

DERIVATION OF A GENERIC MULTI-FIELD TWO-FLUID MODEL

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ABSTRACT

Multiphase computational fluid dynamics (MCFD) simulation based on the two-fluid model has emerged as a valuable tool for reactor thermal-hydraulics design and safety analysis. The classical two-field, two-fluid model treats each phase as a whole, which introduces considerable uncertainties when a phase is comprised of significantly different forms, e.g., liquid droplets and liquid film. This uncertainty becomes particularly important for resolving the multi-dimensional distribution of different fields in CFD applications. In relation to this, a multi-field model is necessary to mechanistically model a wide range of two-phase flow regimes. In this paper, we first derive a generic and rigorous multi-field two-fluid framework based on the local instant formulation of the mass, momentum and energy conservation equations for single phase fluids. An averaging operator is introduced to make the derivation more general than previous studies based on a specific time-, area-, volume-, or ensemble-averaging method. The averaged field conservation equations and interfacial jump conditions are obtained from the local instantaneous formulation through a derivation with minimal assumptions. Based on this framework, a six-field two-fluid model is proposed as a practical model for the entire spectrum of the two-phase flow regimes spanning from bubbly to annular. These six fields include: continuous liquid, two dispersed liquid fields, continuous gas, and two dispersed gas fields. The relationship between the momentum transfer terms in the Eulerian two-fluid model and the particle forces have been established by introducing a statistical averaging and the equation of motion for a single particle. Based on this analysis, the Ishii and Mishima [1] formulation for the interfacial momentum transfer terms is adopted in the current six-field two-fluid model.

KEYWORDS

CFD, two-fluid model, multi-field, averaging, interfacial transfer

1. INTRODUCTION

The two-phase flows found in industrial applications often exhibit very complex flow structures, in which a large number of bubbles, droplets, films, and other flow structures undergo rapid interactions and topological changes. Even with ever increasing computing power, it is not feasible in the near-future to simulate these two-phase flow problems by directly solving the local instant formulations (or the so-called one fluid model [2]) which intends to resolve all the interfaces. Therefore, a proper averaging should be taken over a two-phase flow field to eliminate the unresolved high frequency signals, and hence to significantly reduce the computational cost. When averaging is taken over each phase in a gas-liquid two-phase flow, one obtains the “two-fluid model,” in which the conservation equations are written for gas and liquid separately. Ishii [3] was among the first who rigorously derived the two-fluid model from

the fundamental single phase flow formulation based on time-averaging. Other averaging methods such as space averaging, including area and volume averaging [4], and ensemble averaging [5] were also used to derive the two-fluid model in the literature. The two-fluid model originally consisted of one set of mass, momentum and energy equations for each phase. Therefore, the model does not differentiate interfacial structure forms within each phase such that continuous and dispersed gases (or liquids) are considered as a single fluid field. Continuous and dispersed gases (and liquids) have quite different hydrodynamic behavior in a two-phase system, and their importance in terms of heat transfer is also different. For example, it is the film flow rate rather than the total liquid flow rate (which also includes the droplet flow rate) that determines the occurrence of film dryout, and hence the peak cladding temperature, of a nuclear fuel rod. It is necessary to divide gas and liquid phases into multiple fields and solve separate field equations to achieve better predictions.

Among the different approaches, the four-field two-fluid model proposed by Lahey and Drew [6] is considered generic and covers all the flow regimes from bubbly to annular flow. However, the four-field model treats all the bubbles of different sizes as a single field, which does not reflect the fact that small and large bubbles behave differently in terms of drag, lift, and bubble interaction mechanisms. For example, the lift force changes its direction when a bubble size exceeds a certain limit. This difference is important for a 3-D prediction since it determines whether a wall-peak or a center-peak void profile exists in the flow. In relation to this, a two-group interfacial area transport equation (IATE) approach has been developed by Ishii [7] to model small (group-1) and large bubbles (group-2) separately. This treatment requires the modification of the classical two-fluid model. In this regard, Sun [8] proposed a three-field two-fluid model (also called two-group two-fluid model, as there are two bubble groups). Sun presented the separate conservation equations for group-1 and group-2 bubbles, and the liquid phase. They also proposed a combined gas momentum equation to simplify the system and reduce the computational cost. The combined momentum equation approach in a CFD code was also investigated by Lee *et al.* [19]. The two-group two-fluid model is applicable to bubbly, cap-bubbly, cap-turbulent and churn-turbulent flow regimes. Neither the four-field model nor the two-group two-fluid model was derived from the fundamental conservation equations of single phase fluids. Therefore, the completeness and the accuracy of the field equations cannot be verified. Morel [9] re-examined the four-field two-fluid model by introducing two types of indicator functions, one for different phases, and the other one for different regions, namely, the continuous gas and the continuous liquid region. He was able to derive the four-field two-fluid model from the local instant balance equation of single phase fluids. However, Morel's derivation was specifically for stratified flow regime in horizontal flows. It cannot be applied to flows with both groups of bubbles, or flows with more than four fields.

