentum coupling implicitly, and to treat interfacial heat and mass transfer explicitly. With the time step sizes used in IVA3 for premixing simulations (on the order of 0.1 milliseconds), there is little reason to treat convection and viscous stress implicitly. The kinematic viscosity of liquid water is roughly 10^{-6} m^2/sec; for grid spacings of 0.2 m, the characteristic time is 40,000 sec! For the material convection time, a velocity of 20 m/sec implies a characteristic time of 10 milliseconds. Even the single-phase sonic velocities (300 m/sec for air, 1200 m/sec for water) have characteristic times of 0.7 to 0.2 milliseconds.

Characteristic times for heat, mass and momentum transfer are more difficult to quantify, because of the complicated flow regime and heat transfer regime treatment. Characteristic times shorter than 10 milliseconds are likely to appear in heat and mass transfer, so that implicit treatment of at least some of these terms appears to be a higher priority than implicit convection. There is a special approximation procedure in IVA3 for rapid heat and mass transfer terms, but we have grave reservations about its accuracy. This issue will also be discussed below.

Revision of the IVA3 strategy may prove, upon further study, to be advisable. First, however, we present the finite difference equations in present use, based on the strategy just indicated.

3.2 IVA3 differencing scheme

3.2.1 Staggered grid and index convention

The discretization of the multifield flow equations is based on the staggered grid which is commonly used for fluid dynamics. The computational region is divided into an orthogonal grid of cells. The balances of mass and entropy are written for each cell. Each dependent variable has a principal site for each cell. Material properties of the fields, such as α_ℓ, ρ_ℓ, s_ℓ, and the pressure P have their principal sites at the center of each cell. The cells may thus be referred to as material cells. Velocities have their principal sites at the centers of the cell faces, with each velocity component situated on the cell face to which it is normal.

Three indices i, j, k identify each cell in the grid, specifically the cell center. That is, the index triple (i, j, k) identify the principal site of the material property variables. The principal sites of the velocity components are therefore $(i + 1/2, j, k)$ for u_ℓ; $(i, j + 1/2, k)$ for v_ℓ; and $(i, j, k + 1/2)$ for w_ℓ. These principal sites turn out to be very convenient for writing the finite difference form of the balance equations. However, in several instances, a variable will appear in the finite difference equations at a location other than its principal site, and when this happens, the variable will be expressed in terms of the neighboring principal site values by interpolation.

In order to maintain some readability of the discretized equations, a subscript convention will be used. Any variable taken at its *principal site* will be written with *all indices suppressed.* Only when *secondary sites* appear will indices be written explicitly, and then *only those indices differing from the principal site values need be shown.* (Occasionally for emphasis a principal site index may be written explicitly.) Thus

$$
\begin{aligned}
\alpha_\ell &= (\alpha_\ell)_{i,j,k} \\
(\alpha_\ell)_{i+1/2} &= (\alpha_\ell)_{i+1/2,j,k} \\
u_\ell &= (u_\ell)_{i+1/2,j,k} \\
(u_\ell)_{i+1} &= (u_\ell)_{i+1,j,k} \\
v_\ell &= (v_\ell)_{i,j+1/2,k} \\
(v_\ell)_{i+1} &= (v_\ell)_{i+1,j+1/2,k} \\
w_\ell &= (w_\ell)_{i,j,k+1/2} \\
(w_\ell)_{i+1} &= (w_\ell)_{i+1,j,k+1/2}
\end{aligned}
$$

and so on.

3.2.2 Mass equations

The finite difference form of the mass conservation equation represents the balance in a material cell whose center is the principal site for material properties:

$$
\begin{aligned}
&\frac{\gamma}{\Delta t}\left\{(\alpha_\ell\rho_\ell)^{n+1} - (\alpha_\ell\rho_\ell)^{n}\right\} \\
&+ \left\{\left[\gamma_x(\alpha_\ell\rho_\ell)^{n+1}(u_\ell)^{n+1}\right]_{i+1/2} - \left[\gamma_x(\alpha_\ell\rho_\ell)^{n+1}(u_\ell)^{n+1}\right]_{i-1/2}\right\}/\Delta x \\
&+ \left\{\left[\gamma_y(\alpha_\ell\rho_\ell)^{n+1}(v_\ell)^{n+1}\right]_{j+1/2} - \left[\gamma_y(\alpha_\ell\rho_\ell)^{n+1}(v_\ell)^{n+1}\right]_{j-1/2}\right\}/\Delta y \\
&+ \left\{\left[\gamma_z(\alpha_\ell\rho_\ell)^{n+1}(w_\ell)^{n+1}\right]_{k+1/2} - \left[\gamma_z(\alpha_\ell\rho_\ell)^{n+1}(w_\ell)^{n+1}\right]_{k-1/2}\right\}/\Delta z = \mu_\ell^n
\end{aligned}
\tag{37}
$$

The convected quantity $\alpha_\ell\rho_\ell$ at each material cell face is not at its primary site, and its value is specified by a donor cell rule

$$
\begin{aligned}
[\alpha_\ell\rho_\ell]_{i+1/2} &\equiv \begin{cases} (\alpha_\ell\rho_\ell)_i \text{ if } (u_\ell)_{i+1/2}^{n+1} > 0 \\ (\alpha_\ell\rho_\ell)_{i+1} \text{ if } (u_\ell)_{i+1/2}^{n+1} < 0 \end{cases} \\
[\alpha_\ell\rho_\ell]_{j+1/2} &\equiv \begin{cases} (\alpha_\ell\rho_\ell)_j \text{ if } (v_\ell)_{j+1/2}^{n+1} > 0 \\ (\alpha_\ell\rho_\ell)_{j+1} \text{ if } (v_\ell)_{j+1/2}^{n+1} < 0 \end{cases} \\
[\alpha_\ell\rho_\ell]_{k+1/2} &\equiv \begin{cases} (\alpha_\ell\rho_\ell)_k \text{ if } (w_\ell)_{k+1/2}^{n+1} > 0 \\ (\alpha_\ell\rho_\ell)_{k+1} \text{ if } (w_\ell)_{k+1/2}^{n+1} < 0 \end{cases}
\end{aligned}
$$

Note the somewhat unexpected presence of donor cell rules in a supposedly implicit scheme; the function of donor cell differencing is usually to effectively add numerical dissipation which stabilizes an explicit finite difference scheme. The donor cell rules are convenient however if one decided to convert IVA3 to a scheme which treats convection explicitly.

All quantities used in the evaluation of the phase change rate μ_ℓ^n are taken at the old time level, so the treatment is explicit in mass transfer. This could result in significant restrictions on the size of the time step.

The discrete equation (37) contains the volume porosity factor γ, and additional factors γ_x, γ_y, γ_z in the discrete divergences. These factors describe reduced areas at the material cell faces. In the case of engineering structure represented as a porous medium, these factors γ_x, γ_y, γ_z should all be equal to the volume porosity γ; that is, the effective cell face area should be chosen such that when multiplied by the third linear dimension of the cell (Δx, Δy, or Δz) the volume available to flow is obtained. A proof of this fact can be found in Appendix D of Reed and Stewart (1981). In particular, the factors γ_x, γ_y, γ_z are *not* equal to the fraction of area available to flow at the cell faces. Thus it is somewhat misleading to refer to γ_x, γ_y, γ_z as surface permeabilities.

On the other hand, in cases where one wishes to model an engineering structure which restricts the flow in one of the three orthogonal coordinate directions without significantly reducing the volume available to flow, it would be more appropriate to use γ_x, γ_y, or γ_z (as appropriate) to model the reduced area for flow, and leave $\gamma = 1$. One can also imagine situations in which both approaches might be combined: γ modeling a partial reduction in volume available to flow, and one of γ_x, γ_y, or γ_z set to some value less than γ to model an additional restriction of flow area without further displacement of volume available to flow.

3.2.3 Momentum equations

Next we consider the finite difference form of the momentum equations; for the sake of concreteness and simplicity, we shall write the scalar equation for the component of momentum in the x-direction. The discrete momentum equations represent balances for cells which are not the material cell, but are displaced by one-half grid step in each direction, so that the balance for each velocity component is centered at the principal site for that component.

