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# AN ASSESSMENT OF MULTIPHASE FLOW MODELS USING THE SECOND LAW OF THERMODYNAMICS

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**Abstract**—The constraints implied by the second law of thermodynamics have been used to check the validity of two-fluid models. It has been found that all current generation multiphase computer codes violate these constraints. This implies that the physical models used in these codes are inadequate. Recommendations are given for how to improve two-fluid modeling assumptions and a relatively simple set of closure conditions which satisfy the second law of thermodynamics is presented.

*Key Words:* two-fluid model, multiphase flow, phasic entropy

## INTRODUCTION

The second law of thermodynamics can be used to assess the validity of two-phase flow models. Previous studies have been performed in which the entropy constraint for the mixture as a whole was considered. However, the phasic entropy constraints must also be satisfied for each phase separately.

Green & Naghdi (1971) and Bedford & Ingram (1971) have presented two different methods that have been developed for applying phasic entropy constraints. Green & Naghdi (1971) introduced the free energy function (either that of Gibbs or Helmholtz may be used) and demonstrated that the entropy equation placed limits on the constitution of the phasic free energy. For engineering applications, this approach is not particularly useful, since it does not yield constraints on the state variables of interest.

Bedford & Ingram (1971) substituted constitutive equations into the Clausius–Duhem inequality in such a way that the variables of interest appear explicitly. They then used the definition of an admissible thermodynamic process to conclude that the coefficients of those variables which appear only once in the equality must be equal to zero. When the form of the constitutive equations are known, this approach provides an excellent method for developing constraints on those constitutive equations.

We have used a similar procedure in this work. The Gibbs equation is used to combine the entropy equation and the thermal energy equation to obtain an entropy constraint which is devoid of derivatives of the phasic specific entropy. The result is then used to evaluate the ability of two-fluid two-phase flow models to satisfy the second law.

The local instantaneous entropy equality will be derived first. This equation will then be appropriately averaged and combined with the total energy equation, the mechanical energy equation and the Gibbs equation to yield the desired form of the entropy constraint.

## DISCUSSION

The local instantaneous continuity, momentum, total energy and entropy equations of phase-$k$ are (Ishii 1975):

*continuity*,

$$\partial \rho_k / \partial t + \nabla \cdot (\rho_k \mathbf{V}_k) = 0; \qquad [1]$$

*momentum*,

$$\partial (\rho_k \mathbf{V}_k) / \partial t + \nabla \cdot (\rho_k \mathbf{V}_k \mathbf{V}_k) - \rho_k \mathbf{g}_k - \nabla \cdot \mathbf{T}_k = 0; \qquad [2]$$

*energy*,

$$\partial[\rho_k(u_k + 0.5\mathbf{V}_k\cdot\mathbf{V}_k)]/\partial t + \nabla\cdot[\rho_k\mathbf{V}_k(u_k + 0.5\mathbf{V}_k\cdot\mathbf{V}_k)] + \rho_k\mathbf{g}_k\cdot\mathbf{V}_k - \nabla\cdot(\mathbf{T}_k\cdot\mathbf{V}_k) + \nabla\cdot\mathbf{q}_k'' - q_k''' = 0; \quad [3]$$

*entropy*,

$$\partial(\rho_k s_k)/\partial t + \nabla\cdot(\rho_k s_k\mathbf{V}_k) + \nabla\cdot(\mathbf{q}_k''/T_k) - q_k'''/T_k = \Delta_k \geqslant 0. \quad [4]$$

The mechanical energy equation is formed by taking the dot product of the velocity ($\mathbf{V}_k$) with the momentum equation [2]. Subtracting the resulting mechanical energy equation from the total energy equation yields the so-called internal energy equation:

$$\partial(\rho_k u_k)/\partial t + \nabla\cdot(\rho_k u_k\mathbf{V}_k) + \nabla\cdot\mathbf{q}_k'' - q_k''' - \mathbf{T}_k : \nabla\mathbf{V}_k = 0. \quad [5]$$

The Gibbs equation expressed in terms of the material derivatives of the internal energy, $u_k$, the entropy, $s_k$, and the density $\rho_k$, may be combined with the continuity equation to obtain

$$\mathrm{D}u_k/\mathrm{D}t = T_k\,\mathrm{D}s_k/\mathrm{D}t - (p_k/\rho_k)\,\nabla\cdot\mathbf{V}_k. \quad [6]$$

Combining [6] and [5], and making use of the continuity equation [1], we obtain the following entropy equality:

$$\rho_k\,\mathrm{D}s_k/\mathrm{D}t + \nabla\cdot(\mathbf{q}_k''/T_k) - \mathbf{q}_k''\cdot\nabla(1/T_k) - q_k'''/T_k - (1/T_k)\boldsymbol{\tau}_k : \nabla\mathbf{V}_k = 0, \quad [7]$$

where use has been made of the constitutive assumption

$$\mathbf{T}_k = -p_k\mathbf{I} + \boldsymbol{\tau}_k,$$

where $\mathbf{T}_k$ is the stress tensor, $p$ is the pressure and $\boldsymbol{\tau}_k$ is the viscous stress tensor of phase-$k$; $\mathbf{I}$ is the identity tensor. We may combine [7] with [4] to obtain

$$\partial(\rho_k s_k)/\partial t + \nabla\cdot(\rho_k s_k\mathbf{V}_k) + \nabla\cdot(\mathbf{q}_k''/T_k) - q_k'''/T_k = \Delta_k, \quad [8a]$$

where

$$\Delta_k = \mathbf{q}_k''\cdot\nabla(1/T_k) + (1/T_k)\boldsymbol{\tau}_k : \nabla\mathbf{V}_k \geqslant 0. \quad [8b]$$

Although the terms $\mathbf{q}_k''\cdot\nabla(1/T_k)$ and $(1/T_k)\boldsymbol{\tau}_k : \nabla\mathbf{V}_k$ are not easy to evaluate, [8a,b] are advantageous in that they give the conditions under which the entropy equation becomes an equality.

Let us now derive an appropriate form of the averaged entropy equation. This work makes use of the ensemble average, defined by Drew & Wood (1985) to be

$$\langle f(x, t)\rangle = \int_M f(x, t, \mu)\,\mathrm{d}m(\mu),$$

where $m(\mu)$ is the measure (probability) of observing process $\mu$, and $M$ is the set of all processes. However, the results developed herein apply to any rigorous form of averaging.

Using the notation of Bouré & Delhaye (1981), the ensemble-averaged momentum equation of phase-$k$ is (Arnold 1988)

$$\partial(\alpha_k\langle\rho_k\rangle^x\langle\mathbf{V}_k\rangle^{x\rho})/\partial t + \nabla\cdot(\alpha_k\langle\rho_k\rangle^x\langle\mathbf{V}_k\rangle^{x\rho}\langle\mathbf{V}_k\rangle^{x\rho})$$
$$= \nabla\cdot[\alpha_k(\langle\mathbf{T}_k\rangle^x + \mathbf{T}_k^{\mathrm{Re}})] + \alpha_k\langle\rho_k\rangle^x\mathbf{g}_k + \mathbf{M}_k + \Gamma_k\mathbf{V}_{ki}, \quad [9]$$

where:

$\langle\mathbf{T}_k\rangle^x$—average stress tensor,
$\mathbf{T}_k^{\mathrm{Re}}$—Reynolds stress tensor, $\langle X_k\rho_k\mathbf{V}_k'\mathbf{V}_k'\rangle/\alpha_k$,
$\mathbf{M}_k$—interfacial momentum source, $-\langle\mathbf{T}_k\cdot\nabla X_k\rangle$,
$\Gamma_k$—mass generation rate, $\langle\rho_k(\mathbf{V}_k - \mathbf{V}_{ki})\cdot\nabla X_k\rangle$,
$\mathbf{g}_k$—body force,
$X_k(\mathbf{x}, t)$—phase indicator function $\begin{cases}1, & \text{if phase-}k\text{ is at location }\mathbf{x}\text{ at time }t,\\ 0, & \text{otherwise,}\end{cases}$
$\alpha_k$—average of the phase indicator function, $\langle X_k\rangle$,

and

$\mathbf{V}_k'$—velocity fluctuation, $\mathbf{V}_k - \langle\mathbf{V}_k\rangle^{x\rho}$.

Terms of the form $\Gamma_k \zeta_{ki}$ are averages weighted by the interfacial mass transfer: $\Gamma_k \zeta_{ki} = \langle \rho_k \zeta_k (\mathbf{V}_k - \mathbf{V}_{ki}) \cdot \nabla X_k \rangle$.