In relation to the above, this paper focuses on the development of a generic multi-field two-fluid model for mechanical and thermal non-equilibrium two-phase flows. This will become the foundation of any specific multi-field two-fluid model for a particular flow regime. More importantly, combining with the interfacial area transport equation, a unified two-fluid model framework can be established. Within this framework, flow regime transitions are predicted based on physical models rather than empirical transition criteria, thus preserving the dynamics of two-phase structure and eliminating possible numerical issues.

2. DERIVATION OF A GENERIC MULTI-FIELD TWO-FLUID MODEL

In this section, a detailed derivation of a generic multi-field two-fluid model framework is presented. Similar to the derivation of the classical two-fluid model, it is assumed that the general conservation principles for mass, momentum, and energy, apply to any point in the flow domain at any given time. For the two-phase flow of interest, two important assumptions are also made here. First, the interface is sufficiently smooth and has a zero thickness. Therefore, the derivation is only applicable to immiscible fluids, which are of primary concern in this work. Second, two fields of the same phase do not have

continuous direct contact over a time-averaged relevant time scale. This assumption is made to simplify the classification of different fields within the same phase. If a connected object has to be divided into two different fields, it makes the demarcation extremely difficult both numerically and experimentally because of the complex two-phase flow interfacial structures. Two fields of the same phase may interact in a near instantaneous manner (i.e., a group-1 and group-2 bubble coalescing into a group-2 bubble).

In a multi-field two-fluid model, two fundamental discontinuities appear: 1) the discontinuity due to a physical parameter change across the interface, and, 2) the discontinuity due to the sudden change of the field. In the second case, the discontinuity is artificially created due to the classification of flow fields. The “sharp interface” and “sudden field change” concept may not be desirable for direct numerical simulations. However, these discontinuities in the local instant formulation will be eliminated through certain averaging processes. The resultant two-fluid model is based on the averaged flow parameters which are smooth and quantifiable in nature. The practical engineering application, based on the two-fluid model, will not see these discontinuities caused by either interface or inter-field changes. As discontinuities and Dirac delta functions appear in the derivation, the functions appearing in the local instant formulations should be considered as generalized functions (or distributions). The following convention is adopted for a better representation of the parameters in a multi-field two-phase flow.

1. For phase k , there are N_k fields in total. Similarly, N_l denotes the total number of fields in phase l .
2. For a variable f_{kj} , subscript kj means phase k , field j . $k=g$ for gas, f for liquid. $j=0$ for the continuous field, $1, 2, \dots, N_k - 1$ for dispersed fields.
3. A subscript i in quantity f_i means an interfacial quantity.
4. The subscript $kj - lm$ in quantity $f_{i,kj-lm}$ represents the interface between fields kj and lm .
5. The subscript $kj \rightarrow lm$ in quantity $f_{i,kj \rightarrow lm}$ means a transfer from field kj to lm .
6. The under right arrow, e.g., \underline{v} , indicates a vector. The double under-bar, e.g., $\underline{\underline{\tau}}$, represents a tensor.

2.1. Local Instant Parameters

For a multi-field two-phase flow, one can define the level set representation of field kj as [3] :

$$f_{kj}(\underline{x}, t) \begin{cases} > 0, & \text{inside field } kj \\ = 0, & \text{at the interface} \\ < 0, & \text{outside field } kj \end{cases} \quad (1)$$