In order to motivate the finite difference form of the convection terms, it may be helpful to refer to their derivation from conservative differential form. After subtracting $\mathbf{V}_\ell$ times the mass equation, the two divergence terms are

$$\nabla \cdot (\gamma \alpha_\ell \rho_\ell \mathbf{V}_\ell \mathbf{V}_\ell) - \mathbf{V}_\ell \nabla \cdot (\gamma \alpha_\ell \rho_\ell \mathbf{V}_\ell).$$

Consider just the $\partial/\partial x$ terms in the equation for the velocity component u_ℓ

$$\frac{\partial}{\partial x}(\gamma \alpha_\ell \rho_\ell u_\ell u_\ell) - u_\ell \frac{\partial}{\partial x}(\gamma \alpha_\ell \rho_\ell u_\ell). \tag{38}$$

The first term is discretized about the principal site $(i+1/2, j, k)$ of u_ℓ, locating $\alpha_\ell \rho_\ell u_\ell$ at (i, j, k) and $(i+1, j, k)$ and the second factor u_ℓ by donor cell rules, while the second term is discretized by central differences:

$$\begin{gathered}\left\{\left[(\gamma_x \alpha_\ell \rho_\ell u_\ell)(u_\ell)\right]_{i+1} - \left[(\gamma_x \alpha_\ell \rho_\ell u_\ell)(u_\ell)\right]_i\right\} / \Delta x - \\ (u_\ell)_{i+1/2} \left\{(\gamma_x \alpha_\ell \rho_\ell u_\ell)_{i+1} - (\gamma_x \alpha_\ell \rho_\ell u_\ell)_i\right\} / \Delta x\end{gathered} \tag{39}$$

where

$$(\gamma_x \alpha_\ell \rho_\ell u_\ell)_{i+1} = (\gamma_x \alpha_\ell \rho_\ell)_{i+1} \frac{(u_\ell)_{i+1/2} + (u_\ell)_{i+3/2}}{2} \tag{40}$$

and

$$[u_\ell]_{i+1} \equiv \begin{cases} (u_\ell)_{i+1/2} \text{ if } (\gamma_x \alpha_\ell \rho_\ell u_\ell)_{i+1} > 0 \\ (u_\ell)_{i+3/2} \text{ if } (\gamma_x \alpha_\ell \rho_\ell u_\ell)_{i+1} < 0 \end{cases}$$

Note that the discretized mass balance equation used in the second line of (39) is *not* the finite difference equation (37). Here we use a different form of mass balance, centered at the principal site for u_ℓ and using central differences rather than donor cell rules. This form of mass balance is used solely for the purpose of deriving (or motivating) a discrete momentum balance in material derivative form.

In light of the donor cell rule for u_ℓ (used only in the first line of (39)!), we may rewrite

$$\left[(\gamma_x \alpha_\ell \rho_\ell u_\ell)(u_\ell)\right]_{i+1} / \Delta x - (u_\ell)_{i+1/2} (\gamma_x \alpha_\ell \rho_\ell u_\ell)_{i+1} / \Delta x$$

$$= (\gamma_x \alpha_\ell \rho_\ell u_\ell)_{i+1} \frac{(\Delta u_\ell)_{i+1}}{\Delta x}$$

where

$$\frac{(\Delta u_\ell)_{i+1}^{n+1/2}}{\Delta x} \equiv \begin{cases} 0 \text{ if } (\gamma_x \alpha_\ell \rho_\ell u_\ell)_{i+1} > 0 \\ \dfrac{(u_\ell)_{i+3/2}^{n} - (u_\ell)_{i+1/2}^{n+1}}{\Delta x} \text{ if } (\gamma_x \alpha_\ell \rho_\ell u_\ell)_{i+1} < 0 \end{cases} \tag{41}$$

Note that time levels have been indicated, as they are coded in IVA3; the mixed time levels will be further discussed below.

Because the discrete mass balance used in (39) is *not* the same as equation (37), the discrete momentum equations will not be strictly conservative—small numerical sinks or sources of momentum will be present as part of the truncation error for the spatial derivatives. In view of the other uncertainties in the momentum balances, this departure from strict momentum conservation in the discrete formulation is not a serious concern.

Similarly rewriting the remaining two terms in the expression (39) yields the expression

$$(\gamma_x \alpha_\ell \rho_\ell u_\ell)_{i+1}^{n} \frac{(\Delta u_\ell)_{i+1}^{n+1/2}}{\Delta x} + (\gamma_x \alpha_\ell \rho_\ell u_\ell)_{i}^{n} \frac{(\Delta u_\ell)_{i}^{n+1/2}}{\Delta x}$$

as an approximation to the differential expression (38). The definition of

$$\frac{(\Delta u_\ell)_{i}^{n+1/2}}{\Delta x} \equiv \begin{cases} 0 \text{ if } (\gamma_x \alpha_\ell \rho_\ell u_\ell)_{i} > 0 \\ \dfrac{(u_\ell)_{i+1/2}^{n+1} - (u_\ell)_{i-1/2}^{n}}{\Delta x} \text{ if } (\gamma_x \alpha_\ell \rho_\ell u_\ell)_{i} < 0 \end{cases} \tag{42}$$

is precisely analogous in its spatial indices to the preceding definition in eq. (41) of $(\Delta u_\ell)_{i+1}^{n+1/2}/\Delta x$, but is repeated to specify the mixed time level coded in IVA3. It is now evident that the new time level is chosen whenever u_ℓ appears at the central principal site. This introduces minimal extra complication in the numerical procedure for advancing the finite difference solution one time step. While it is true that this partially implicit treatment of convection is unconditionally stable, its truncation error grows significantly worse when the time step exceeds the CFL convection limit, and for this reason the use of new time levels exclusively would usually be the preferred form of implicit differencing.

Difference forms of the expressions for the $\partial/\partial y$ and $\partial/\partial z$ terms can be written similarly. The interpolations to secondary sites for $(\gamma_y \alpha_\ell \rho_\ell v_\ell)_{j+1/2}$ and for $(\gamma_z \alpha_\ell \rho_\ell w_\ell)_{k+1/2}$ are more elaborate than eq. (40). This is because

$(i+1/2, j+1/2, k)$ as a secondary site for v_ℓ is best interpolated from the values of v_ℓ at four surrounding principal sites, and similarly for w_ℓ. Again the differences of u_ℓ in the y and z directions use new time level for the central site and old time level for the surrounding sites.

With this motivation, the discrete momentum equation for u_ℓ is

$$\begin{gathered}
\frac{1}{\Delta t}\left\{\gamma\alpha_\ell\rho_\ell(u_\ell^{n+1}-u_\ell^n)\right\}_{i+1/2} + (\gamma\alpha_\ell)^n_{i+1/2}\left\{P^{n+1}_{i+1}-P^{n+1}_i\right\}/\Delta x + \\
(\gamma_x\alpha_\ell\rho_\ell u_\ell)^n_{i+1}\frac{(\Delta u_\ell)^{n+1/2}_{i+1}}{\Delta x} + (\gamma_x\alpha_\ell\rho_\ell u_\ell)^n_i\frac{(\Delta u_\ell)^{n+1/2}_i}{\Delta x} + \\
(\gamma_y\alpha_\ell\rho_\ell v_\ell)^n_{i+1/2,j+1/2}\frac{(\Delta u_\ell)^{n+1/2}_{i+1/2,j+1/2}}{\Delta y} + (\gamma_y\alpha_\ell\rho_\ell v_\ell)^n_{i+1/2,j-1/2}\frac{(\Delta u_\ell)^{n+1/2}_{i+1/2,j-1/2}}{\Delta y} + \\
(\gamma_z\alpha_\ell\rho_\ell w_\ell)^n_{i+1/2,k+1/2}\frac{(\Delta u_\ell)^{n+1/2}_{i+1/2,k+1/2}}{\Delta z} + (\gamma_z\alpha_\ell\rho_\ell w_\ell)^n_{i+1/2,k-1/2}\frac{(\Delta u_\ell)^{n+1/2}_{i+1/2,k-1/2}}{\Delta z} + \\
= (\alpha_\ell\rho_\ell\nu_\ell)_{i+1/2}(\nabla^2\gamma u_\ell)^{n+1/2}_{i+1/2} + F^{n+1/2}_{\ell i,x} + \mu^n_\ell(u^{n+1}_{\ell i} - u^{n+1}_\ell)
\end{gathered} \tag{43}$$

where

$$\begin{aligned}
(\nabla^2\gamma u_\ell)^{n+1/2}_{i+1/2} \equiv {} & \left\{\frac{\gamma_{i+1}}{\Delta x_{i+1}}\left[(u_\ell^n)_{i+3/2} - (u_\ell^{n+1})\right] - \frac{\gamma_i}{\Delta x_i}\left[(u_\ell^{n+1}) - (u_\ell^n)_{i-1/2}\right]\right\}/\Delta x \\
& + \left\{\frac{\gamma_{j+1/2}}{\Delta y_{j+1/2}}\left[(u_\ell^n)_{j+1} - (u_\ell^{n+1})\right] - \frac{\gamma_{j-1/2}}{\Delta y_{j-1/2}}\left[(u_\ell^{n+1}) - (u_\ell^n)_{j-1}\right]\right\}/\Delta x \\
& + \left\{\frac{\gamma_{k+1/2}}{\Delta z_{k+1/2}}\left[(u_\ell^n)_{k+1} - (u_\ell^{n+1})\right] - \frac{\gamma_{k+1/2}}{\Delta z_{k-1/2}}\left[(u_\ell^{n+1}) - (u_\ell^n)_{k-1}\right]\right\}/\Delta x
\end{aligned}$$

Again the choice of time level for u_ℓ in the viscous stress terms is mixed, with new time level at the central site and old time level for surrounding sites. This is much easier to solve than fully implicit differencing, and is unconditionally stable, but again the accuracy deteriorates significantly if the time step exceeds the characteristic time associated with viscous stress on the discrete spatial grid.

The discretization of the drag and the time derivative part of the added mass is straightforward. We use the example of bubble flow. Since u_ℓ is only required at the principal site, the drag term can be treated implicitly:

$$F_{21,x}^{n+1/2} = \left[(C_{21}^d)_{i+1/2}^n + (C_{21}^{vm})_{i+1/2}^n/\Delta t\right](u_2^{n+1}-u_1^{n+1})-(C_{21}^{vm})_{i+1/2}^n/\Delta t(u_2^n-u_1^n)$$

The coefficients $(C_{21}^d)_{i+1/2}^n$ and $(C_{21}^{vm})_{i+1/2}^n$ are evaluated using material properties appropriately interpolated to the secondary site $(i+1/2, j, k)$; examples for α_ℓ and $\alpha_\ell\rho_\ell$ are shown below.