Similarly, the averaged total energy equation is

$$\begin{aligned}
&\partial[\alpha_k \langle \rho_k \rangle^x (\langle u_k \rangle^{x\rho} + 0.5 \langle \mathbf{V}_k \rangle^{x\rho} \cdot \langle \mathbf{V}_k \rangle^{x\rho} + U_k^{\mathrm{Re}})]/\partial t + \nabla \cdot [\alpha_k \langle p \rangle_k^x \langle \mathbf{V} \rangle_k^{x\rho} (\langle u \rangle_k^{x\rho} \\
&\quad + 0.5 \langle \mathbf{v}_k \rangle^{x\rho} \cdot \langle \mathbf{V}_k \rangle^{x\rho} + U_k^{\mathrm{Re}})] = \nabla \cdot [\alpha_k (\langle \mathbf{T}_k \rangle^x + \mathbf{T}_k^{\mathrm{Re}}) \cdot \langle \mathbf{V}_k \rangle^{x\rho}] - \nabla \cdot \alpha_k (\langle \mathbf{q}_k'' \rangle^x + \mathbf{q}_k^{\mathrm{Re}}) \\
&\quad + \alpha_k \langle q_k''' \rangle^x + \alpha_k \langle \rho_k \rangle^x \mathbf{g}_k \cdot \langle \mathbf{V} \rangle_k^{x\rho} + E_k + W_{ki} + \Gamma_k [u_{ki} + 0.5 (\mathbf{V}_k \cdot \mathbf{V}_k)_{\mathrm{i}}],
\end{aligned} \qquad [10]$$

where:

$u_k$—internal energy,
$U_k^{\mathrm{Re}}$—turbulent kinetic energy, $0.5 \langle X_k \rho_k \mathbf{V}_k' \cdot \mathbf{V}_k' \rangle / \alpha_k \langle \rho_k \rangle^x$,
$\langle \mathbf{q}_k'' \rangle^x$—average heat flux, $\langle X_k \mathbf{q}_k'' \rangle / \alpha_k$,
$\mathbf{q}_k^{\mathrm{Re}}$—composed of various energy terms, $\mathbf{q}_k^{\mathrm{p}} + \mathbf{q}_k^{\mathrm{t}} + \mathbf{q}_k^{\mathrm{k}} + \mathbf{q}_k^{\mathrm{r}}$,
  $\mathbf{q}_k^{\mathrm{p}} = \langle X_k p_k \mathbf{V}_k' \rangle / \alpha_k$,
  $\mathbf{q}_k^{\mathrm{t}} = -\langle X_k \boldsymbol{\tau}_k \cdot \mathbf{V}_k' \rangle / \alpha_k$,
  $\mathbf{q}_k^{\mathrm{k}} = \frac{1}{2} \langle X_k \rho_k \mathbf{V}_k' \mathbf{V}_k' \cdot \mathbf{V}_k' \rangle / \alpha_k$,
  $\mathbf{q}_k^{\mathrm{r}} = \langle X_k \rho_k \mathbf{V}_k' u_k' \rangle / \alpha_k$,
$\boldsymbol{\tau}_k$—viscous stress tensor,
$q_k'''$—volumetric heat generation rate,
$E_k$—interfacial heat source, $\langle \mathbf{q}_k'' \cdot \nabla X_k \rangle$,

and

$w_{ki}$—so-called interfacial work,† $-\langle \mathbf{T}_k \cdot \mathbf{V}_k \cdot \nabla X_k \rangle$.

The mechanical energy equation is obtained by taking the dot product of the momentum equation with the average velocity. Expanding derivatives in the total energy equation and subtracting the mechanical energy equation, one obtains a form of the averaged internal energy equation:

$$\begin{aligned}
&\alpha_k \langle \rho_k \rangle^x \mathrm{D}(\langle u_k \rangle^{x\rho} + U_k^{\mathrm{Re}})/\mathrm{D}t = \alpha_k \langle \mathbf{T}_k \rangle^x : \nabla \langle \mathbf{V}_k \rangle^{x\rho} + \alpha_k \mathbf{T}^{\mathrm{Re}} : \nabla \langle \mathbf{V}_k \rangle^{x\rho} + W_{k\mathrm{i}} - \mathbf{M}_k \cdot \langle \mathbf{V}_k \rangle^{x\rho} \\
&\quad - \nabla \cdot \alpha_k \langle \mathbf{q}_k'' \rangle^x - \nabla \cdot \alpha_k \mathbf{q}_k^{\mathrm{Re}} + \alpha_k \langle q_k''' \rangle^x + E_k \\
&\quad + \Gamma_k [(u_{ki} - \langle u_k \rangle^{x\rho}) + \tfrac{1}{2} (\mathbf{V}_k \cdot \mathbf{V}_k)_i - (\mathbf{V}_k)_i \cdot \langle \mathbf{V}_k \rangle^{x\rho} + \tfrac{1}{2} \langle \mathbf{V}_k \rangle^{x\rho} \cdot \langle \mathbf{V}_k \rangle^{x\rho} - U_k^{\mathrm{Re}}].
\end{aligned} \qquad [11]$$

The density-weighted average internal energy can now be expressed in terms of the density-weighted average entropy and the phase-weighted average density. Expanding the internal energy with a first-order Taylor series in terms of entropy and density perturbations and then averaging yields (Arnold 1988):

$$\langle u_k \rangle^{x\rho} = u_k (\langle s_k \rangle^{x\rho}, \langle \rho_k \rangle^x) + \langle (\partial u_k / \partial s_k) s_k' \rangle^{x\rho} + \langle (\partial u_k / \partial \rho_k) \rho_k' \rangle^{x\rho}.$$

Noting that (Callen 1985)

$$\partial u_k / \partial s_k = T_k$$

and

$$\partial u_k / \partial \rho_k = p_k / \rho_k^2,$$

we obtain

$$\langle u_k \rangle^{x\rho} = u_k (\langle s_k \rangle^{x\rho}, \langle \rho_k \rangle^x) + \langle T_{ks} s_k' \rangle^{x\rho} + \langle (p_{ks} / \langle \rho_k \rangle^{x2}) \rho_k' \rangle^{x\rho}, \qquad [12]$$

where $T_{ks}$ and $p_{ks}$ are evaluated at the average entropy and density.

The term $\langle T_{ks} s_k' \rangle^{x\rho}$ is zero because $T_{ks}$ is a constant and $s_k' = s_k - \langle s_k \rangle^{x\rho}$, thus $\langle s_k' \rangle^{x\rho} = 0$. Therefore,

$$\langle u_k \rangle^{x\rho} = u_k (\langle s_k \rangle^{x\rho}, \langle \rho_k \rangle^x) + (p_{ks} / \langle \rho_k \rangle^{x2}) \langle \rho_k' \rangle^{x\rho}. \qquad [13]$$

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†Actually this term is a power production density term.

Taking the material derivative of both sides, one obtains

$$\mathrm{D}\langle u_k\rangle^{x\rho}/\mathrm{D}t = T_{k\mathrm{s}}\,\mathrm{D}\langle s_k\rangle^{x\rho}/\mathrm{D}t + (p_{k\mathrm{s}}/\langle\rho_k\rangle^{x^2})\mathrm{D}\langle\rho_k\rangle^{x}/\mathrm{D}t + \mathrm{D}[(p_{k\mathrm{s}}/\langle\rho_k\rangle^{x^2})\langle\rho'_k\rangle^{x\rho}]/\mathrm{D}t. \quad [14]$$

The averaged entropy equation is obtained by multiplying [8a,b] by the phase indicator function and averaging. Expressed in terms of the material derivative of entropy, this gives (Arnold 1988):

$$\begin{aligned}\alpha_k\langle\rho_k\rangle^{x}\,\mathrm{D}\langle s_k\rangle^{x\rho}/\mathrm{D}t = {} & -\nabla\cdot[\alpha_k(\langle\mathbf{q}''_k/T^{x}_k\rangle + \alpha_k\langle\rho_k\rangle^{x}\langle s'_k\mathbf{V}'_k\rangle^{x\rho})] \\ & + \alpha_k\langle q'''_k/T_k\rangle^{x} + \langle(\mathbf{q}''_k T_k)\cdot\nabla X_k\rangle + \Gamma_k(s_{k\mathrm{i}} - \langle s_k\rangle^{x\rho}) \\ & + \langle X_k\mathbf{q}''_k\cdot\nabla(1/T_k)\rangle + \langle X_k(1/T_k)\boldsymbol{\tau}_k : \nabla\mathbf{V}_k\rangle, \end{aligned} \quad [15]$$

where we know that from [8b], $\langle X_k\mathbf{q}''_k\cdot\nabla(1/T_k)\rangle + \langle X_k(1/T_k)\boldsymbol{\tau}_k : \nabla\mathbf{V}_k\rangle) \geqslant 0$. Substituting [14] and [15] into [11], we obtain the averaged entropy equation:

$$\begin{aligned} & \alpha_k(\langle\mathbf{T}_k\rangle^{x} + \mathbf{T}^{\mathrm{Re}}_k) : \nabla\langle\mathbf{V}_k\rangle^{x\rho} + W_{k\mathrm{i}} - \mathbf{M}_k\cdot\langle\mathbf{V}_k\rangle^{x\rho} + T_{k\mathrm{s}}\nabla\cdot\langle X_k\mathbf{q}''_k/T_k\rangle \\ & - \nabla\cdot\alpha_k(\langle\mathbf{q}''_k\rangle^{x} + \mathbf{q}^{\mathrm{r}}_k + \mathbf{q}^{\mathrm{p}}_k + \mathbf{q}^{\mathrm{t}}_k + \mathbf{q}^{\mathrm{k}}_k) + T_{k\mathrm{s}}\nabla\cdot\alpha_k\langle\rho_k\rangle^{x}\langle s'_k\mathbf{V}'_k\rangle^{x\rho} + \alpha_k\langle q'''_k\rangle^{x} \\ & - T_{k\mathrm{s}}\langle X_k q'''_k/T_k\rangle + E_k - T_{k\mathrm{s}}\langle(\mathbf{q}''_k/T_k)\cdot\nabla X_k\rangle \\ & - \alpha_k\langle\rho_k\rangle^{x}\,\mathrm{D}[(p_{k\mathrm{s}}/\langle\rho_k\rangle^{x^2})\langle\rho'_k\rangle^{x\rho}]/\mathrm{D}t - (\alpha_k p_{k\mathrm{s}}/\langle\rho_k\rangle^{x})\mathrm{D}\langle\rho_k\rangle^{x}/\mathrm{D}t \\ & - \alpha_k\langle\rho_k\rangle^{x}\,\mathrm{D}U^{\mathrm{Re}}_k/\mathrm{D}t + \Gamma_k[(u_{k\mathrm{i}} - \langle u_k\rangle^{x\rho}) - U^{\mathrm{Re}}_k + (1/2)(\mathbf{V}_k\cdot\mathbf{V}_k)_{\mathrm{i}} \\ & - \langle\mathbf{V}_k\rangle^{x\rho}\cdot(\mathbf{V}_k)_{\mathrm{i}} + 1/2\langle\mathbf{V}_k\rangle^{x\rho}\cdot\langle\mathbf{V}_k\rangle^{x\rho} - T_{k\mathrm{s}}(s_{k\mathrm{i}} - \langle s_k\rangle^{x\rho})] \\ & = T_{k\mathrm{s}}[\langle X_k\mathbf{q}''_k\cdot\nabla(1/T_k)\rangle + \langle X_k(1/T_k)\boldsymbol{\tau}_k : \nabla\mathbf{V}_k\rangle] \geqslant 0. \end{aligned} \quad [16]$$

This form of the second law is a generalization of the corresponding results for single-phase flow (Aris 1962). While the physical meaning of some of these terms is clear, others are more obscure.

It is advantageous now to consider grouping some of these terms, and partitioning others. If use is again made of the constitutive assumption

$$\mathbf{T}_k = -p_k\mathbf{I} + \boldsymbol{\tau}_k.$$

The interfacial work term becomes

$$W_{k\mathrm{i}} = \langle p_k\mathbf{V}_k\cdot\nabla X_k\rangle - \langle\boldsymbol{\tau}_k\cdot\mathbf{V}_k\cdot\nabla X_k\rangle.$$

This can also be expressed as

$$W_{k\mathrm{i}} = \langle\mathbf{V}_k\rangle_{\mathrm{i}}\cdot(\langle p_k\rangle_{\mathrm{i}}\mathbf{I} - \langle\boldsymbol{\tau}_k\rangle_{\mathrm{i}})\cdot\nabla\alpha_k + W''_{k\mathrm{i}} + \langle\mathbf{V}_k\rangle_{\mathrm{i}}\cdot(\mathbf{M}_{k\mathrm{p}} + \mathbf{M}_{k\mathrm{t}}), \quad [17]$$

where:

$\mathbf{M}_{k\mathrm{p}}$—interfacial pressure force, $\langle(p_k - \langle p_k\rangle_{\mathrm{i}})\cdot\nabla X_k\rangle$,
$\mathbf{M}_{k\mathrm{t}}$—interfacial shear force, $-\langle(\boldsymbol{\tau}_k - \langle\boldsymbol{\tau}_k\rangle_{\mathrm{i}})\cdot\nabla X_k\rangle$,

and

$W''_{k\mathrm{i}}$—interfacial "extra" work term, $\langle(\mathbf{V}_k - \langle\mathbf{V}_k\rangle_{\mathrm{i}})\cdot(p_k\mathbf{I} - \boldsymbol{\tau}_k)\cdot\nabla X_k\rangle$.

Similarly, the phasic interfacial momentum source term ($\mathbf{M}_k$) may be expressed as

$$\mathbf{M}_k = \mathbf{M}_{k\mathrm{p}} + \mathbf{M}_{k\mathrm{t}} + (\langle p_k\rangle_{\mathrm{i}}\mathbf{I} - \langle\boldsymbol{\tau}_k\rangle_{\mathrm{i}})\cdot\nabla\alpha_k. \quad [18]$$

Under normal flow conditions, perturbations of the fluid state are expected to be relatively small; i.e. the perturbation in any state variable divided by the average value of that variable is small. Fluid properties which are dependent upon the state variables will thus also have relatively small perturbations. Hence, the product of perturbations of two state variables, a state variable and a fluid property, or of two fluid properties may be assumed to be small enough to ignore.

Products of velocity perturbations on the other hand are not necessarily small. Indeed, an instantaneous perturbation in the velocity of a fluid may be greater than the average velocity. Thus, all products of velocity perturbations will be retained. Similarly, products of velocity perturbations with perturbations of fluid state variables or properties are also retained.

Neglecting terms which are quadratic in fluid property perturbations, one obtains (Arnold 1988):

$$\langle u_k \rangle^{x\rho} = u_{ks}, \tag*{[19a]}$$

$$\langle T_k \rangle^{x\rho} = T_{ks} \tag*{[19b]}$$

$$\Gamma_k(u_{ki} - \langle u_k \rangle^{x\rho}) + T_{ks}\Gamma_k(\langle s_k \rangle^{x\rho} - s_{ki}) = \Gamma_k p_{ks}(\rho_{ki} - \langle \rho_k \rangle)^x / \langle \rho_k \rangle^{x^2}, \tag*{[20]}$$

$$p_{ks} - \langle p_k \rangle^x = 0, \tag*{[21]}$$

$$\langle X_k q_k''' \rangle - \langle T_k \rangle^{x\rho} \langle X_k q_k''' / T_k \rangle = 0, \tag*{[22]}$$

$$\langle T_k \rangle^{x\rho}\, \nabla \cdot \alpha_k \langle \rho_k \rangle^x \langle s_k' \mathbf{V}_k' \rangle^{x\rho} - \nabla \cdot \alpha_k \mathbf{q}_k^{\mathrm{r}} = -\alpha_k \langle \rho_k \rangle^x \langle s_k' \mathbf{V}_k' \rangle^{x\rho} \cdot \nabla \langle T_k \rangle^{x\rho}, \tag*{[23]}$$

$$\langle T_k \rangle^{x\rho}\, \nabla \cdot \alpha_k \langle \mathbf{q}_k'' / T_k \rangle^x - \nabla \cdot \alpha_k \langle \mathbf{q}_k'' \rangle^x = -\alpha_k \langle \mathbf{q}_k'' \rangle^x / \langle T_k \rangle^{x\rho} \cdot \nabla \langle T_k \rangle^{x\rho} \tag*{[24]}$$

and

$$\langle \mathbf{q}_k'' \cdot \nabla X_k \rangle - \langle T_k \rangle^{x\rho} \langle \mathbf{q}_k'' / T_k \cdot \nabla X_k \rangle = \langle \mathbf{q}_k'' \cdot \nabla X_k \rangle \langle T_k' \rangle^x / \langle T_k \rangle^{x\rho}. \tag*{[25]}$$

Substitution of [19]–[25] into [16] yields:

$$\begin{aligned}
&\alpha_k(\langle \boldsymbol{\tau}_k \rangle^x + \mathbf{T}_{\mathrm{k}}^{\mathrm{Re}}) : \mathbf{D}_k + (\mathbf{M}_{k\mathrm{p}} + \mathbf{M}_{k\mathrm{t}}) \cdot (\langle \mathbf{V}_k \rangle_{\mathrm{i}} - \langle \mathbf{V}_k \rangle^{x\rho}) + W_{k\mathrm{i}}'' \\
&\quad + (\langle \mathbf{V}_k \rangle_{\mathrm{i}} - \langle \mathbf{V}_k \rangle^{x\rho}) \cdot (\langle p_k \rangle_{\mathrm{i}} \mathbf{I} - \langle \boldsymbol{\tau}_k \rangle_{\mathrm{i}}) \cdot \nabla \alpha_k - \alpha_k / \langle T_k \rangle^{x\rho} \langle \mathbf{q}_k'' \rangle^x \cdot \nabla \langle T_k \rangle^{x\rho} \\
&\quad - \nabla \cdot \alpha_k (\mathbf{q}_k^{\mathrm{p}} + \mathbf{q}_k^{\mathrm{t}} + \mathbf{q}_k^{\mathrm{k}}) - \alpha_k \langle \rho_k \rangle^x \langle s_k' \mathbf{V}_k' \rangle^{x\rho} \cdot \nabla \langle T_k \rangle^{x\rho} - \alpha_k \langle \rho_k \rangle^x \, \mathrm{D} U_k^{\mathrm{Re}} / \mathrm{D}t \\
&\quad + \langle p_k \rangle^x \, \mathrm{D}\alpha_k / \mathrm{D}t + \Gamma_k \langle p_k \rangle^x [\rho_{k\mathrm{i}} - 2\langle \rho_k \rangle^x] / \langle \rho_k \rangle^{x^2} + \Gamma_k [0.5(\mathbf{V}_k \cdot \mathbf{V}_k)_{\mathrm{i}} - \langle \mathbf{V}_k \rangle^{x\rho} \cdot (\mathbf{V}_k) \\
&\quad + 0.5 \langle \mathbf{V}_k \rangle^{x\dot{\rho}} \cdot \langle \mathbf{V}_k \rangle^{x\rho} - U_k^{\mathrm{Re}}] = \langle T_k \rangle^{x\rho} [\langle X_k \mathbf{q}_k'' \cdot \nabla(1/T_k) \rangle + \langle (X_k / T_k) \boldsymbol{\tau}_k : \nabla \mathbf{V}_k \rangle] \geqslant 0,
\end{aligned} \tag*{[26]}$$

where, $\mathbf{D}_k$ is the phasic deformation tensor, given by

$$\mathbf{D}_k = 0.5[\nabla \langle \mathbf{V}_k \rangle^{x\rho} + (\nabla \langle \mathbf{V}_k \rangle^{x\rho})^{\mathrm{T}}]. \tag*{[27]}$$