For multi-particle systems, one may define f_{kj} for the surface of each particle. A new function obtained from the product of all those f_{kj} 's has the same properties as those shown in Eq. (1). Therefore, function f_{kj} appeared in the following discussions may represent either a single or multiple interfaces. The phase indicator function χ_k can be extended to the field indicator function as:

$$\chi_{kj}(\underline{x}, t) = H_f(f_{kj}(\underline{x}, t)) = \begin{cases} 1, & (\underline{x}, t) \text{ occupied by field } kj \\ 0, & \text{otherwise} \end{cases} \quad (2)$$

where H_f is the Heaviside function. Each field indicator function is defined over the entire spatial and temporal domain $T \times \Omega : \{-\infty < t < \infty, \bar{x} \in R^3\}$. The local instant interfacial area concentration for field kj can be written as:

$$a_{i,kj} = |\nabla \chi_{kj}| = \delta(f_{kj}) |\nabla f_{kj}|. \quad (3)$$

Here δ is the Dirac delta function. For multi-field two-phase flows, it is proper to further divide the interfacial area into several interface pairs:

$$a_{i,kj-lm} = \begin{cases} a_{i,kj}, & \text{at the interface between fields } kj \text{ and } lm \\ 0, & \text{otherwise} \end{cases} \quad (4)$$

Here subscript $kj - lm$ represents the interface between fields kj and lm . The total interfacial area surrounding field kj can be given as:

$$a_{i,kj} = \sum_{\substack{l \neq k \\ m=0, \dots, N_l-1}} a_{i,kj-lm} \quad (5)$$

2.2 Filter Function, Convolution and Averaging

Averaging a two-phase flow is a low pass filtering process to eliminate unwanted high frequency signals from local instant fluctuations of variables [1]. In the present study, an averaging concept based on filter functions [10] is utilized to ensure the generality of the derived two-fluid model. In other words, the derivation can be applied to time-averaging, area-averaging, volume-averaging, or any combination using these averages. A filter function (or a kernel function) $G(\underline{x}, t)$ is defined on the time-spatial domain $T \times \Omega : \{-\infty < t < \infty, \bar{x} \in R^3\}$ with a compact support. Averaging can be realized by taking the convolution of a field parameter $f(\underline{x}, t)$ and a filter function given by the following expression:

$$\bar{f}^A(\underline{x}, t) = G^A(\underline{x}, t) * f(\underline{x}, t) = \int_{T \times \Omega} G^A(\underline{x}', t') f(\underline{x} - \underline{x}', t - t') dx' dy' dz' dt' \quad (6)$$

Here, the over bar indicates an averaged value. Superscript 'A' means averaging method, it could be 'T', 'V' and 'S' representing time, volume and area averaging, respectively. For time-averaging, the filter function is defined as:

$$G^T(\underline{x}, t) = \begin{cases} \frac{1}{\Delta T} \delta(\underline{x}), & |t| \leq \Delta T / 2 \\ 0, & |t| > \Delta T / 2 \end{cases} \quad (7)$$

By the definition given in Eq. (6), the time-averaged value for a field quantity f is:

$$\bar{f}^T(\underline{x}, t) = \int_{T \times \Omega} G(\underline{x}', t') f(\underline{x} - \underline{x}', t - t') dx' dy' dz' dt' = \frac{1}{\Delta T} \int_{t-\Delta T/2}^{t+\Delta T/2} f(\underline{x}, t') dt' \quad (8)$$

This is identical to the definition given by Ishii [3]. Essentially, by introducing the Dirac delta function in the kernel, the averaging is frozen at the given point. The examples and filter functions can also be given for line-, area-, and volume-averaging, and any combination of those operations in a similar way [10]. The convolution has the following properties which can be carried forward to the averaging operator:

$$\begin{aligned} G * f &= f * G, \\ G * (af_1 + bf_2) &= aG * f_1 + bG * f_2, \\ \frac{\partial(G * f)}{\partial t} &= G * \frac{\partial f}{\partial t}, \\ \nabla(G * f) &= G * \nabla f. \end{aligned} \quad (9)$$

In the current averaging scheme, the integral is taken over the entire spatial and temporal domain $T \times \Omega : \{-\infty < t < \infty, \bar{x} \in R^3\}$, and the field quantity f is well defined over this domain. The averaging operator commutes with time and spatial derivatives. This is different from the Ishii approach [3], in which the integration range contains several discrete time intervals and they are dependent on location. In that case, the Leibnitz rule has to be used to convert the time/space derivatives of the average to the average of these derivatives.