The phase change contribution is conveniently discretized with new time levels for the velocities, which again appear only at the central principal site:

$$\mu_\ell^n(u_{\ell i}^{n+1} - u_\ell^{n+1}) = \mu_{evap}^n(u_2^{n+1} - u_1^{n+1})$$

All quantities used in the evaluation of the phase change rate μ_ℓ^n are again taken at the old time level, so the treatment is again explicit.

Other quantities in the discrete momentum equation which appear at secondary sites are defined as follows:

$$(\gamma\alpha_\ell)_{i+1/2} \equiv \frac{(\gamma\Delta x\alpha_\ell)_{i+1} + (\gamma\Delta x\alpha_\ell)_i}{(\gamma\Delta x)_{i+1} + (\gamma\Delta x)_i}$$

$$(\gamma\alpha_\ell\rho_\ell)_{i+1/2} \equiv \frac{(\gamma\Delta x\alpha_\ell\rho_\ell)_{i+1} + (\gamma\Delta x\alpha_\ell\rho_\ell)_i}{(\gamma\Delta x)_{i+1} + (\gamma\Delta x)_i}$$

3.2.4 Entropy and concentration equations

The discrete forms of the entropy and concentration balances are very similar to the mass balances. Since entropies and concentrations are material properties, the discrete balances are again written with reference to the material cell whose center is the principal site (i, j, k) for all material properties.

Material derivative forms are used for the discrete entropy and concentration balances. As with the momentum equations, the spatial derivative term $\gamma\alpha_\ell\rho_\ell\mathbf{V}_\ell \cdot \nabla s_\ell$ is expressed as a difference

$$\nabla \cdot (\gamma \alpha_\ell \rho_\ell s_\ell \mathbf{V}_\ell) - s_\ell \nabla \cdot (\gamma \alpha_\ell \rho_\ell \mathbf{V}_\ell)$$

However, in contrast with the momentum equations, the discrete form for $\nabla \cdot (\gamma \alpha_\ell \rho_\ell \mathbf{V}_\ell)$ used in the entropy equation *is* identical with the form used in the discrete mass balance

$$[\nabla \cdot (\gamma \alpha_\ell \rho_\ell \mathbf{V}_\ell)]_{ijk}^{n+1} =$$

$$+\left\{[\gamma_x (\alpha_\ell \rho_\ell)^{n+1} (u_\ell)^{n+1}]_{i+1/2} - [\gamma_x (\alpha_\ell \rho_\ell)^{n+1} (u_\ell)^{n+1}]_{i-1/2}\right\} / \triangle x$$

$$+\left\{[\gamma_y (\alpha_\ell \rho_\ell)^{n+1} (v_\ell)^{n+1}]_{j+1/2} - [\gamma_y (\alpha_\ell \rho_\ell)^{n+1} (v_\ell)^{n+1}]_{j-1/2}\right\} / \triangle y$$

$$+\left\{[\gamma_z (\alpha_\ell \rho_\ell)^{n+1} (w_\ell)^{n+1}]_{k+1/2} - [\gamma_z (\alpha_\ell \rho_\ell)^{n+1} (w_\ell)^{n+1}]_{k-1/2}\right\} / \triangle z$$

The term $\nabla \cdot (\gamma \alpha_\ell \rho_\ell s_\ell \mathbf{V}_\ell)$ is discretized in precisely analogous fashion,

$$[\nabla \cdot (\gamma \alpha_\ell \rho_\ell s_\ell \mathbf{V}_\ell)]_{ijk}^{n+1} =$$

$$+\left\{[\gamma_x (\alpha_\ell \rho_\ell s_\ell)^{n+1} (u_\ell)^{n+1}]_{i+1/2} - [\gamma_x (\alpha_\ell \rho_\ell s_\ell)^{n+1} (u_\ell)^{n+1}]_{i-1/2}\right\} / \triangle x$$

$$+\left\{[\gamma_y (\alpha_\ell \rho_\ell s_\ell)^{n+1} (v_\ell)^{n+1}]_{j+1/2} - [\gamma_y (\alpha_\ell \rho_\ell s_\ell)^{n+1} (v_\ell)^{n+1}]_{j-1/2}\right\} / \triangle y$$

$$+\left\{[\gamma_z (\alpha_\ell \rho_\ell s_\ell)^{n+1} (w_\ell)^{n+1}]_{k+1/2} - [\gamma_z (\alpha_\ell \rho_\ell s_\ell)^{n+1} (w_\ell)^{n+1}]_{k-1/2}\right\} / \triangle z$$

and using donor cell rules

$$[\alpha_\ell \rho_\ell s_\ell]_{i+1/2} \equiv \begin{cases} (\alpha_\ell \rho_\ell s_\ell)_i \text{ if } (u_\ell)_{i+1/2}^{n+1} > 0 \\ (\alpha_\ell \rho_\ell s_\ell)_{i+1} \text{ if } (u_\ell)_{i+1/2}^{n+1} < 0 \end{cases}$$

and so on. The discrete entropy balance for field 1 is then

$$\frac{\alpha_1 \rho_1 \gamma}{\Delta t} \{(s_1)^{n+1} - (s_1)^n\}$$

$$+[\nabla \cdot (\gamma \alpha_1 \rho_1 s_1 \mathbf{V}_1)]_{ijk}^{n+1} - s_1^{n+1} [\nabla \cdot (\gamma \alpha_1 \rho_1 \mathbf{V}_1)]_{ijk}^{n+1} = \tag{44}$$

$$\left\{+\tfrac{1}{2}\mu_{evap}^n [(\mathbf{V}_2 - \mathbf{V}_1)_{ijk}^n]^2 + Q_1^n\right\} / T_1^n + \mu_{evap}^n (s_{1,sat}^n - s_1^{n+1})$$

Because the term $\nabla \cdot (\gamma\alpha_1\rho_1\mathbf{V}_1)$ is discretized here exactly as in the mass equation, the discrete entropy balance is strictly conservative in the spatial derivative terms; that is, the sum of all the discrete fluxes of entropy across all the material cells is zero for a closed region. Thus there are no numerical sources or sinks of entropy associated with the spatial discretization. This is a desirable property for the finite difference equations; it is most consequential in the simulation of very slow transients or steady states, where total energy and mass conservation is assured.

In IVA3, this discrete conservation is achieved while simultaneously benefiting from a favorable property of the material derivative form of entropy balance: namely, the largest portion $\mu_{evap}(s_{1,sat} - s_2)$ of the entropy carried by phase change is absent from the calculation of the entropy balance for field 1, for example. If the material derivative form were not used, the term $\mu_{evap}(s_{1,sat} - s_2)$ together with an opposing term $s_1\{\partial(\gamma\alpha_1\rho_1)/\partial t + \nabla \cdot (\gamma\alpha_1\rho_1\mathbf{V}_1)\}$ might dominate the remaining terms in cases of very rapid phase change. The absence of these two large terms which nearly cancel each other makes the calculation of the remaining terms in eq. (44) less susceptible to numerical error. The penalty paid for these advantages is the cost of computing $\nabla \cdot (\gamma\alpha_\ell\rho_\ell s_\ell\mathbf{V}_\ell) - s_\ell\nabla \cdot (\gamma\alpha_\ell\rho_\ell\mathbf{V}_\ell)$ in place of $\gamma\alpha_\ell\rho_\ell\mathbf{V}_\ell \cdot \nabla s_\ell$ or $\nabla \cdot (\gamma\alpha_\ell\rho_\ell s_\ell\mathbf{V}_\ell)$, and this cost is not great because $\nabla \cdot (\gamma\alpha_\ell\rho_\ell\mathbf{V}_\ell)$ has already been computed for the mass balances.

In short, this semi-conservative finite differencing of the entropy balance combines advantageous properties of both the fully conservative form and the material derivative form.

3.2.5 Approximation of heat transfer terms

In addition to the discrete approximations detailed above, there is one further aspect of the discretization which must be described. Some of the heat transfer terms comprising Q_ℓ and μ_ℓ are modified by factors intended to provide a better approximation of their temporal evolution than can be obtained from a first-order explicit differencing scheme. For example, in the case of the convective heat transfer contribution in eq. (23), instead of Q_{conv}, IVA3 uses

$$\overline{Q}_{conv} = Q_{conv} f$$

where

$$f = \frac{\tau_3^*}{\Delta t}(1 - e^{-\Delta t/\tau_3^*}),$$
$$\tau_3^* = \frac{D_3 \rho_3 c_{P3}}{6\alpha_c}.$$

The factor f involves the ratio of the discrete time step size Δt to a characteristic time τ_3^* for this heat transfer process, and can be motivated by the following consideration. Suppose we consider a highly simplified entropy balance for field 3,

$$\alpha_3 \rho_3 T_3 \frac{\partial s_3}{\partial t} = \alpha_3 \rho_3 c_{P3} \frac{\partial T_3}{\partial t} = Q_3 = Q_{conv}$$
$$= (\frac{6\alpha_3}{D_3})\alpha_c(T_2 - T_3)$$

Suppose further that during the time Δt, the value of T_2 remains sensibly constant; then T_3 relaxes toward the value T_2 with the characteristic time τ_3^* according to

$$\frac{\partial T_3}{\partial t} = \frac{(T_2 - T_3)}{\tau_3^*}$$

Under these assumptions, the value of T_3^{n+1} at the end of the time step Δt would satisfy

$$T_3^{n+1} - T_2 = (T_3^{n+1} - T_2)e^{-\Delta t/\tau_3^*}.$$

The same value of T_3^{n+1} would be obtained from an explicit finite difference equation

$$\frac{(T_3^{n+1} - T_3^n)}{\Delta t} = \frac{(T_2 - T_3^n)}{\tau_3^*} f$$

where the value of f may be determined by rewriting

$$T_3^{n+1} - T_3^n = T_3^{n+1} - T_2 + (T_2 - T_3^n)$$

$$= (T_2 - T_3^n)(1 - e^{-\Delta t/\tau_3^*}).$$

From this it follows that the value of f must be as stated above.