Let us now consider the Lagrangian form of the local instantaneous phasic entropy equation given by

$$\mathrm{D}(\rho_k s_k)/\mathrm{D}t + \nabla \cdot (\mathbf{q}_k'' / T_k) - q_k''' / T_k = \mathbf{q}_k'' \cdot \nabla(1/T_k) + (1/T_k) \boldsymbol{\tau}_k : \nabla \mathbf{V}_k \geqslant \, = 0. \tag*{[28]}$$

This tells us that the rate of change of the specific entropy must exceed the entropy source, and that it does so by an amount equal to

$$\mathbf{q}_l'' \cdot \nabla(1/T_k) + (1/T_k) \boldsymbol{\tau}_k : \nabla \mathbf{V}_k.$$

This means that there may be energy transfer from the macroscale to the microscale that is in excess of that which can be accounted for by the "local instantaneous" parameters,

$$-\nabla \cdot (\mathbf{q}_k'' / T_k) + q_k''' / T_k.$$

We see a similar effect in the averaged entropy equation [26]. The rate of change of the specific averaged entropy must exceed the entropy sources, which are expressed in terms of averaged parameters. If all terms in this equation are properly constituted, then we should find that the resulting entropy equation is always satisfied. Alternatively, if the constitutive equations do not always satisfy the entropy equation, then we know that dissipation (i.e. energy transfer to the microscale) is not being correctly predicted.

In a system of averaged balance equations, the solution of the energy equation will only be a valid solution for the energy partition of the system if all terms within the energy equation accurately model the desired phenomena. If the constitutive equations used to obtain closure for the system of equations do not accurately model dissipation, then they will yield an inaccurate-energy partition.

The entropy equation is an inequality. Accordingly, one might expect that the inability of constitutive equations to satisfy the entropy equation implies that dissipation is being under-predicted. However, it can be shown (Arnold 1988) that the inability to satisfy the entropy equation can lead to either over-prediction or under-prediction of dissipation, depending on the flow situation.

Averaged flow, and particularly averaged multiphase flow, has more sources of dissipation than does the corresponding local instantaneous flow. Additional sources of dissipation include two-phase turbulent dissipation and interfacial dissipation. These add further complications to consideration of the second law.

In order to assess the validity of [26], it can be shown (Arnold 1988) that the averaged entropy constraint is trivially satisfied for the exact constitutive equations which can be derived by a modified cell model averaging technique (Nigmatulin 1979) for the liquid phase of a bubbly two-phase flow of an inviscid liquid.

It is worth noting that [26] accounts for both recoverable and nonrecoverable turbulent kinetic energy. In two-phase flows, one of the primary sources of turbulent kinetic energy is through interfacial work. These work terms appear in [26] as terms having the generalized form, $\langle \mathbf{T} : \nabla \nabla X \rangle$. Several of these terms appear because [26] has been partitioned into more recognizable terms. When interfacial work is performed on the continuous phase, these work terms are a positive source of dissipation. However, turbulent kinetic energy appears in the equation in the form of $-\alpha_k \langle \rho_k \rangle^x \mathrm{D}U_k^{\mathrm{Re}}/\mathrm{D}t$, which during the production of turbulent kinetic energy acts to reduce the source of dissipation. Thus, we can see that turbulent kinetic energy acts to temporarily store energy. If later interfacial work acts to reduce the turbulent kinetic energy, then that energy may be reversibly recovered, and never actually appear as dissipation. If, however, turbulence is reduced by diffusion $(-\nabla \cdot \alpha_k \mathbf{g}_k^{\mathrm{k}})$, the rate of reduction in turbulent kinetic energy $(-\alpha_k \langle \rho_k \rangle^x \mathrm{D}U_k^{\mathrm{Re}}/\mathrm{D}t)$ can result in dissipation. This dissipation represents the excess of that product less that which diffuses away.

## *Computer Code Models*

Let us now consider the sets of two-fluid conservation and constitutive equations in use in some state-of-the-art transient two-phase flow codes. We will demonstrate that all such models violate the second law of thermodynamics.

Our averaged entropy equation is based upon rigorously derived balance equations. The only terms that have been neglected are terms that we have demonstrated to be small under the circumstances of interest. The result is an entropy equation which we may partition as required to be compatible with the partitioning of any mathematically correct set of conservation equations.

Unfortunately, the systems of conservation equations used in many computer codes are not complete. Some common inadequacies found within these codes include:

(1) The energy equations do not include interfacial work.
(2) The conservation equations disregard turbulent phenomena.
(3) The systems of equations do not properly account for the interfacial energy and momentum transfers due to phase change.
(4) The energy equation disregards turbulent kinetic energy and energy fluxes.
(5) Viscous effects are disregarded.

All codes investigated use one pressure for both phases so we may assume $\langle p_k \rangle_{\mathrm{i}} = \langle p_k \rangle^x = p$. Additionally, in all cases the following terms were neglected: $W''_{k\mathrm{i}}$, $\langle \boldsymbol{\tau}_k \rangle_{\mathrm{i}}$, $\mathbf{q}_k^{\mathrm{p}} + \mathbf{q}_k^{\mathrm{t}} + \mathbf{q}_k^{\mathrm{k}}$ and $U_k^{\mathrm{Re}}$.

Most codes also neglect kinetic energy and use either enthalpy or internal energy as the state variable in the energy equation. We derived the entropy equation starting with the ensemble-averaged total energy equation. It is also possible to derive an entropy equation starting with the averaged internal energy equation. Such an averaged entropy equation looks quite different from the entropy constraint equation given by [26]. However, it is possible to demonstrate that they are equivalent (Arnold 1988). For example, the entropy constraint derived from the internal energy equation does not contain interfacial work terms explicitly. However, it contains the term

$$\alpha_k \langle \boldsymbol{\tau}_k : \nabla \mathbf{V}'_k \rangle^x.$$

We may partition this term as

$$\alpha_k \langle \boldsymbol{\tau}_k : \nabla \mathbf{V}'_k \rangle^x = \nabla \cdot \langle X_k \boldsymbol{\tau}_k \cdot \mathbf{V}'_k \rangle^x - W_{k_{\mathrm{ti}}} - \mathbf{M}_{k\mathrm{t}} \cdot \langle \mathbf{V}_k \rangle_{\mathrm{i}} - \langle X_k \mathbf{V}'_k \cdot \nabla \cdot \boldsymbol{\tau}_k \rangle^x.$$

The first term on the r.h.s. is the turbulent shear work $(\alpha_k \mathbf{q}_k^{\mathrm{t}})$, the second term is the viscous component of the interfacial work and the third term is the dot product of the interfacial viscous drag force with the average interfacial velocity. These are all terms which appear explicitly in [26]. Thus, the dissipative terms explicitly present in the entropy equation given by [26] are present in the internal energy equation based form of the entropy equation.

We will now apply the phasic entropy constraint equation [26] to the constitutive equations for the continuous liquid phase of a two-phase flow. Let us begin by considering the COMMIX-2 code.

### *COMMIX-2*

The COMMIX-2 code (ANL 1985) is a three-dimensional computer code for the analysis of steady-state and transient single-phase and two-phase flows. It contains a 5-equation two-phase flow model and makes use of a mixture energy equation.

If we compare the mixture energy equation used in COMMIX-2 to the complete mixture energy equation we find that all dissipation terms are disregarded by COMMIX-2.

The COMMIX-2 constitutive equations for the continuous liquid phase are listed in table 1.

Because of the donor-cell method that is used for the interfacial momentum flux in COMMIX-2, the entropy equation will be different depending on whether evaporation or condensation is occurring. Moreover, the interfacial velocity of the liquid phase is treated by the same donor-cell method.