In the following derivation, an over bar is used to represent an arbitrary averaging operator:

$$\bar{f} = G * f . \quad (10)$$

The specific averaging, *i.e.*, time-averaging, space-averaging, or the combination of the two, can be determined by the kernel function. The properties of the averaging operator expressed in Eq.(9) will be used in the later derivation. Note that the properties of the averaging operator are similar to the ensemble-averaging. Therefore, the following derivation also applies to the ensemble-averaging used by Drew and Lahey [5].

2.3 Averaged Generalized Balance Equation

The following averaged quantities are introduced first:

$$\begin{aligned} \bar{f}_{kj} &= G * (\chi_{kj} f) = \overline{\chi_{kj} f} , \\ \bar{f}_{kj} &= \frac{G * (\chi_{kj} f)}{G * \chi_{kj}} = \frac{\overline{\chi_{kj} f}}{\alpha_{kj}} , \\ \hat{f}_{kj} &= \frac{G * (\chi_{kj} \rho f)}{G * (\chi_{kj} \rho)} = \frac{\overline{(\rho f)_{kj}}}{\bar{\rho}_{kj}} . \end{aligned} \quad (11)$$

Here, $\overline{(\)}_{kj}$, $\overline{\overline{(\)}}_{kj}$ and $\widehat{(\)}_{kj}$ represent the mean value of a field *kj* property, the phase-weighted average, and the mass-weighted- (or Favre-) average, respectively. The derivation of the two-fluid model starts from the generalized balance equation of single phase fluids. For an intensive quantity *c* of the fluids, the generalized balance equation in differential form is given as [11] :

$$\frac{\partial}{\partial t}(\rho c) + \nabla \cdot (\rho c \underline{v}) = -\nabla \cdot \underline{J} + \rho \phi . \quad (12)$$

Here \underline{J} and ϕ are surface flux and volume source terms, respectively. Following a procedure similar to Drew and Lahey's [5], one first multiplies the generalized local instant balance equation, Eq. (12), by the field indicator function, χ_{kj} , and rearrange to get:

$$\left[\frac{\partial}{\partial t}(\chi_{kj} \rho c) + \nabla \cdot (\chi_{kj} \rho c \underline{v}) + \nabla \cdot (\chi_{kj} \underline{J}) - \chi_{kj} \rho \phi \right] - \rho c \left[\frac{\partial}{\partial t}(\chi_{kj}) + \underline{v} \cdot \nabla \chi_{kj} \right] - \nabla \chi_{kj} \cdot \underline{J} = 0 . \quad (13)$$

Applying the generic averaging operator to Eq. (13), one gets:

$$\frac{\partial}{\partial t}(\overline{\chi_{kj} \rho c}) + \nabla \cdot (\overline{\chi_{kj} \rho c \underline{v}}) = -\nabla \cdot (\overline{\chi_{kj} \underline{J}}) + \overline{\chi_{kj} \rho \phi} + \rho c \left[\frac{\partial}{\partial t}(\overline{\chi_{kj}}) + \underline{v} \cdot \nabla \overline{\chi_{kj}} \right] + \overline{\nabla \chi_{kj} \cdot \underline{J}} . \quad (14)$$

The properties of the averaging operators are used in the above derivation. Based on the definitions given in Eq (11), Eq. (14) can be written as:

$$\frac{\partial}{\partial t}(\alpha_{kj} \bar{\rho}_{kj} \hat{c}_{kj}) + \nabla \cdot (\alpha_{kj} \bar{\rho}_{kj} (\underline{c \underline{v}})_{kj}) = -\nabla \cdot (\alpha_{kj} \bar{\underline{J}}_{kj}) + \alpha_{kj} \bar{\rho}_{kj} \hat{\phi}_{kj} + \rho c \left[\frac{\partial}{\partial t}(\overline{\chi_{kj}}) + \underline{v} \cdot \nabla \overline{\chi_{kj}} \right] + \overline{\nabla \chi_{kj} \cdot \underline{J}} . \quad (15)$$

In order to take into account the fluctuating component effect caused by turbulence, one can decompose the property *c* as follows:

$$c = \hat{c}_{kj} + c'_{kj} . \quad (16)$$

Then:

$$\hat{c}_{kj} = \widehat{(c_{kj})_{kj}} + \widehat{(c'_{kj})_{kj}} . \quad (17)$$