It should be particularly noted that the value of f approaches the very small value $\tau_3^*/\Delta t$ when the time step size Δt is much larger than the characteristic time τ_3^*. In other words, the heat transfer is sharply reduced to such an extent that the characteristic time for change in T_3 is made equal to Δt. Thus the possibility that explicit differencing of the heat transfer terms would produce numerical instability for $\Delta t > \tau_3^*$ is eliminated. Similar approximation factors f are introduced into the heat transfer and phase change contributions in other heat transfer regimes.

The assumptions on which this approximation rests are a highly simplistic entropy balance, and the constancy of T_2. These assumptions are unlikely to be valid in actual simulations of complex phenomena like premixing or detonation of steam explosions. Furthermore, it should be noted that where flow and heat transfer regimes dictate multiple contributions to the total heat transfer, IVA3 may apply several approximation factors f based on contradictory assumptions, for example, that T_2 is sensibly constant in deriving one approximation factor f while assuming that T_2 relaxes with a characteristic time in deriving another factor f in a separate heat transfer contribution.

Finally, it must be recognized that these approximation factors have as a consequence the very undesirable property that the magnitude of heat transfer contributions will depend on the time step size Δt. When Δt is larger than the characteristic time for any given heat transfer contribution, doubling Δt will halve the heat transfer contribution.

The possibility of significant errors caused by these approximation factors f in the heat transfer terms is a serious cause for concern about the accuracy of IVA3, and calls for a careful and detailed investigation, to be outlined at the end of this report.

3.3 Semi-implicit differencing

Although IVA3 uses a fully implicit treatment of sonic propagation, convection, and viscous stress, we have seen that the treatment of convection and viscous stress in the momentum equations uses mixed time levels which have poor accuracy for large time step sizes. This causes no practical difficulties because the very rapid evolution of a premixing transient means that time step sizes must in any case be held below the material convective limit. In view of this, it must be asked what is the cost in computational effort required for implicit convection, and whether it might be more efficient to adopt a different overall strategy and treat all aspects of material convection with explicit differences. In particular, the divergences in the mass and entropy balances could then be written with the material properties at the old time level, retaining new time levels only for the velocities. As we shall see in the next section, this would result in a significant simplification of the IVA3 numerical solution procedure.

Here, for comparison, we give the semi-implicit difference equation for mass balance:

$$\begin{aligned}
&\frac{\gamma}{\Delta t}\left[(\alpha_\ell\rho_\ell)^{n+1} - (\alpha_\ell\rho_\ell)^n\right] \\
&+ \left\{[\gamma_x(\alpha_\ell\rho_\ell)^n(u_\ell)^{n+1}]_{i+1/2} - [\gamma_x(\alpha_\ell\rho_\ell)^n(u_\ell)^{n+1}]_{i-1/2}\right\}/\Delta x \\
&+ \left\{[\gamma_y(\alpha_\ell\rho_\ell)^n(v_\ell)^{n+1}]_{j+1/2} - [\gamma_y(\alpha_\ell\rho_\ell)^n(v_\ell)^{n+1}]_{j-1/2}\right\}/\Delta y \\
&+ \left\{[\gamma_z(\alpha_\ell\rho_\ell)^n(w_\ell)^{n+1}]_{k+1/2} - [\gamma_z(\alpha_\ell\rho_\ell)^n(w_\ell)^{n+1}]_{k-1/2}\right\}/\Delta z = \mu_\ell^n
\end{aligned}$$

Again donor cell rules are used for the convected densities; the spatial indexing is exactly as given previously for eq. (37), with only the time level changed from $n+1$ to n.

Semi-implicit entropy and concentration balances would be written in completely analogous fashion.

It is possible, and sometimes desirable, to treat the phase change terms with more implicitness. For example, semi-implicit difference schemes typically admit new time levels for any material properties appearing in the phase change terms:

$$\mu_\ell^{n+1/2} = \mu_\ell(\boldsymbol{\alpha}^{n+1}, \mathbf{T}^{n+1}, P^{n+1}, \mathbf{V}_1^n, \mathbf{V}_2^n, \mathbf{V}_3^n)$$

where $\boldsymbol{\alpha} = \{\alpha_1, \alpha_2, \alpha_3\}$ and $\mathbf{T} = \{T_1, T_2, T_3\}$. Similarly, material properties (especially $\mathbf{T}$ and P) appearing in the heat transfer terms in the entropy balances may be taken at the new time level.

An efficient and reliable solution procedure incorporating this alternative numerical strategy is described in Reed and Stewart (1981).

4 Numerical Solution Procedure

Having once indicated the details of the finite difference equations, let us now consider a more concise description of these equations which will serve to describe the numerical solution procedure while suppressing unnecessary detail. The discrete mass balance (37) may be written as

$$\frac{\gamma}{\Delta t}\left[(\alpha_\ell\rho_\ell)^{n+1}-(\alpha_\ell\rho_\ell)^n\right]+\nabla\cdot\left[\gamma(\alpha_\ell\rho_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}\right]=\mu_\ell^n \tag{45}$$

keeping in mind that the discrete divergence involves each velocity component whose principal site is a material cell face; furthermore, the macroscopic densities $\alpha_\ell\rho_\ell$ in the discrete divergence are given by donor cell rules, so that values in adjacent material cells appear for each cell face having inward flow.

The discrete momentum equation (43) in the x direction is written compactly as

$$\begin{gathered}\frac{1}{\Delta t}\left[\gamma\alpha_\ell\rho_\ell(u_\ell^{n+1}-u_\ell^n)\right]_{i+1/2}+(\gamma\alpha_\ell)_{i+1/2}^n\left[P_{i+1}^{n+1}-P_i^{n+1}\right]/\Delta x+\\ (\gamma\alpha_\ell\rho_\ell\mathbf{V}_\ell)_{i+1/2}^n\cdot\nabla(u_\ell)_{i+1/2}^{n+1/2}=[\alpha_\ell\rho_\ell\nu_\ell]_{i+1/2}(\nabla^2\gamma u_\ell)_{i+1/2}^{n+1/2}\\ +F_{\ell i,x}^{n+1/2}((u_1)_{i+1/2}^{n+1},(u_2)_{i+1/2}^{n+1},(u_3)_{i+1/2}^{n+1})+\mu_\ell^n(u_{\ell i}^{n+1}-u_\ell^{n+1})\end{gathered} \tag{46}$$

keeping in mind that velocities u_ℓ at sites other than $(i+1/2,j,k)$ appear only in the convection and viscous stress terms (second line above), taken at the old time level. Only velocities u_ℓ at the central site $(i+1/2,j,k)$ are at the new time level.

Our compact form for the discrete entropy balance eq. (44) is

$$\begin{gathered}\frac{\alpha_1\rho_1\gamma}{\Delta t}[(s_1)^{n+1}-(s_1)^n]\\ +\nabla\cdot[(\gamma\alpha_1\rho_1 s_1)^{n+1}(\mathbf{V}_1)^{n+1}]-s_1^{n+1}\nabla\cdot[(\gamma\alpha_1\rho_1)^{n+1}(\mathbf{V}_1)^{n+1}]=\\ +\left\{\tfrac{1}{2}\mu_{evap}^n[(\mathbf{V}_2-\mathbf{V}_1)_{ijk}^n]^2+Q_1^n\right\}/T_1^n+\mu_{evap}^n(s_{1,sat}^n-s_1^{n+1})\end{gathered} \tag{47}$$

This equation is identical in structure to the mass balance: new time level velocity components at material cell faces, new time level material properties at the material cell center, and in adjacent cells when flow across a cell face is directed inward.

4.1 Outer iteration

Because of the multiple appearances of new time level quantities in the finite difference equations, often in nonlinear combinations (e.g. $\alpha_1\rho_1 s_1 \mathbf{V}_1$), no direct solution procedure is available. IVA3 uses an iterative procedure, with each iteration consisting essentially of two phases.

In the first phase of the outer iteration, the volume fractions, concentrations, and entropies are held fixed; the densities change only through changes in pressure. The momentum equations are combined with a mixture volume conservation equation, and solved simultaneously for estimates of the new velocities and pressures. This is achieved by first eliminating all velocities to obtain a set of simultaneous equations for the pressures in all cells, then solving this Poisson problem using one of several standard elliptic solvers. In this phase, the physical phenomena of sonic propagation, interfacial momentum exchange, and momentum convection are resolved through the implicit terms in the momentum equations, and the new time level velocities in the divergence terms of the mixture mass conservation equation.