Let us now consider the entropy equation for the liquid phase where the accompanying vapor phase is undergoing condensation. The entropy constraint, with $\epsilon$ representing the void fraction, is

$$
\begin{aligned}
&(1-\epsilon)\mu_L \nabla\langle \mathbf{V}_L\rangle^{x\rho} : D_L + K(\langle \mathbf{V}_G\rangle^{x\rho} - \langle \mathbf{V}_L\rangle^{x\rho})\cdot(\langle \mathbf{V}_G\rangle^{x\rho} - \langle \mathbf{V}_L\rangle^{x\rho}) \\
&\quad - \langle p_L\rangle^{x}(\langle \mathbf{V}_G\rangle^{x\rho} - \langle \mathbf{V}_L\rangle^{x\rho})\cdot\nabla\epsilon - (1-\epsilon)\langle \rho_L\rangle^{x}\langle s_L'\mathbf{V}_L'\rangle^{x\rho}\cdot\nabla\langle T_L\rangle^{x\rho} - \langle p_L\rangle^{x}\,\mathrm{D}\epsilon/\mathrm{D}t \\
&\quad + \underline{\Gamma\langle p_L\rangle^{x}/\langle \rho_L\rangle^{x}} - \Gamma[0.5(\langle \mathbf{V}_G\rangle - \langle \mathbf{V}_L\rangle)\cdot(\langle \mathbf{V}_G\rangle - \langle \mathbf{V}_L\rangle)] \geqslant 0.
\end{aligned}
\qquad [29]
$$

It should be noted that the flow work term, which is underlined in [29], does not appear in the energy equation used by COMMIX and should thus be set equal to zero in [29] to be consistent. However, as we will see, this term is necessary to satisfy the second law.

Since for condensation $\Gamma$ is negative, the term

$$
(1-\epsilon)\mu_L\nabla\langle \mathbf{V}_L\rangle^{x\rho} : \mathbf{D}_L + K(\mathbf{V}_G - \mathbf{V}_L)\cdot(\mathbf{V}_G - \mathbf{V}_L) - \Gamma[0.5(\mathbf{V}_G - \mathbf{V}_L)\cdot(\mathbf{V}_G - \mathbf{V}_L)]
$$

is always positive.

We expect that the turbulent entropy flux, $\langle s_L'\mathbf{V}_L'\rangle^{x\rho}$, is positive in the direction that the entropy decreases most rapidly. In fact, it is reasonable to constitute the turbulent entropy flux as

$$
\langle s_L'\mathbf{V}_L'\rangle^{x\rho} = -k_s\nabla\langle s_L\rangle^{x\rho},
$$

where $k_s$ is a positive turbulent diffusivity coefficient for entropy transport. If we consider a case with uniform pressure, the Gibbs equation may be represented as

$$
\mathrm{d}h = T\,\mathrm{d}s.
$$

Table 1. COMMIX-2 constitutive equations for a continuous liquid phase

$$
\begin{aligned}
\langle \boldsymbol{\tau}_L\rangle^{x} &= -[\mu_L\nabla\langle \mathbf{V}_L\rangle^{x}] \\
\mathbf{T}_L^{Re} &= 0 \\
\mathbf{M}_{Lp} &= 0 \\
\mathbf{M}_{Lt} &= K(\langle \mathbf{V}_G\rangle^{x\rho} - \langle \mathbf{V}_L\rangle^{x\rho}) \\
\langle \mathbf{q}_k''\rangle^{x} &= 0 \\
\Gamma\mathbf{V}_{Li} &= \begin{cases} \Gamma\langle \mathbf{V}_G\rangle^{x\rho}, & \text{for condensation} \\ \Gamma\langle \mathbf{V}_L\rangle^{x\rho}, & \text{for evaporation} \end{cases} \\
\mathbf{V}_{Li} &= \begin{cases} \langle \mathbf{V}_G\rangle^{x\rho}, & \text{for condensation} \\ \langle \mathbf{V}_L\rangle^{x\rho}, & \text{for evaporization} \end{cases} \\
\Gamma\langle p_L\rangle^{x}/\langle \rho_L\rangle^{x} &= 0
\end{aligned}
$$

Using the relationship $\mathrm{d}h = c_p\,\mathrm{d}T$, we may represent this version of the Gibbs equation in terms of temperature and entropy gradients as

$$\nabla s = (c_p/T)\nabla T.$$

Hence in [29] we may express minus the value of the dot product of the turbulent entropy flux with the temperature gradient as

$$-(1-\epsilon)\langle\rho_L\rangle^x\langle s'_L\mathbf{V}'_L\rangle^{x\rho}\cdot\nabla\langle T_L\rangle^{x\rho} = (1-\epsilon)\langle\rho_L\rangle^x k_s(c_p/\langle T_L\rangle^{x\rho})\nabla\langle T_L\rangle^{x\rho}\cdot\nabla\langle T_L\rangle^{x\rho}.$$

This term is obviously positive, and will remain positive. This conclusion is valid as long as pressure gradients are not large (e.g. shocks).

The material derivative of the void fraction may be either positive or negative. We stated earlier that the mixture energy equation in COMMIX-2 disregarded the flow work term, $\Gamma\langle p_L\rangle^x/\langle\rho_L\rangle^x$. In order to understand the implications of this assumption, we note that for uniform phasic pressure and density (as assumed in the COMMIX-2 code):

$$\Gamma\langle p_L\rangle^x/\langle\rho_L\rangle^x \equiv \Gamma(p_L/\rho_L)_i = -\langle(p_L/\rho_L)\rho_L(\mathbf{V}_L-\mathbf{V}_i)\cdot\nabla X_L\rangle,$$

$$\Gamma\langle p_L\rangle^x/\langle\rho_L\rangle^x = -\langle p_L\rangle^x\langle[(\mathbf{V}_L-\langle\mathbf{V}_L\rangle^{x\rho})+(\langle\mathbf{V}_L\rangle^{x\rho}-\mathbf{V}_i)]\cdot\nabla X_L\rangle,$$

$$\Gamma\langle p_L\rangle^x/\langle\rho_L\rangle^x = -\langle p_L\rangle^x[\langle\mathbf{V}'_L\cdot\nabla X_L\rangle - \partial\epsilon/\partial t - \langle\mathbf{V}_L\rangle^{x\rho}\cdot\nabla\epsilon]$$

and

$$\Gamma\langle p_L\rangle^x/\langle\rho_L\rangle^x = \langle p_L\rangle^x\,\mathrm{D}\epsilon/\mathrm{D}t - \langle p_L\rangle^x\langle\mathbf{V}'_L\cdot\nabla X_L\rangle. \qquad [30]$$

We see from [29] and [30] that the inclusion of this phase change terms causes a cancellation which prevents the $\langle p_L\rangle^x\,\mathrm{D}\epsilon/\mathrm{D}t$ term from violating the second law. Additionally, [29] contains the term

$$-\langle p_L\rangle^x(\langle\mathbf{V}_G\rangle^{x\rho}-\langle\mathbf{V}_L\rangle^{x\rho})\cdot\nabla\epsilon.$$

Assuming that for condensation the interfacial velocity is the average vapor phase velocity, we may constitute $\langle p_L\rangle^x\langle\mathbf{V}'_L\cdot\nabla X_L\rangle$ in [30] as minus this term so that it also would not violate the second law. In fact, to be consistent with the donor-cell formulation of the interfacial momentum flux, we should constitute this term as

$$\langle\mathbf{V}'_L\cdot\nabla X_L\rangle = \begin{cases} -(\langle\mathbf{V}_G\rangle^{x\rho}-\langle\mathbf{V}_L\rangle^{x\rho})\cdot\nabla\epsilon, & \text{for condensation,}\\ 0.0, & \text{for evaporation.}\end{cases}$$

Now let us consider the case of the continuous liquid phase undergoing evaporation. For this case, the entropy equation becomes

$$(1-\epsilon)\mu_L\nabla\langle\mathbf{V}_L\rangle^{x\rho}:\mathbf{D}_L - \epsilon\langle\rho_L\rangle^x\langle s'_L\mathbf{V}'_L\rangle^{x\rho}\cdot\nabla\langle T_L\rangle^{x\rho} - \langle p_L\rangle^x\,\mathrm{D}\epsilon/\mathrm{D}t + \Gamma\langle p_L\rangle^x/\langle\rho_L\rangle^x \geqslant 0. \qquad [31]$$

Again, we see that this equation cannot be satisfied for all possible two-phase flow situations. But, as can be seen in [30], inclusion of the underlined flow work term $\Gamma\langle p_L\rangle^x/\langle\rho_L\rangle^x$, can correct this. However, it should be noted that while the second law may be satisfied if flow work is properly included, the model used for interfacial velocity is inadequate, and should also be changed to improve model predictions.

### *RELAP5*

The RELAP5 code is an advanced one-dimensional fast-running transient system analysis code designed for the analysis of light-water nuclear reactor (LWR) accidents. It is based on a nonequilibrium two-fluid hydrodynamic model.

The RELAP5/MOD1 code (Ransom *et al.* 1982) uses a mixture energy equation while the RELAP5/MOD2 code (Ransom *et al.* 1985) used an energy equation for each phase. The conservation equations neglect turbulent stresses, turbulent kinetic energy, turbulent energy fluxes, convective heat flux, many interfacial momentum sources, interfacial work, viscous stress and volumetric heat generation.