Similar to the derivation of the Reynolds-Averaged Navier-Stokes (RANS) equation, one can assume the average is idempotent:

$$\widehat{(\hat{c}_{kj} f)}_{kj} = \hat{c}_{kj} \hat{f}_{kj} , \quad (18)$$

Based on the above decomposition, Eq. (15) becomes:

$$\begin{aligned} \frac{\partial}{\partial t} (\alpha_{kj} \bar{\rho}_{kj} \hat{c}_{kj}) + \nabla \cdot (\alpha_{kj} \bar{\rho}_{kj} \hat{c}_{kj} \underline{v}_{kj}) = & -\nabla \cdot (\alpha_{kj} \bar{J}_{kj}) - \nabla \cdot \left[\alpha_{kj} \bar{\rho}_{kj} \widehat{(c'_{kj} v'_{kj})_{kj}} \right] + \alpha_{kj} \bar{\rho}_{kj} \hat{\phi}_{kj} \\ & + \rho c \overline{\left[\frac{\partial}{\partial t} (\chi_{kj}) + \underline{v} \cdot \nabla \chi_{kj} \right]} + \overline{\nabla \chi_{kj} \cdot \underline{J}} . \end{aligned} \quad (19)$$

The second to the last term in Eq. (19) can be rearranged as a material derivative form:

$$\rho c \left[\frac{\partial}{\partial t} (\chi_{kj}) + \underline{v} \cdot \nabla \chi_{kj} \right] = \rho c \frac{D\chi_{kj}}{Dt} . \quad (20)$$

To properly account for the inter-phase and inter-field mass transfers, $\frac{D\chi_{kj}}{Dt}$ is partitioned as follows:

$$\frac{D\chi_{kj}}{Dt} = \frac{D\chi_{kj}}{Dt} \Big|_{\text{phase}} + \frac{D\chi_{kj}}{Dt} \Big|_{\text{field}} , \quad (21)$$

where,

$$\frac{D\chi_{kj}}{Dt} \Big|_{\text{phase}} = \begin{cases} \frac{D\chi_{kj}}{Dt} , & \text{fluid changes phase} \\ 0 , & \text{otherwise} \end{cases} \quad (22)$$

and

$$\frac{D\chi_{kj}}{Dt} \Big|_{\text{field}} = \begin{cases} \frac{D\chi_{kj}}{Dt} , & \text{fluid changes field without phase change} \\ 0 , & \text{otherwise} \end{cases} \quad (23)$$

In the classical two-fluid model, each phase contains only one field. The following equality holds as long as the field on either side of an interface remains constant [12]:

$$\frac{\partial \chi_{kj}}{\partial t} + \underline{v}_{i,kj} \cdot \nabla \chi_{kj} = 0 . \quad (24)$$

The above equation is also called the phase topological equation, in which $\underline{v}_{i,kj}$ is the interfacial velocity. Considering Equations (20) and (24), one can obtain:

$$\overline{\rho c \frac{D\chi_{kj}}{Dt}} = \overline{\rho c \left[(\underline{v} - \underline{v}_{i,kj}) \cdot \nabla \chi_{kj} \right]} = \Gamma_{kj} \hat{c}_{i,kj} \quad (25)$$

For the multi-field two-fluid model, the phase change term can be expressed as follows:

$$\overline{\rho c \frac{D\chi_{kj}}{Dt}} \Big|_{\text{phase}} = \rho c \sum_{\substack{l \neq k \\ m=0, \dots, N_f-1}} \overline{\frac{D\chi_{kj}}{Dt}} \Big|_{kj-lm} = \sum_{\substack{l \neq k \\ m=0, \dots, N_f-1}} \Gamma_{kj-lm} \hat{c}_{i,kj-lm} . \quad (26)$$

Here Γ_{kj-lm} and $\hat{c}_{i,kj-lm}$ are the mass transfer rate due to phase change, and the averaged value of c during the phase change, at the interface between fields kj and lm .

The term $\left. \frac{D\chi_{kj}}{Dt} \right|_{\text{field}}$ becomes nontrivial due to field change that occurs within the same phase. In this case, Eq. (24) does not hold. The field change is a result of the topological change of the two-phase flow structures, not an event at a single point. Therefore, it cannot be modeled by the local instant equation alone. The averaged two-fluid model based on the local instant equation does not have that capability either. One must use a Boltzmann statistical description or a phenomenological approach to model the field change rate in a two-phase flow system. Following a similar path as the two-group IATE [7], field changes can be divided into a source and a sink term. Each is further attributed to various physical mechanisms:

$$\left. \frac{D\chi_{kj}}{Dt} \right|_{\text{field}} = \sum_{\substack{m=0,\dots,N_k-1 \\ m \neq j}} \left. \frac{D\chi_{kj}}{Dt} \right|_{km \rightarrow kj} + \sum_{\substack{m=0,\dots,N_k-1 \\ m \neq j}} \left. \frac{D\chi_{kj}}{Dt} \right|_{kj \rightarrow km}, \quad (27)$$

where, the subscript $km \rightarrow kj$ stands for the change from field km to kj , and vice versa. Therefore, the first and second terms on the RHS of Eq. (27) represent the gain and the loss of field kj , respectively. Averaging Eq. (27), one obtains:

$$\overline{\rho c \left. \frac{D\chi_{kj}}{Dt} \right|_{\text{field}}} = \sum_{\substack{m=0,\dots,N_k-1 \\ m \neq j}} \dot{m}_{km \rightarrow kj} \hat{c}_{km \rightarrow kj} - \sum_{\substack{m=0,\dots,N_k-1 \\ m \neq j}} \dot{m}_{kj \rightarrow km} \hat{c}_{kj \rightarrow km}, \quad (28)$$

where,

$$\dot{m}_{km \rightarrow kj} = \rho \overline{\left. \frac{D\chi_{kj}}{Dt} \right|_{km \rightarrow kj}}, \quad (29)$$

and

$$\hat{c}_{km \rightarrow kj} = \frac{\overline{\left. \frac{D\chi_{kj}}{Dt} \right|_{km \rightarrow kj}}}{\dot{m}_{km \rightarrow kj}}. \quad (30)$$

$\left. \frac{D\chi_{kj}}{Dt} \right|_{km \rightarrow kj}$ is zero everywhere except where the fluid field changes from km to kj . Therefore, property

$\hat{c}_{km \rightarrow kj}$ means the averaged value of c during the transfer from field km to kj . Note the difference between the field transfer subscript $kj \rightarrow km$, in which the arrow indicates the direction of the field change. The direction of phase change is neither considered in the classical two-fluid model, nor in the two-group two-fluid model. One reason is that phase change is usually assumed to be unidirectional at a given point in the flow domain at a given time. However, field transfer could be caused by many different mechanisms and each one of them could result in significantly different momentum and energy exchanges. Considering annular flow, for example, entrainment and deposition are common transfer mechanisms between the film and the droplets. The governing hydrodynamics are quite different between the entrainment and deposition processes. The entrainment and deposition velocities are also different and they must be treated separately in the momentum equation.

Substituting Eqs. (26) and (28) into Eq. (19), the averaged generalized balance equation takes the following form:

$$\begin{aligned}
\frac{\partial}{\partial t}(\alpha_{kj}\bar{\rho}_{kj}\hat{c}_{kj}) + \nabla \cdot (\alpha_{kj}\bar{\rho}_{kj}\hat{c}_{kj}\hat{v}_{kj}) = & -\nabla \cdot (\alpha_{kj}\bar{J}_{kj}) - \nabla \cdot \left[\alpha_{kj}\bar{\rho}_{kj}(\widehat{c'_{kj}v'_{kj}})_{kj} \right] + \alpha_{kj}\bar{\rho}_{kj}\hat{\phi}_{kj} \\
& + \sum_{\substack{l \neq k \\ m=0, \dots, N_l-1}} \Gamma_{kj-lm}\hat{c}_{i,kj-lm} + \sum_{\substack{m=0, \dots, N_k-1 \\ m \neq j}} \dot{m}_{km \rightarrow kj}\hat{c}_{km \rightarrow kj} - \sum_{\substack{m=0, \dots, N_k-1 \\ m \neq j}} \dot{m}_{kj \rightarrow km}\hat{c}_{kj \rightarrow km} \\
& + \nabla \chi_{kj} \cdot \underline{J}.
\end{aligned} \tag{31}$$

2.4 Field Equations in the Multi-field Two-fluid Model

As no specific assumptions are made, Eq. (31) is applicable to any field of either phase in a two-phase flow system. By specifying corresponding c , J , and ϕ for the conservations of mass, momentum and energy [11], the following averaged equations for field kj , can be obtained:

Continuity equation

$$\frac{\partial}{\partial t}(\alpha_{kj}\bar{\rho}_{kj}) + \nabla \cdot (\alpha_{kj}\bar{\rho}_{kj}\hat{v}_{kj}) = \sum_{\substack{l \neq k \\ m=0, \dots, N_l-1}} \Gamma_{kj-lm} + \sum_{\substack{m=0, \dots, N_k-1 \\ m \neq j}} \dot{m}_{km \rightarrow kj} - \sum_{\substack{m=0, \dots, N_k-1 \\ m \neq j}} \dot{m}_{kj \rightarrow km}. \tag{32}$$

Momentum equation

$$\begin{aligned}
\frac{\partial}{\partial t}(\alpha_{kj}\bar{\rho}_{kj}\hat{v}_{kj}) + \nabla \cdot (\alpha_{kj}\bar{\rho}_{kj}\hat{v}_{kj}\hat{v}_{kj}) = & -\nabla(\alpha_{kj}\bar{p}_{kj}) + \nabla \cdot \left[\alpha_{kj} \left(\overline{\underline{\tau}^\mu} \right)_{kj} + \underline{\tau}_{kj}^T \right] + \alpha_{kj}\bar{\rho}_{kj}\hat{g}_{kj} \\
& + \sum_{\substack{l \neq k \\ m=0, \dots, N_l-1}} \Gamma_{kj-lm}\hat{v}_{i,kj-lm} + \sum_{\substack{m=0, \dots, N_k-1 \\ m \neq j}} \dot{m}_{km \rightarrow kj}\hat{v}_{km \rightarrow kj} - \sum_{\substack{m=0, \dots, N_k-1 \\ m \neq j}} \dot{m}_{kj \rightarrow km}\hat{v}_{kj \rightarrow km} \\
& + \bar{p}_{i,kj}\nabla\alpha_{kj} - \nabla\alpha_{kj} \cdot \overline{\underline{\tau}^\mu} + \sum_{\substack{l \neq k \\ m=0, \dots, N_l-1}} \underline{M}_{i,kj-lm}.
\end{aligned} \tag{33}$$

Enthalpy energy equation

$$\begin{aligned}
\frac{\partial}{\partial t}(\alpha_{kj}\bar{\rho}_{kj}\hat{h}_{kj}) + \nabla \cdot (\alpha_{kj}\bar{\rho}_{kj}\hat{h}_{kj}\hat{v}_{kj}) = & -\nabla \cdot \left[\alpha_{kj}(\bar{q}_{kj} + \underline{q}_{kj}^T) \right] \\
& + \sum_{\substack{l \neq k \\ m=0, \dots, N_l-1}} \Gamma_{kj-lm}\hat{h}_{i,kj-lm} + \sum_{\substack{m=0, \dots, N_k-1 \\ m \neq j}} \dot{m}_{km \rightarrow kj}\hat{h}_{km \rightarrow kj} - \sum_{\substack{m=0, \dots, N_k-1 \\ m \neq j}} \dot{m}_{kj \rightarrow km}\hat{h}_{kj \rightarrow km} \\
& + \sum_{\substack{l \neq k \\ m=0, \dots, N_l-1}} \bar{a}_{i,kj-lm}\bar{q}_{i,kj-lm} + \alpha_{kj}\bar{q}_{kj} + \alpha_{kj}\left(\frac{Dp}{Dt}\right)_{kj} + \Phi_{kj}.
\end{aligned} \tag{34}$$

The interfacial force term in (33) are defined as:

$$\begin{aligned}
\underline{M}_{i,kj-lm} &= \underline{M}_{kj-lm}^n + \underline{M}_{kj-lm}^t, \\
\underline{M}_{kj-lm}^n &= \overline{(\nabla\chi)_{kj-lm}}(p - \bar{p}_{i,kj}), \\
\underline{M}_{kj-lm}^t &= -\overline{(\nabla\chi)_{kj-lm}} \cdot \left(\underline{\tau}^\mu - \overline{(\underline{\tau}^\mu)_{i,kj}} \right).
\end{aligned} \tag{35}$$

This term will be discussed in detail in section 2.8. Following Ishii and Mishima [1], interfacial jump conditions can be given for each interface pair in a multi-field two-fluid model:

$$\begin{cases} \Gamma_{kj-lm} = -\Gamma_{lm-kj}, \\ \underline{M}_{i,kj-lm} = -\underline{M}_{i,lm-kj}, \\ \Gamma_{kj-lm}\hat{h}_{i,kj-lm} + \bar{a}_{i,kj-lm}\bar{q}_{i,kj-lm} = -\left(\Gamma_{lm-kj}\hat{h}_{i,lm-kj} + \bar{a}_{i,lm-kj}\bar{q}_{i,lm-kj} \right). \end{cases} \tag{36}$$