In the second phase of the outer iteration, the pressures and velocities are held fixed; the densities change only through changes in entropies and concentrations. The individual field balance equations for masses, entropies, concentrations, and particle number densities are solved for estimates of the new volume fractions, entropies, concentrations, and particle number densities. This is achieved by a Gauss-Seidel iteration over all cells for each balance equation. In this phase, the physical phenomena of material convection is resolved through the new time level material properties in the divergence terms of the individual field material balance equations; the physical phenomenon of thermal expansion is resolved by computing density changes resulting from changes in entropy, and conservation of volume is reconciled. Because the heat and mass transfer terms have been differenced explicitly, we prefer *not* to say that these physical phenomena are resolved here, but rather that they are incorporated in the resolution of material convection and thermal expansion.

Each outer iterations carries out the first, pressure-velocity phase, and then the second, material convection phase. There is no relaxation or other adjustment to aid convergence. Because of the decoupling of physical phenomena in the two separate phases of each outer iteration, the overall solution cannot be considered as a generalized Newton or secant iteration for the full set of difference equations. Thus in contrast to other procedures such as the semi-implicit method of the THERMIT, TRAC, and other codes, the convergence of the IVA3 outer iterations cannot in general be guaranteed. In practical application to premixing analysis, the time step sizes used appear to decouple the equations, that is, to minimize the influence of the first phase estimates on the second phase, sufficiently that the outer iterations usually converge very rapidly after the first two outer iterations. However, in some cases, the result of the first outer iteration is observed to be erratic, and this can be attributed to the decoupled solution strategy. A more extensively coupled solution method such as used in THERMIT, for example, would in most instances avoid this erratic behavior of the first iteration.

4.2 Pressure-velocity phase

In this phase, the volume fractions, concentrations, and entropies are held fixed; the densities change only through changes in pressure. The momentum equations (46) are combined with a mixture volume conservation equation, and solved simultaneously for estimates of the new velocities and pressures.

The mixture volume conservation equation is obtained from a sum of the individual field mass balances, weighted by the specific volume ($= \rho_\ell^{-1}$) of each field. The purpose of this equation is to determine the relation between pressure changes in a cell and mass fluxes across the cell faces, independent of any changes of volume fractions. Returning to the differential form of mass balance,

$$\frac{\partial}{\partial t}(\alpha_\ell \rho_\ell) + \nabla \cdot (\alpha_\ell \rho_\ell \mathbf{V}_\ell) = \mu_\ell$$

we expand the time derivative

$$\frac{\partial}{\partial t}(\alpha_\ell \rho_\ell) = \rho_\ell \frac{\partial \alpha_\ell}{\partial t} + \alpha_\ell \frac{\partial \rho_\ell}{\partial t}$$

$$= \rho_\ell \frac{\partial \alpha_\ell}{\partial t} + \alpha_\ell \left(\frac{\partial \rho_\ell}{\partial P}\frac{\partial P}{\partial t} + \frac{\partial \rho_\ell}{\partial s_\ell}\frac{\partial s_\ell}{\partial t} + \frac{\partial \rho_\ell}{\partial c_\ell}\frac{\partial c_\ell}{\partial t} \right)$$

Now take the specific volume weighted sum of the balances for the individual fields:

$$\sum_\ell \frac{\partial \alpha_\ell}{\partial t} + \sum_\ell \frac{\alpha_\ell}{\rho_\ell}\left(\frac{\partial \rho_\ell}{\partial P}\frac{\partial P}{\partial t} + \frac{\partial \rho_\ell}{\partial s_\ell}\frac{\partial s_\ell}{\partial t} + \frac{\partial \rho_\ell}{\partial c_\ell}\frac{\partial c_\ell}{\partial t}\right)$$

$$+\sum_\ell \rho_\ell^{-1}\nabla \cdot (\alpha_\ell \rho_\ell \mathbf{V}_\ell) = \sum_\ell \rho_\ell^{-1}\mu_\ell$$

Of course $\sum_\ell \partial\alpha_\ell/\partial t = 0$; the elimination of time derivatives of the volume fractions was the goal of weighting by specific volume. We might have contemplated a mixture mass conservation equation, and simply ignored the effect of the changes in α_ℓ^{n+1} from the second, material convection phase of the outer iteration; but in that case, the decoupling of the pressure-velocity phase from the material convection phase would not be so effective, and the convergence of outer iterations would be impeded. Note however that the coupling of the two solution phases through entropy changes still exists. In particular, a change in density due to entropy change (i.e. thermal expansion) is not recognized in the pressure-velocity problem at the first outer iteration, because the entropy change will only be manifest in the second, material convection phase. This is the reason for the erratic behavior of the first outer iteration which is sometimes observed in IVA3. This design of the outer iteration will in principal also cause some deterioration in the rate of convergence in subsequent outer iterations, but any such deterioration appears to be much less dramatic than the effect on the first iteration.

These difficulties might be partly corrected by revising the outer iteration so that the material convection phase (including heat transfer) is performed *before* the pressure-velocity phase; this might reduce the erratic behavior of the first iteration. A better approach, although more difficult to implement, would be to more fully couple the solution procedure, including heat transfer effects in the pressure-velocity phase; this might improve both the initial iterations and the final convergence. This would correspond to the approach described in Reed and Stewart (1981).

The discrete form of the mixture volume conservation equation in IVA3 is

$$\begin{aligned}&\left[\gamma \textstyle\sum_\ell \dfrac{\alpha_\ell^{n+1}}{\rho_\ell^n}\left(\dfrac{\partial \rho_\ell}{\partial P}\right)^n\right]\dfrac{(P^{n+1}-P^n)}{\Delta t}+\textstyle\sum_\ell \nabla\cdot\left[\gamma(\alpha_\ell\rho_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}\right]/\rho_\ell^n \\ &=\textstyle\sum_\ell \dfrac{\mu_\ell^n}{\rho_\ell^n}-\gamma\textstyle\sum_\ell \dfrac{\alpha_\ell^{n+1}}{\rho_\ell^n}\left[\left(\dfrac{\partial \rho_\ell}{\partial s_\ell}\right)^n\dfrac{(s_\ell^{n+1}-s_\ell^n)}{\Delta t}+\left(\dfrac{\partial \rho_\ell}{\partial c_\ell}\right)^n\dfrac{(c_\ell^{n+1}-c_\ell^n)}{\Delta t}\right]\end{aligned} \qquad (48)$$

We now consider fixed all quantities in eq. (48) to be updated in the material convection phase of the outer iteration: the volume fractions α_ℓ^{n+1}, the entropies s_ℓ^{n+1}, the concentrations c_ℓ^{n+1}, and the convected macroscopic densities $(\alpha_\ell\rho_\ell)^{n+1}$ appearing in the discrete divergences. With these quantities considered fixed, the remaining new time level variables describe a relation between the cell face velocities and the change in pressure within the cell associated with the combined compressibility of the fields. The expression

$$\sum_\ell \frac{\alpha_\ell}{\rho_\ell}\left(\frac{\partial \rho_\ell}{\partial P}\right)=\frac{1}{\left(\sum_\ell \alpha_\ell\rho_\ell\right)a^2}$$

relates this combined compressibility to the sound speed a of the multifield mixture in mechanical equilibrium, i.e. all field velocities equal.

The velocities can be eliminated from the mixture volume concentration in favor of the pressure gradients across each cell face by using the momentum equations for each field and each velocity component. Keeping in mind that the partly implicit convection and viscous stress terms in the discrete momentum equation (46) involve new time level velocities only at the central site $(i+1/2, j, k)$ for u_ℓ, the discrete momentum equations for the three fields may be written as linear relationships

$$a_{11}u_1^{n+1}+a_{12}u_2^{n+1}+a_{13}u_3^{n+1}+b_1(P_{i+1}^{n+1}-P_i^{n+1})=c_1$$

$$a_{21}u_1^{n+1}+a_{22}u_2^{n+1}+a_{23}u_3^{n+1}+b_2(P_{i+1}^{n+1}-P_i^{n+1})=c_2$$

$$a_{31}u_1^{n+1}+a_{32}u_2^{n+1}+a_{33}u_3^{n+1}+b_3(P_{i+1}^{n+1}-P_i^{n+1})=c_3$$

Here the diagonal coefficients $a_{\ell\ell}$ involve the terms in eq. (46) where u_ℓ^{n+1} appears in the field ℓ balance, namely the time derivative, convection, viscous stress, drag, virtual mass, and phase change terms; the off-diagonal coefficients involve only the drag, virtual mass and phase change terms describing interfacial momentum exchange.