Table 2. RELAP5 constitutive equations for a continuous liquid phase

$$\langle \boldsymbol{\tau}_{\rm L} \rangle^{x} = 0$$

$$\mathbf{T}_{\rm L}^{\rm Re} = 0$$

$$M_{\rm Lp} = C\epsilon(1-\epsilon)\rho_{\rm m}[{\rm D_G}\langle V_{\rm L}\rangle^{x\rho}/{\rm D}t - {\rm D_L}\langle V_{\rm G}\rangle^{x\rho}/{\rm D}t] \quad \text{(MOD1)}$$

$$M_{\rm Lp} = C\epsilon(1-\epsilon)\rho_{\rm m}[\partial\langle V_{\rm L}\rangle^{x\rho}/\partial t - \partial\langle V_{\rm G}\rangle^{x\rho}/\partial t] \quad \text{(MOD2)}$$

where

$$C = 1.5/\epsilon - 1.0 \qquad \epsilon > 0.5$$

$$C = 0.5/(1-\epsilon) + \epsilon/(1-\epsilon) \qquad \epsilon \leqslant 0.5$$

$$M_{\rm Lt} = (1-\epsilon)\langle \rho_{\rm L}\rangle^{x}\,{\rm FIF}(\langle V_{\rm G}\rangle^{x\rho} - \langle V_{\rm L}\rangle^{x\rho}) - (1-\epsilon)\langle \rho_{\rm L}\rangle^{x}\,{\rm FWF}\langle V_{\rm L}\rangle^{x\rho}$$

$$\langle \mathbf{q}_{\rm L}'' \rangle^{x} = 0$$

$$\Gamma V_{\rm Gi} = \Gamma V_{\rm Li} = \Gamma(1-\eta_{\rm m})\langle V_{\rm G}\rangle^{x\rho} + \Gamma\eta_{\rm m}\langle V_{\rm L}\rangle^{x\rho}$$

$$\eta_{\rm m} = \begin{cases} 0, & \text{for condensation} \\ 1, & \text{for evaporation} \end{cases}$$

$$\langle V_{\rm L}\rangle_{\rm i} = (1-\eta_{\rm m})\langle V_{\rm G}\rangle^{x\rho} + \eta_{\rm m}\langle V_{\rm L}\rangle^{x\rho}$$

The constitutive equations used by RELAP5 for the continuous phase are listed in table 2. It is significant to note that the flow work term, $\Gamma\langle p_{\rm L}\rangle/\langle \rho_{\rm L}\rangle$, is neglected in the internal energy equation in RELAP5. Substituting these into the entropy equation for the liquid phase, we obtain for evaporative flow,

$$-(1-\epsilon)\langle \rho_{\rm L}\rangle^{x}\langle s_{\rm L}' V_{\rm L}'\rangle^{x\rho}\cdot\nabla\langle T_{\rm L}\rangle^{x\rho} - \langle p_{\rm L}\rangle^{x}\,{\rm D}\epsilon/{\rm D}t + \Gamma\langle p_{\rm L}\rangle^{x}/\langle \rho_{\rm L}\rangle^{x} \geqslant 0. \qquad [32]$$

We see again, as in the case of the COMMIX-2 code, the RELAP5 code requires the $\Gamma\langle p_{\rm L}\rangle/\langle \rho_{\rm L}\rangle$ term in the energy equation if the second law is to be satisfied.

For a condensing flow the entropy equation becomes:

$$\begin{aligned} &-(1-\epsilon)\langle \rho_{\rm L}\rangle^{x}\langle s_{\rm L}' V_{\rm L}'\rangle^{x\rho}\cdot\nabla\langle T_{\rm L}\rangle^{x\rho} - \langle p_{\rm L}\rangle^{x}\,{\rm D}\epsilon/{\rm D}t + \Gamma\langle p_{\rm L}\rangle^{x}/\langle \rho_{\rm L}\rangle^{x} \\ &- \langle p_{\rm L}\rangle^{x}(\langle V_{\rm G}\rangle^{x\rho} - \langle V_{\rm L}\rangle^{x\rho})\cdot\nabla\epsilon - \Gamma[0.5(\langle V_{\rm G}\rangle^{x\rho} - \langle V_{\rm L}\rangle^{x\rho})^{2}] \\ &+ C\epsilon(1-\epsilon)\rho_{\rm m}[{\rm D_G}\langle V_{\rm L}\rangle^{x\rho}/{\rm D}t - {\rm D_L}\langle V_{\rm G}\rangle^{x\rho}/{\rm D}t](\langle V_{\rm G}\rangle^{x\rho} - \langle V_{\rm L}\rangle^{x\rho}) \\ &+ (1-\epsilon)\langle \rho_{\rm L}\rangle^{x}\,{\rm FIF}(\langle V_{\rm G}\rangle^{x\rho} - \langle V_{\rm L}\rangle^{x\rho})^{2} \geqslant 0. \end{aligned} \qquad [33]$$

The RELAP5/MOD2 version of this equation differs only in that the virtual mass term contains only the partial time derivatives of the phase velocities rather than material derivatives.

The first four terms are all either properly dissipative or we have discussed their implications previously. Since this equation is for condensing flow, $\Gamma$ is negative. Also, be definition, the interfacial friction factor, FIF, is always positive. Hence, the term,

$$-\Gamma[\tfrac{1}{2}(\langle V_{\rm G}\rangle^{x\rho} - \langle V_{\rm L}\rangle^{x\rho})^{2}] + (1-\epsilon)\langle \rho_{\rm L}\rangle^{x}\,{\rm FIF}(\langle V_{\rm G}\rangle^{x\rho} - \langle V_{\rm L}\rangle^{x\rho})^{2}$$

is never negative. The virtual mass force appears in the entropy equation as

$$C\epsilon(1-\epsilon)\rho_{\rm m}[{\rm D_G}\langle V_{\rm L}\rangle^{x\rho}/{\rm D}t - {\rm D_L}\langle V_{\rm G}\rangle^{x\rho}/{\rm D}t](\langle V_{\rm G}\rangle^{x\rho} - \langle V_{\rm L}\rangle^{x\rho}).$$

For accelerating two-phase flow this term can be negative and can cause the second law constraints to be violated. This implies that somewhere within the balance equations, a term has been neglected which should result in an acceleration times the relative velocity in the entropy equation. Inviscid flow calculations (Arnold 1988) demonstrate the existence of the time derivative of the relative velocity times the relative velocity within the extra interfacial work term, $W_{\rm i}''$. Additionally, the material derivative of the turbulent kinetic energy, a term appearing in the entropy equation, if properly constituted, will result in an acceleration times the relative velocity. We see that with the inclusion of the virtual mass force in the momentum equation we need some corresponding term(s) to prevent a violation of the entropy constraint.

In order for the RELAP5 constitutive equations to satisfy the entropy equation we must:

(1) Include in the energy equation, and properly constitute, the term:

$$-\Gamma_G\langle p_L\rangle^x/\langle \rho_L\rangle^x.$$

This term should be constituted as previously recommended for the COMMIX-2 code, [30].

(2) Either the interfacial work must be included and constituted in such a way that it negates the virtual mass work appearing in the entropy equation, or the turbulent kinetic energy must be included and constituted properly.

### *TRAC-PF1/MOD1*

The TRAC-PF1 code (LANL *et al.* 1986) is a thermal-hydraulic transient analysis code for the simulation of accidents in pressurized water nuclear reactors (PWR). The TRAC-BD1 code (Taylor *et al.* 1984) is a boiling water reactor (BWRs) version of the same code.

The conservation equations solved by the TRAC code in the three-dimensional reactor vessel are fairly standard multiphase conservation equations. In particular, they include the phasic continuity and momentum equations, and the vapor phase and mixture energy equations. The constitutive equations used for the continuous liquid phase are listed in table 3.

These constitutive equations are sufficiently similar to those of the COMMIX-2 code that we can immediately recognize that the inclusion of the $\Gamma\langle p_L\rangle^x/\langle\rho_L\rangle^x$ term in the internal energy equation will permit these constitutive equations to satisfy second law constraints.

Prior to continuing, it is enlightening to discuss two aspects of current generation computer codes that this analysis has revealed. The phasic interfacial average velocity occurs numerous times in the entropy constraint, [26], which indicates that this velocity is an important parameter in satisfying the second law of thermodynamics. It is obvious that fluid at an interface does not move at the phase average velocity. Rather, it must move at some velocity that is between the phase average velocity of the two phases present at the interface.

With the exception of RELAP5, all computer models examined use a donor-cell formulation for the interfacial velocity. Unfortunately, this is physically incorrect. Nevertheless, such a formulation is capable in many instances of satisfying second law constraints. This is a good example of why satisfaction of second law constraints, although necessary, is not sufficient to demonstrate that the constitutive model is correct.

It has been demonstrated that energy equations used in all current generation computer codes neglect the phase change flow work term, $-\Gamma_k(p_k/\rho_k)_i$. That is, the energy equations, which are expressed as balance equations for phasic average internal energy or enthalpy, use as the interfacial energy flux the interfacial enthalpy rather than the interfacial internal energy. It has been shown (Arnold 1988) that the term $\Gamma_k(p_k/\rho_k)_i$ is an interfacial source of turbulent kinetic energy, and not an interfacial source of internal energy. The neglect of this term in the computer codes is due to the confusion concerning the definition of the dependent variable of the energy equation.