By inverting the 3×3 matrix $[a]$ this system can be simplified to a system

$$\begin{aligned} u_1^{n+1} + B_1(P_{i+1}^{n+1} - P_i^{n+1}) &= C_1 \\ u_2^{n+1} + B_2(P_{i+1}^{n+1} - P_i^{n+1}) &= C_2 \\ u_3^{n+1} + B_3(P_{i+1}^{n+1} - P_i^{n+1}) &= C_3 \end{aligned} \tag{49}$$

These relations at $(i+1/2, j, k)$ and the corresponding ones at $(i-1/2, j, k)$ can now be used to eliminate the cell face velocities from the $\partial/\partial x$ component of the divergences in the mixture volume conservation equation (48) in favor of the pressures P_{i+1}^{n+1}, P_i^{n+1}, and P_{i-1}^{n+1}. Similarly, the momentum equations for v_ℓ and w_ℓ lead to equations used to eliminate the remaining velocities from (48). The result is an equation for each cell involving the new time level pressures in the cell and in the six adjacent cells on both sides in the three coordinate directions. This system of equations for the pressures is elliptic. It can be shown that diagonal dominance is assured when at least one field is compressible and the interfacial drag coefficients are non-negative; see Reed and Stewart (1981) for a proof in the case of two velocity fields. The diagonal dominance is proportional to the ratio of the CFL sonic time step limit to the time step size Δt, and is of the order of the off-diagonal terms when Δt is of the order of the CFL sonic limit.

The pressure problem can be solved by any standard elliptic solver. IVA3 offers a choice of line or plane SOR; these methods should be entirely adequate for premixing analysis where the time step sizes are typically much smaller than the CFL sonic limit. If changes in the numerical method were to allow larger time step sizes, more efficient elliptic solvers, such as an incomplete Cholesky conjugate gradient method, might be preferred.

Once the pressure problem is solved, the equations (49) are used to infer the new time level velocities. This completes the pressure-velocity phase of the outer iteration.

The pressure-velocity phase of the outer iteration involves several subroutines in IVA3. The equations (49) do not change from one outer iteration to the next, and can be pre-computed before the outer iterations begin. This is done in subroutine I2DIV, which in turn calls I2DIVU, I2DIVV, and I2DIVW to compute the momentum convection, viscous stress, and phase change terms, subroutine DRAG00 for the interfacial drag and virtual mass terms, and subroutine RELI which assembles the momentum equations and inverts the 3 × 3 matrices to obtain the velocity-pressure gradient relations (49). The coefficients B are stored as variables RUU, RVV, and RWW for the u_ℓ, v_ℓ, and w_ℓ equations; the remainders C are stored as DUU, DVV, and DWW.

The mixture volume conservation equation must be recomputed for each outer iteration; this is done in subroutine ASSCO1, along with the reduction to the Poisson problem. The variant Poisson solvers are subroutines POISZY, POISFL, POISRE, and POISON. The backward substitution of the new pressures into equations (49) for the new velocities is done in subroutine I2GESH. Finally, in the case of cylindrical geometry, the velocities at azimuthal angle zero and at angle 2π must be identified, and this is done in subroutine ZYKLUS. This concludes the pressure-velocity phase of the outer iteration.

4.3 Material convection phase

In this phase, the pressures and velocities are held fixed; the densities change only through changes in entropies and concentrations. The individual field balance equations for masses, entropies, concentrations, and particle number densities are solved for estimates of the new volume fractions, entropies, concentrations, and particle number densities. This is achieved by a Gauss-Seidel iteration over all cells for each balance equation. Let us first see how this applies to an individual field mass balance equation

$$\frac{\gamma}{\Delta t}\left[(\alpha_\ell\rho_\ell)^{n+1} - (\alpha_\ell\rho_\ell)^n\right] + \nabla\cdot\left[\gamma(\alpha_\ell\rho_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}\right] = \mu_\ell^n$$

For each cell, it is convenient to divide the terms in the discrete divergence into two groups, fluxes of mass leaving a cell, and fluxes of mass entering the cell:

$$\nabla\cdot[\gamma(\alpha_\ell\rho_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}] =$$

$$\nabla\cdot[\gamma(\alpha_\ell\rho_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}]_{out} + \nabla\cdot[\gamma(\alpha_\ell\rho_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}]_{in}$$

Because of the donor cell rules for the mass fluxes, the $[\ ]_{out}$ fluxes involve only the macroscopic density $\alpha_\ell\rho_\ell$ in the cell (i,j,k), so

$$\nabla\cdot\left[\gamma(\alpha_\ell\rho_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}\right]_{out} = (\alpha_\ell\rho_\ell)_{ijk}^{n+1}\nabla\cdot\left[\gamma(\mathbf{V}_\ell)^{n+1}\right]_{out}$$

On the other hand, the $[\ ]_{in}$ fluxes involve exclusively macroscopic densities in the neighboring cells. This partitioning is the basis for a Gauss-Seidel iterative solution for the new time level macroscopic densities. Marching over the cells in a fixed sequence, a new estimate for α_ℓ^{n+1} is obtained as

$$\alpha_\ell^{n+1} = \frac{\gamma\left(\dfrac{\alpha_\ell^n\rho_\ell^n}{\Delta t} + \mu_\ell^n\right) + \nabla\cdot\left[\gamma(\alpha_\ell\rho_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}\right]_{in}}{\left(\dfrac{\gamma}{\Delta t} + \nabla\cdot\left[\gamma(\mathbf{V}_\ell)^{n+1}\right]_{out}\right)\rho_\ell^{n+1}} \tag{50}$$

Always the latest available values for the macroscopic densities $\alpha_\ell\rho_\ell$ in the neighboring cells are used in computing the $[\ ]_{in}$ fluxes: for neighbors preceding cell (i,j,k) in the marching sequence, macroscopic densities from the current Gauss-Seidel iteration are used, while for neighbors succeeding cell (i,j,k) in the marching sequence, macroscopic densities from the previous Gauss-Seidel iteration are taken.

A similar approach is used for the entropy balance. Both divergences are decomposed into incoming and outgoing fluxes, and the double decomposition is simplified as follows:

$$\begin{gathered}
\nabla\cdot\left[(\gamma\alpha_\ell\rho_\ell s_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}\right] - s_\ell^{n+1}\nabla\cdot\left[(\gamma\alpha_\ell\rho_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}\right] = \\
\nabla\cdot\left[(\gamma\alpha_\ell\rho_\ell s_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}\right]_{in} + (\alpha_\ell\rho_\ell s_\ell)_{ijk}^{n+1}\nabla\cdot\left[\gamma(\mathbf{V}_\ell)^{n+1}\right]_{out} \\
-s_\ell^{n+1}\nabla\cdot\left[(\gamma\alpha_\ell\rho_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}\right]_{in} - s_\ell^{n+1}(\alpha_\ell\rho_\ell)_{ijk}^{n+1}\nabla\cdot\left[\gamma(\mathbf{V}_\ell)^{n+1}\right]_{out} = \\
\nabla\cdot\left[(\gamma\alpha_\ell\rho_\ell s_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}\right]_{in} - s_\ell^{n+1}\nabla\cdot\left[(\gamma\alpha_\ell\rho_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}\right]_{in}
\end{gathered}$$

In the final line, we again have neighboring cell entropies exclusively in one term, and the entropy in cell (i,j,k) exclusively in the other term. Thus each step in the Gauss-Seidel iteration solves for

$$s_\ell^{n+1} = \frac{\gamma\left(\dfrac{\alpha_\ell^n\rho_\ell^n s_\ell^n}{\Delta t} + S_\ell^n\right) + \nabla\cdot\left[\gamma(\alpha_\ell\rho_\ell s_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}\right]_{in}}{\gamma\left(\dfrac{\alpha_\ell^n\rho_\ell^n}{\Delta t} + S_\ell^{n+1}\right) + \nabla\cdot\left[(\gamma\alpha_\ell\rho_\ell)^{n+1}(\mathbf{V}_\ell)^{n+1}\right]_{in}} \tag{51}$$

where (taking the example of field 1)

$$S_1^n = \left\{ \tfrac{1}{2}\mu_{evap}^n [(\mathbf{V}_2 - \mathbf{V}_1)_{ijk}^n]^2 + Q_1^n \right\} / T_1^n + \mu_{evap}^n s_{1,sat}^n$$

$$S_1^{n+1} = \mu_{evap}^n$$

The new concentrations c_ℓ and particle number densities n_ℓ are found in analogous fashion.

We can now summarize the Gauss-Seidel iterative procedure for estimating α_ℓ^{n+1}, s_ℓ^{n+1}, c_ℓ^{n+1}, n_ℓ^{n+1}, T_ℓ^{n+1}, and ρ_ℓ^{n+1} as follows:

1. For each Gauss-Seidel iteration, loop over cell in ascending order of indices; the z (or azimuthal) direction is the innermost loop, the x (or radial) direction is next, and the y (or axial) direction is the outermost loop. Inside all spatial index loops, loop over fields $\ell = 1, 2, 3$.

2. Compute new estimate of α_ℓ^{n+1} using eq. (50), new estimate of s_ℓ^{n+1} using eq. (51), and new estimate of c_ℓ^{n+1} similarly.

3. Compute new estimate of temperature T_ℓ^{n+1} and density ρ_ℓ^{n+1} by linear perturbation from the old time level values T_ℓ^n and ρ_ℓ^n :

$$T_\ell^{n+1} = T_\ell^n + (P^{n+1} - P^n)\frac{\partial T_\ell}{\partial P} + (c_\ell^{n+1} - c_\ell^n)\frac{\partial T_\ell}{\partial c_\ell} + (s_\ell^{n+1} - s_\ell^n)\frac{\partial T_\ell}{\partial s_\ell}$$

$$\rho_\ell^{n+1} = \rho_\ell^n + (P^{n+1} - P^n)\frac{\partial \rho_\ell}{\partial P} + (c_\ell^{n+1} - c_\ell^n)\frac{\partial \rho_\ell}{\partial c_\ell} + (s_\ell^{n+1} - s_\ell^n)\frac{\partial \rho_\ell}{\partial s_\ell}$$

In particular, the effect of thermal expansion is resolved in the last term perturbing ρ_ℓ^{n+1}.

4. Check that $\rho_\ell^{n+1} > 0$; check that $T_\ell^{n+1} - T_\ell^n$ does not exceed allowed limit.

5. Compute new estimate of particle number density n_ℓ^{n+1}.

6. Because there is no guarantee that $\sum_\ell \alpha_\ell = 1$ at this stage, the conservation of volume may have to be reconciled by adjusting one (or more) of the α_ℓ; currently in IVA3 this is done by adjusting the largest of the three α_ℓ.

7. If the change in α_ℓ^{n+1} for this cell from its value at the previous Gauss-Seidel iteration is larger than the corresponding change for preceding cells in the sweep, record the change (to check convergence of the Gauss-Seidel iterations); likewise for s_ℓ^{n+1} and c_ℓ^{n+1}.

8. If any cell does not meet the convergence criterion, repeat the entire procedure; however, no more than 10 Gauss-Seidel iterations are performed.

Since the Gauss-Seidel iteration is done mainly for the purpose of resolving material convection, the iteration should converge quickly when the time step size is much smaller than the material convection CFL limit. However, for larger time step sizes, the order in which cells are visited during the Gauss-Seidel iteration becomes important. When cells are visited in the same sequence as the direction of flow, the effect of convection is propagated over many cells in a single iteration. However, if the sequence of visiting cells opposes the direction of flow, convergence propagates by only one cell per iteration. In flow-through applications, a fixed sequence of visiting cells (as in IVA3) would be effective; but in problems in closed regions, where there is no preferred direction for convection, it would be much more effective to alternate the sequence of visiting cells from one Gauss-Seidel iteration to the next. However, we do not advocate such a modification to IVA3 for premixing; in view of the small time step sizes used in practice, it would be preferable to avoid the question of Gauss-Seidel iterative convergence entirely by treating material convection with explicit finite differences.

The Gauss-Seidel iterations would be unnecessary if convection were to be treated explicitly, so that the material properties in the discrete divergences were taken at the old time level. However, it might be preferable in that case to update the entropy first, permitting the temperature to be updated and the corresponding adjustment of density to be made before the new volume fraction is determined from the mass balance. Or a coupled simultaneous update of entropy and volume fraction in each cell may prove necessary.

The source terms μ_ℓ are treated explicitly in IVA3, and can therefore be computed once before the beginning of the outer iterations. This is done in subroutine INTGRA. The complete Gauss-Seidel iteration process is done in subroutine I4ALEN.

4.4 Automatic time step selection

For efficient computation of transients, it is desirable to choose the time step size during computation with an adaptive algorithm. Ideally the time step size should be just below the threshold of numerical instability, and just small enough to maintain reasonable truncation error.

IVA3 includes algorithms for automatic time step size selection. The principal criteria are limits on the magnitude of change in key variables (pressure, temperatures, volume fractions, velocities) during each time step. By limiting the changes per time step, truncation error is presumably kept at acceptable levels.

As noted above, IVA3 treats all heat and mass transfer processes with explicit finite differences. This implies some stability limit on time step size, involving certain characteristic times for the heat and mass transfer processes. Because of the complex interdependence of the mass and energy balances, it is difficult to analyze the characteristic times definitively. Rough estimates can be obtained using simplistic assumptions, as in Section 3.2.5 above. IVA3 uses some estimates of characteristic times to modify heat and mass transfer terms to effectively reduce the characteristic times and guarantee stability; but this is done at the cost of jeopardizing the accuracy, perhaps seriously. It would be safer in terms of accuracy to use the estimates of characteristic times to limit the time step size, but this could increase the computational effort. In the long run, an implicit or selectively implicit treatment of heat and mass transfer may be required for best accuracy and efficiency.

At present, even the adjustments to heat transfer may not insure numerical stability. Only some contributions are adjusted; it is far from clear that these are the only contributions of significance for stability. Furthermore, even if all contributions were analyzed and adjusted, the simplistic analyses might not be conclusive for the stability of the coupled system of equations.

If numerical instabilities should develop during a simulation due to strong heat and mass transfer, they will probably be eventually damped out by the automatic time step selection. Typical numerical instabilities generate growing oscillations with a period of two time steps. Such oscillations superposed on the underlying (physical) trends in the variables will substantially increase the magnitude of changes during each time step. If the limits on changes per time step are chosen carefully, the growing numerical instability will cause the time step to be reduced before the oscillations reach catastrophic proportions.

Although the adaptive selection of time step size is in one sense a desirable means of balancing accuracy and efficiency, in another sense it might possibly conceal a multitude of sins. If the explicit treatment of heat transfer terms implies strong constraints on the time step size, these constraints will be realized through the time step size selection. Oscillatory numerical instabilities will continually erupt and be gradually damped out, introducing inaccuracies that would not be present if the time step could be chosen more rationally. If only the variable changes from the previous time step are checked, there is no way of knowing whether the time step size is a result of unavoidable accuracy requirements for a very rapid transient phenomenon, or on the other hand if the time step size is small simply because of unrecognized numerical instabilities.

If numerical instabilities are present, it would be typical that the time step size itself would oscillate over periods of many time steps. On the other hand, if the time step constraints are purely physical, and unrelated to numerical instability, one would expect a more steady evolution of the time step size, with substantial changes occurring only when unusual physical events occur, e.g. a large slug of liquid impacting on a rigid structure.

In typical premixing simulations, IVA3 does exhibit large swings in time step size over many time steps, consistent with the eruption and suppression of numerical instabilities. Note that this indication by itself is consistent with, but does not necessarily imply, numerical instability problems; it could be that these swings in time step size are purely physical in origin. If however they are symptoms of time step constraints due to explicit treatment of heat and mass transfer, then a more implicit coupled treatment could result in the ability to use substantially large time step sizes, with corresponding improvements in computational efficiency.

There are at least two more incisive tests for potential numerical instabilities. One is to extend the analysis of characteristic times to all heat transfer contributions. This has value, but is difficult to extend beyond the simplistic analysis of individual contributions. Another approach would be more refined empirical evaluation of the numerical solution. For instance, one could save key solution variables over several time steps and examine them in the time domain for evidence of a strong component with a period of two time steps. In addition, spatial domain analysis could be performed to identify any spatial oscillations with a period of two spatial grid steps.

While it is certainly possible to implement such diagnostics as automatic algorithms within IVA3, the evaluation would be greatly facilitated by developing diagnostic tools using interactive graphic analysis. For example, an interactive version of IVA3 could repeat a small time slice of simulation following an intermediate dump, with visualization of solution variables under user control as the simulation steps forward. This would eliminate some of the missed opportunities for diagnosis which are inevitably dictated by the vast amounts of data generated and the limitations of storage media. Such an interactive visualization capability would certainly be of great benefit in evaluating the physics of IVA3 simulations, as well as any numerical problems.

5 Recommendations

The foregoing assessment has lead to six specific recommendations for future assessment and improvement of the IVA3 model and code. Briefly, they are: (1) improve code efficiency in the numerical treatment of material convection; (2) improve code efficiency (and perhaps accuracy) in numerical treatment of heat and mass transfer; (3) implement a more consistent representation of virtual mass and drag forces; (4) investigate the model sensitivity to the magnitude of viscous stresses; (5) develop improved visualization techniques to assess numerical stability and accuracy problems which may be masked by automatic time step size selection; and (6) apply state-of-the-art software tools to further improve code documentation.

The first recommendation is actually a series of suggestions concerning the implicit treatment of material convection, and the material convection phase of the outer iteration. The concern here is with computational efficiency; there is little doubt that in this regard the accuracy of the current scheme is acceptable. However, an execution profile of IVA3 carried out by M. Lummer has shown that about 40 percent of CPU time in a typical simulation is consumed in subroutine I4ALEN where the material convection phase is computed. Furthermore, it is typical to use as many as six Gauss-Seidel iterations in this phase. This means that there is substantial room for improvement in efficiency if the number of iterations can be reduced. If nothing else, it should be possible to save some time by allowing less convergence of the Gauss-Seidel iterations during the first few outer iterations, either by relaxing tolerances or by limiting the number of iterations. However, even better strategies are available.

A full Gauss-Seidel iteration of all cells is only required if there is substantial coupling among cells due to convection. However, in almost all cells the field velocities in typical premixing simulations are at least an order of magnitude smaller than $\Delta x/\Delta t$, so the convective coupling is in fact very weak. Therefore, the repeated Gauss-Seidel iterations are almost certainly being used to resolve coupling among the volume fractions, entropies, and concentrations in each cell separately. It is highly unlikely that as many as six iterations are required to resolve these couplings in every cell simultaneously. Therefore a next level of improvement could be obtained by eliminating the Gauss-Seidel full sweep, and only iterating in each cell as often as required for that cell. This could be done whenever the convective coupling is determined to be small. If one were to change the overall strategy to an explicit treatment of material convection, the convective coupling would automatically become null. In fact, just the simplification of computing the convective terms only once in each material convection phase should by itself create a considerable saving of computational effort.