To understand how this may have occurred we need to examine the energy equation; or more correctly, the energy equations. It is possible to distinguish three distinct types of energy and three

Table 3. TRAC-PF1 constitutive equations for the continuous liquid phase

$$\langle \boldsymbol{\tau}_L\rangle^x = 0$$

$$\mathbf{T}_L^{Re} = 0$$

$$\mathbf{M}_{Lt} = \mathbf{f}_i = C_i(\langle \mathbf{V}_G\rangle^{x\rho} - \langle \mathbf{V}_L\rangle^{x\rho}|\langle \mathbf{V}_G\rangle^{x\rho} - \langle \mathbf{V}_L\rangle^{x\rho}|$$

$$\mathbf{M}_{Lp} = 0$$

$$\langle \mathbf{q}_L''\rangle^x = 0$$

$$\Gamma \mathbf{V}_{Li} = \begin{cases} \Gamma\langle \mathbf{V}_G\rangle^{x\rho}, & \text{for condensation} \\ \Gamma\langle \mathbf{V}_L\rangle^{x\rho}, & \text{for evaporation} \end{cases}$$

$$\langle \mathbf{V}_L\rangle_i = \begin{cases} \langle \mathbf{V}_G\rangle^{x\rho}, & \text{for condensation} \\ \langle \mathbf{V}_L\rangle^{x\rho}, & \text{for evaporation} \end{cases}$$

distinct energy equations for multiphase flow. Herein they are called mechanical energy, turbulent kinetic energy and internal energy. Some consider mechanical energy to be the sum of the turbulent kinetic energy and what is called here mechanical energy, however, even then there are three distinct forms of energy. Balance equations for these three forms of energy may be derived as follows:

- The mechanical energy equation is simply the vector dot product of the phasic average momentum equation with the phasic average velocity, and is satisfied whenever the momentum equation is satisfied.
- The turbulent kinetic energy equation is found by subtracting the mechanical energy equation from the phasic average of the vector dot product of the local instantaneous momentum equation with the local instantaneous velocity.
- The internal energy equation is found by averaging the total energy equation, and then subtracting off the mechanical energy and the turbulent kinetic energy equations. Alternatively, using ensemble-averaging techniques, the local instantaneous internal energy equation may be directly averaged to obtain the phasic internal energy equation.

Rigorous time- and volume-averaging techniques have generally relied upon a "standard" form of balance equation (e.g. Ishii 1975, equation V.1.1). The averaging is performed on the generalized balance equation. The individual averaged balance equations are then formulated from the averaged generalized balance equation. This process has been used by Ishii (1975) and Drew & Wood (1985) as well as many others. One problem with this process is that the local instantaneous internal energy equation does not fit the form of the generalized balance equation. Hence derivation of the averaged internal energy equation must be performed using the more elaborate and indirect method just discussed.

Ishii (1975) defines the effective internal energy. It is the sum of the phasic average internal energy and the turbulent kinetic energy. He then derives a balance equation for it by subtracting the mechanical energy equation from the averaged total energy equation. Ishii's internal energy equation is the sum of what is herein called the internal energy equation and the turbulent kinetic energy equations. It is a valid energy equation, however care must be taken to ensure that constituted interfacial sources include both interfacial sources of internal energy and interfacial sources of turbulent kinetic energy. This Ishii has done in the constitutive relations he recommends (Ishii 1975).

Examination of the energy equations in all of the computer codes examined in this paper demonstrates a remarkable similarity between them and Ishii's internal energy equation. We conjecture that these energy equations were derived in a manner similar to Ishii's, and that they are indeed balance equations for the "effective" internal energy, and not just for the phasic internal energy. However, the dependent variable of these energy equations is treated as the internal energy (or in some cases enthalpy) and the turbulent kinetic energy component is disregarded. Thus, improper interpretation of the dependent variables of these equations has apparently led to the problems which have been discussed.

### *An Acceptable Set of Constitutive Equations*

The second law of thermodynamics cannot tell us which constitutive laws are correct, it can only detect which sets of constitutive equations are incompatible with specific physical requirements. An acceptable set of constitutive equations should:

(1) Be reasonably brief.
(2) Include all important effects.
(3) Be compatible with the second law of thermodynamics.
(4) Be compatible with the principle of objectivity (Draw & Lahey 1979).
(5) Lead to a well-posed two-fluid model.
(6) Predict the available data.

As an example of how the entropy constraint should be used to assess candidate constitutive laws, let us evaluate a proposed set. One possible set of constitutive equations is listed in table 4. Arnold *et al.* (1988) have justified the existence of these constitutive equations using cell model ensemble

Table 4. An acceptable set of liquid-phase constitutive equations for bubbly flow

$$
\begin{aligned}
\mathbf{T}_{\mathrm{L}}^{\mathrm{Re}} &= 0.05\epsilon\langle\rho\rangle^{x}[3a_1 U_{\mathrm{R}}^2\mathbf{I} + a_2\mathbf{U}_{\mathrm{R}}\mathbf{U}_{\mathrm{R}}] \\
\langle\boldsymbol{\tau}_{\mathrm{L}}\rangle^{x} &= 0 \\
\mathbf{V}_{\mathrm{Li}} &= \langle\mathbf{V}_{\mathrm{L}}\rangle^{x\rho} + (1-\eta_{\mathrm{m}})\mathbf{U}_{\mathrm{R}} \\
\langle p_{\mathrm{L}}\rangle^{x} - \langle p_{\mathrm{L}}\rangle_{\mathrm{i}} &= 0.25(1-\epsilon)\langle\rho_{\mathrm{L}}\rangle^{x}U_{\mathrm{R}}^2 \\
\mathbf{M}_{\mathrm{Lp}} &= \epsilon\langle\rho_{\mathrm{L}}\rangle^{x}C_{\mathrm{vm}}\mathbf{a}^{*} + 0.5C_{\mathrm{r}}\langle\rho_{\mathrm{L}}\rangle^{x}\,\mathrm{D}_{\mathrm{G}}\epsilon/\mathrm{D}t\,\mathbf{U}_{\mathrm{R}} - C_{\mathrm{n}}\langle\rho_{\mathrm{L}}\rangle^{x}\mathbf{U}_{\mathrm{R}}\cdot\nabla\epsilon\,\mathbf{U}_{\mathrm{R}} \\
\mathbf{M}_{\mathrm{Lt}} &= 0.375C_{\mathrm{D}}U_{\mathrm{R}}\epsilon\langle\rho_{\mathrm{L}}\rangle^{x}/R_{\mathrm{b}}\mathbf{U}_{\mathrm{R}} \\
W_{\mathrm{LP}}'' &= (1-\eta_{\mathrm{m}})\langle p_{\mathrm{L}}\rangle^{x}\mathbf{U}_{\mathrm{R}}\cdot\nabla\epsilon + \langle p_{\mathrm{L}}\rangle^{x}\,\mathrm{D}_{\mathrm{L}}\epsilon/\mathrm{D}t \\
&\quad + 0.15a_1(1-\epsilon)\epsilon\langle\rho_{\mathrm{L}}\rangle^{x}U_{\mathrm{R}}\,\mathrm{tr}(\mathbf{D}_{\mathrm{L}}) - 0.45a_1(1-\epsilon)\epsilon\langle\rho_{\mathrm{L}}\rangle^{x}\mathbf{U}_{\mathrm{R}}\mathbf{U}_{\mathrm{R}}:\mathbf{D}_{\mathrm{L}} \\
&\quad - 0.05(9a_1+a_2)(1-\epsilon)\epsilon\langle\rho_{\mathrm{L}}\rangle^{x}\mathbf{U}_{\mathrm{R}}\mathbf{U}_{\mathrm{R}}:\nabla\mathbf{U}_{\mathrm{R}} + \Gamma_{\mathrm{L}}\langle p_{\mathrm{L}}\rangle_{\mathrm{i}}/\langle\rho_{\mathrm{L}}\rangle^{x} \\
\mathbf{q}_{\mathrm{L}}^{\mathrm{p}} + \mathbf{q}_{\mathrm{L}}^{\mathrm{k}} + \mathbf{q}_{\mathrm{L}}^{\mathrm{r}} &= 0 \\
W_{\mathrm{L}i}'' &= 0 \\
\langle\boldsymbol{\tau}_{\mathrm{L}}\rangle_{\mathrm{i}} &= 0 \\
\mathbf{q}_{\mathrm{L}}^{\mathrm{t}} &= 0 \\
\langle\mathbf{q}_{\mathrm{L}}''\rangle^{x} &= -K_{\mathrm{t}}k_{\mathrm{L}}\nabla\langle T_{\mathrm{L}}\rangle^{x\rho} \\
U_{\mathrm{L}}^{\mathrm{Re}} &= 0.025(9_1 a + {}_2 a)\alpha_{\mathrm{R}}U^2 \\
\Gamma_k\mathbf{V}_{ki} &= \Gamma_k[\langle\mathbf{V}_k\rangle^{x\rho} + (1-\eta_{\mathrm{m}})\mathbf{U}_{\mathrm{R}}] \\
\Gamma_k(\mathbf{V}_k\cdot\mathbf{V}_k)_{\mathrm{i}} &= \Gamma_k[\langle\mathbf{V}_k\rangle^{x\rho}\cdot\langle\mathbf{V}_k\rangle^{x\rho} + 0.5\mathbf{U}_{\mathrm{R}}^2 + 2(1-\eta_{\mathrm{m}})\langle\mathbf{V}_k\rangle^{x\rho}\cdot\mathbf{U}_{\mathrm{R}}]
\end{aligned}
$$