Another level of improvement could be gained by noting that the coupling among variables in each cell separately (in particular the coupling of density and entropy through thermal expansion) is a relatively simple problem for which a set of simultaneous equations could be developed and solved rather easily.

A final improvement might involve incorporating these simultaneous equations into the pressure-velocity phase of the outer iteration. This might improve convergence of the outer iterations, make convergence more reliable (i.e. cut down on the need for time step reduction), and help the erratic behavior sometimes seen in the first iteration. Actually, this last problem, which is the most obviously vexing one, might be cured by simply reversing the order of the two phases in the outer iteration, as noted in Section 4.2 above.

If the explicit numerical treatment of material convection is adopted, then it would be preferable to make the treatment of momentum convection explicit as well. While this would not change the computational efficiency, it would remove any possible concern about the accuracy of the mixed time level differencing.

The second recommendation is for a detailed investigation of the treatment of heat and mass transfer, particularly whether there are numerical stability problems associated with the explicit treatment which are being masked by the automatic time step size algorithm. The adjustments to the heat transfer terms for time averaging should be examined to see if characteristic times are ever much shorter than the time step size. If so, the adjustments may seriously effect accuracy, and should be removed; if not, the adjustments have virtually no effect, and for safety's sake they should be removed.

With the adjustments removed, simulations should be diagnosed for any signs of numerical instability, that is, oscillations with a period of two discrete steps in either time or space. If any such evidence is found, further analysis should attempt to determine what heat and mass transfer regimes and contributions are responsible, whether a selectively implicit treatment is feasible, and whether it would substantially increase the allowable time step size. (That is, in addition to knowing the time step limitation which actually controls, one should look at the magnitudes of other limitations which would come into play if the strategy were modified.)

If no evidence is found that time step size selection is controlling numerical instabilities, then it is probably the case that physical rates of change inherent in the problem itself are limiting the time step size which can be used for accurate solutions. This should be carefully confirmed, since the time step sizes currently used in IVA3 appear to be smaller even than the CFL limit associated with single-phase sonic propagation, and one would therefore want to consider the extra simplicity and efficiency of a fully explicit numerical scheme.

A complete, accurate, and readable documentation of the entire logic of flow regime selection, heat transfer regime selection, and all heat and mass transfer correlations would be helpful in implementing this recommendation.

The third recommendation is to review the treatment of virtual mass and lift terms. The virtual mass could be neglected altogether in the more dense field; on the other hand, the spatial derivative terms and the lift force should be included in the less dense fields. Although these changes are limited in scope, it would be preferable to defer them until the issue of material convection is resolved. If convection is treated with explicit differences, the treatment of spatial derivatives in virtual mass and lift should be explicit also, and this would be simpler and more straightforward to implement.

The fourth recommendation is to perform sensitivity studies of the effect of the magnitude of the viscous stress terms. Although little is known about turbulent shear stress, it would be enlightening to know whether a large increase in the single-phase kinematic viscosity coefficient would have any significant impact on a typical simulation. Furthermore, the use of donor cell rules in the differencing scheme is known to introduce an artificial viscosity which is proportional to the truncation error. The magnitude of this artificial viscosity is roughly equal to the largest viscosity which can be stably computed with an explicit difference scheme for the viscous stress term. By introducing an appropriate *negative* viscosity into the model, one can therefore effectively reduce the artificial viscosity, and hence get some idea of the effect which would be obtained by refining the mesh.

Of course viscosity relates only to the truncation error in the momentum equations. It is tempting to introduce mass and entropy diffusion terms into the model for the purpose of studying the sensitivity to possible turbulent diffusion, and estimating the truncation error due to the donor cell rules in the mass and entropy equations. However, it might be preferable to introduce instead a partial donor cell rule, in which the convected quantities in the divergence terms are taken at some location interpolated between the donor and the acceptor cell.

The fifth recommendation is to develop an interactive visualization capability for IVA3. This would help considerably in implementing the second recommendation, and would undoubtedly have great benefits for the assessment of the physics of simulations as well. The most powerful visualization tool would be based on a version of IVA3 executing on a workstation; since execution times may be much longer than on a mainframe, one would like to be able to use the workstation version to pick up from an intermediate dump created by a mainframe run. By performing the visualization interactively on the workstation while the simulation is in progress, one would be able to edit the output in the most productive way, for example recording time histories in specific cells identified as being of particular interest. This would provide much more effectively targeted visualization than is possible from batch runs, where the sheer volume of computed results precludes storage of all quantities of possible interest.

The sixth recommendation is to exploit state-of-the-art software tools to generate even better documentation of IVA3. Specifically, this report has been prepared using the $\TeX$ text formatting and typesetting system. There is a powerful software environment for code development, known as Web, originally developed by the same D. Knuth who originated $\TeX$. Web combines the facilities of $\TeX$ for documentation with any of several standard compilers, including Fortran. Sophisticated use of Web involves developing both code and documentation from a single source. This is said by its advocates to profoundly alter the process of code development, supporting and promoting greater clarity in basic code design. At the same time, code documentation benefits from improved clarity and reliability, which in turn promotes better code efficiency, reliability, and easier maintenance. Using Web at this level should be seriously considered in any new code development to supplement or supersede IVA3.

In the meantime, Web could be used at a simpler level to improve the documentation of IVA3. It would be possible to develop a unified source from which it would be possible to automatically generate an extended version of this report with the inclusion of appropriate segments of source code for reference, and also to generate source program listings in which portions of this report are included as comments. Even at this very simple level, the use of Web might provide substantial benefits. Much of the work needed to accomplish this has already been done by preparing this report with TEX.

BIBLIOGRAPHY

Amarasooriya, W.H., and Theofanous, T.G. (1991) Premixing of steam explosions: a three-fluid model. *Nucl. Eng. Des.* **126** 23-39.

Arnold, G.S. (1988) Entropy and objectivity as constraints upon constitutive equations for two-fluid modeling of multiphase flow. Ph.D. Thesis, Rensselaer Polytechnic Institute, Troy, N.Y.

Arnold, G.S., Drew, D.A., and Lahey, R.T. (1990) An assessment of multiphase flow models using the second law of thermodynamics. *Int. J. Multiphase Flow* **16**, 481-494.

Biesheuvel, A. and van Wijngaarden, L. (1984) Two-phase flow equations for a dilute dispersion of gas bubbles in liquid. *J. Fluid Mech.* **148**, 301-318.

Birkhoff, G. (1964) Averaged conservation laws in pipes. it J. Math. Anal. Appl. **8**, 66-77.

Bouré, J. and Delhaye, J.-M. (1981) General equations and two-phase flow modeling. In Hestroni, G. (ed.), *Handbook of Multiphase Systems*, Chapter 1.2, pp. 1-36 to 1-95. Hemisphere, Washington.

Drew, D.A. and Lahey, R.T. (1987) The virtual mass and lift force on a sphere in rotating and straining inviscid flow. *Int. J. Multiphase Flow* **13**, 113-121.

Ishii, M. (1975) *Thermo-fluid Dynamic Theory of Two-Phase Flow.* Eyrolles, Paris.

Kolev, N. (1991a) Derivatives for the equations of state of multicomponent mixtures for universal multicomponent flow models. *Nucl. Sci. Eng.* **108**, 74-87.

Kolev, N.I. (1991b) A three-field model of transient 3D multiphase, three-component flow for the computer code IVA3. Part 1: Theoretical basis: conservation and state equations, numerics. Report KFK 4948.

Kolev, N.I. (1991c) A three-field model of transient 3D multiphase, three-component flow for the computer code IVA3. Part 2: Models for the interfacial transport phenomena. Code validation. Report KFK 4949.

Kolev, N.I. (1991d) IVA3: Computer code for modelling of transient three-dimensional three phase flow in complicated geometry. Program documentation: Input description. Report KFK 4950.

Kolev, N.I. (1994a) The code IVA-4 - Modeling of mass conservation in multiphase multicomponent flows in heterogeneous porous-media. *Kerntechnik* **59**, 226-237.

Kolev, N.I. (1994b) The code IVA-4 - Modeling of momentum conservation in multiphase multicomponent flows in heterogeneous porous-media. *Kerntechnik* **59**, 249-258.

Kolev, N.I. (1995) The code IVA-4 - Modeling of entropy conservation in multiphase multicomponent flows in heterogeneous porous-media. *Kerntechnik*, in press.

Lahey, R.T., and Drew, D.A. (1989) The three-dimensional time and volume averaged conservation equations of two-phase flow. In *Advances in Nuclear Science and Technology*, Volume 20, pp. 1-69.

Lahey, R.T., Drew, D.A., Kalkach-Navarro, S., and Park, J.-W. (1992) The relationship between void waves and flow regime transition. Preprint.

Nigmatulin, R.I. (1979) Spatial averaging in the mechanics of heterogeneous and dispersed systems. *Int. J. Multiphase Flow* **5**, 353-385.

Park, J.W. (1992) Void wave propagation in two-phase flow. Ph.D. Thesis, Rensselaer Polytechnic Institute, Troy, N.Y.

Reed, W.H., and Stewart, H.B. (1981) THERMIT: A computer program for three-dimensional thermal-hydraulic analysis of light water reactor cores. Report EPRI NP-2032.