where

$\epsilon$—volume fraction of the dispersed vapor phase

$R_{\mathrm{b}}$—bubble radius

$\mathrm{D}_k/\mathrm{D}t$—material derivative following phase-$k$

$\mathbf{a}^{*}$—objective acceleration, given by

$\mathbf{a}^{*} = \mathrm{D}_{\mathrm{G}}\mathbf{V}_{\mathrm{G}}/\mathrm{D}t - \mathrm{D}_{\mathrm{L}}\mathbf{V}_{\mathrm{L}}/\mathrm{D}t + \mathbf{U}_{\mathrm{R}}\times\nabla\times\mathbf{V}_{\mathrm{L}}$

averaging of potential flow around a spherical bubble. Unspecified coefficients are assumed to be sufficient to account for differences between actual flow and the idealized flow conditions used for the calculations. The entropy equation gives us the necessary constraints upon these coefficients. It should be recognized that these closure conditions are fairly simple and can be improved. For example, the turbulent stresses ($\mathbf{T}^{\mathrm{Re}}$) are only due to "bubble-induced" effects. To include shear-induced effects, more realistic turbulence models (e.g. $\tau$–$\epsilon$ models) are necessary.

Let us substitute these equations into the entropy constraint [26] and use the following relations:

$$
\mathrm{D}_{\mathrm{G}}\epsilon/\mathrm{D}t = \partial\epsilon/\partial t + \langle\mathbf{V}_{\mathrm{L}}\rangle^{x\rho}\cdot\nabla\epsilon + \mathbf{U}_{\mathrm{R}}\cdot\nabla\epsilon = \mathrm{D}_{\mathrm{L}}\epsilon/\mathrm{D}t + U_{\mathrm{R}}\cdot\nabla\epsilon,
$$

$$
\mathbf{U}_{\mathrm{R}}\cdot\mathrm{D}_{\mathrm{L}}\mathbf{U}_{\mathrm{R}}/\mathrm{D}t = \mathbf{U}_{\mathrm{R}}\cdot\mathbf{a}^{*} - \mathbf{U}_{\mathrm{R}}\mathbf{U}_{\mathrm{R}}:\mathbf{D}_{\mathrm{L}} - \mathbf{U}_{\mathrm{R}}\mathbf{U}_{\mathrm{R}}:\nabla\mathbf{U}_{\mathrm{R}}
$$

and

$$
\Gamma\rho_{ki} = \Gamma\langle\rho_k\rangle^{x},
$$

where

$$
\mathbf{U}_{\mathrm{R}} = \langle\mathbf{V}_{\mathrm{G}}\rangle^{x\rho} - \langle\mathbf{V}_{\mathrm{L}}\rangle^{x\rho}.
$$

After we do this and collect terms, the entropy equation becomes

$$
\begin{aligned}
&0.375C_{\mathrm{D}}\epsilon\langle\rho_{\mathrm{L}}\rangle^{x}/R_{\mathrm{b}}U_{\mathrm{R}}^2\,|U_{\mathrm{R}}| + (1-\epsilon)K_{\mathrm{t}}k_{\mathrm{L}}(\nabla\langle T_k\rangle^{x\rho})^2/\langle T_k\rangle^{x\rho} \\
&\quad - \epsilon\langle\rho_{\mathrm{L}}\rangle^{x}\langle s_{\mathrm{L}}'\mathbf{V}_{\mathrm{L}}'\rangle^{x\rho}\cdot\nabla\langle T_{\mathrm{L}}\rangle^{x\rho} + \epsilon\langle\rho_{\mathrm{L}}\rangle^{x}\mathbf{a}^{*}\cdot\mathbf{U}_{R}[(1-\eta_{\mathrm{m}})C_{\mathrm{vm}} - 0.05(1-\epsilon)(9a_1+a_2)] \\
&\quad + \langle\rho_k\rangle^{x}U_{\mathrm{R}}^2\mathbf{U}_{\mathrm{R}}\cdot\nabla\epsilon[(1-\eta_{\mathrm{m}}) - 0.45C_{\mathrm{n}} + 0.25(1-\epsilon) + 0.5C_{\mathrm{r}}] \\
&\quad + \langle\rho_k\rangle^{x}U_{\mathrm{R}}^2\,\mathrm{D}_{\mathrm{L}}\epsilon/\mathrm{D}t[0.5(1-\eta_{\mathrm{m}})C_{\mathrm{r}} - 0.025(1-\epsilon)(9a_1+a_2)] \\
&\quad + \Gamma_{\mathrm{L}}\langle\rho_{\mathrm{L}}\rangle^{x}U_{\mathrm{R}}^2[0.25 - 0.25(1-\epsilon) - 0.025\epsilon(9a_1+a_2)] \geqslant 0.
\end{aligned}
\qquad [34]
$$

The first two terms are positive definite, and, as discussed previously, the third is assumed to be. Thus, we can assure that the entropy equation is always satisfied by requiring that the rest of the equation be equal to zero. This requirement gives us:

$$9a_1 + a_2 = 10, \qquad [35]$$

$$1 - n_{\mathrm{m}} = (1 - \epsilon)/2C_{\mathrm{vm}}, \qquad [36]$$

$$-C_{\mathrm{n}} + 0.25(1 - \epsilon) + 0.5C_{\mathrm{r}} = 0 \qquad [37]$$

and

$$0.5(1 - \eta_{\mathrm{m}})C_{\mathrm{r}} - 0.25(1 - \epsilon) = 0. \qquad [38]$$

The values of $a_1$ and $a_2$ found by inviscid flow calculations are

$$a_1 = a_2 = 1.$$

These values satisfy [35] and are recommended. There are numerous correlations available for the virtual mass coefficient ($C_{\mathrm{vm}}$). The correlation proposed (Ruggles *et al.* 1988) appears to be the best. Nevertheless, using any specific correlation for $C_{\mathrm{vm}}$, [35]–[37] may be solved. This gives us

$$\eta_{\mathrm{m}} = 1 - (1 - \epsilon)/2C_{\mathrm{vm}},$$

$$C_{\mathrm{r}} = C_{\mathrm{vm}}$$

and

$$C_{\mathrm{n}} = (1 - \epsilon)/4 + C_{\mathrm{vm}}/2.$$

## SUMMARY AND CONCLUSION

We have derived an appropriately averaged entropy equation in which derivatives of entropy do not occur. This entropy constraint was applied to sets of constitutive equations found in several state-of-the-art transient multiphase flow computer codes. It was found that all current generation multiphase computer codes violate the second law of thermodynamics. It was found that the conservation and constitutive equations used neglected some interfacial effects. In particular, an interfacial flow work term, $\Gamma_{\mathrm{L}}(p_{\mathrm{L}}/\rho_{\mathrm{L}})_{\mathrm{i}}$, was neglected in all codes.

The analysis of the code's constitutive equations also demonstrated that when physically-based terms, such as the virtual mass force, are added to the conservation equations to improve accuracy when analyzing accelerating two-phase flows, other terms must also be included in the energy equation to prevent violation of the second law.

Examination of the entropy constraint, [26], reveals that the interfacial velocity compliance coefficient ($\eta_{\mathrm{m}}$) is an important parameter in determining phasic dissipation. This fact has been recognized previously (Wallis 1969), however the donor-cell treatment of the interfacial velocity used in most two-fluid computer codes is inadequate.

It is important to remember that dissipative terms may be small, thus a violation of the second law constraints does not necessarily imply a large error in calculated parameters (e.g. flow quality). Nevertheless, a violation of the second law is a clear warning that the physics used in the model should be re-examined.

One acceptable set of constitutive equations for a continuous liquid phase containing a discrete phase was presented. This set of equations had a realistic treatment of interfacial effects and was based on rigorous averaging of the flow parameters for an idealized bubbly flow situation. While it was not demonstrated that this model is well-posed or agrees with the available data, it was shown that this set of constitutive equations is capable of satisfying the second law.

It should be obvious that consideration of second law constraints on multiphase flow models is an important means for assessing those models. The approach discussed herein was restricted to consideration of the continuous liquid-phase conservation equations and their associated closure conditions. However, this approach can be readily extended to the assessment of the modeling of the discrete phase, as well as to models for the corresponding mixture equations and to the equations of the interfacial jump conditions. Indeed, such an analysis may well be capable of demonstrating the incompatibility of the equal phase pressure assumption that is often used. Hence, the entropy constraint given by [26] appears to be a very useful method of filtering out unacceptable two-fluid modeling assumptions.

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