In the above field and jump equations, the interfacial transfer terms Γ_{kj-lm} , $\underline{M}_{i,kj-lm}$ and $\bar{a}_{i,kj-lm}\bar{q}_{i,kj-lm}$ are similar to those in the original two-fluid model. The number of these interfacial terms has increased due

to the classification of more fields and interface pairs. The terms related to $\dot{m}_{km \rightarrow kj}$ and $\dot{m}_{kj \rightarrow km}$ are not found in the original model. These terms represent the inter-field transfers of mass, momentum and energy due to the introduction of the additional fields in each phase. Here the inter-field transfer rates in each direction are explicitly expressed because these bidirectional transfers may involve different mechanisms. Examples are the interexchange between group-1 and group-2 bubbles, and droplet entrainment and deposition.

2.5 Six-field Two-fluid Model

A previous study [10] has shown that very complicated two-phase structures could exist in the churn-turbulent to annular transitional flow, in which various forms of gases and liquids are observed. Fig. 1 shows a typical image taken of a 200 mm x 10 mm rectangular duct. As the figure shows, the gas phase consists of particles of various length scales, from small group-1 bubbles (less than 10 mm) to large group-2 bubbles (up to a few centimeters), up to a continuous gas core. The same wide range of length scales can also be found in the liquid phase. It is shown that both small (below 1 mm) and large (a few millimeters) droplets exist in the gas core. More interestingly, a large liquid bridge (up to 5 cm in length) containing small group-1 bubbles is also seen in the same snapshot. Indeed, this flow condition encompasses a variety of gas and liquid interfacial structures, of which the length scales range from the smallest one that is of practical interest (e.g., a sub-micron droplet), all the way up to a continuous phase scale on the order of the test duct.

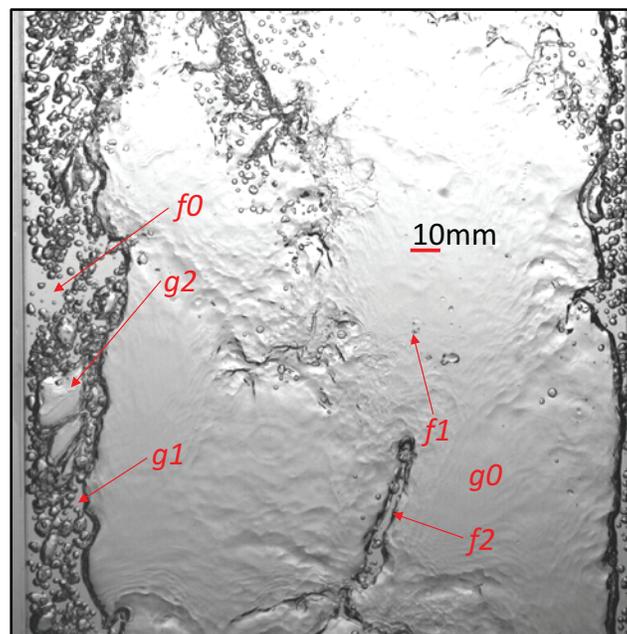


Fig. 1 Typical two-phase structures in the churn-turbulent to annular transitional flow.

The more fields accounted for in either the gas or liquid phase means a potentially more accurate description of the phenomena can be obtained. However, several issues arise if we divide each phase into fine groups. First, computational cost grows with additional fields. The associated numerical issues such as convergence become more problematic. Second, sophisticated instrumentation is not available at the moment to allow detailed measurement of such a transition to annular flow. Third, more fluid fields require more closures for interfacial terms, inter-field terms, and turbulence terms. Without the support of experimental data, it is almost impossible to develop accurate and physical closures for such complicated phenomena. In relation to this, a six-field two-fluid model is proposed as a generic framework for churn-turbulent to annular transitional flows and can be applied to all other two-phase flow regimes. In this

model, the gases are classified into three fields: small bubbles ($g1$, or $DV1$), large bubbles ($g2$, or $DV2$) and continuous gas ($g0$, or CV). The liquids are classified into three similar fields: small droplets ($f1$, or $DL1$), large droplets ($f2$, or $DL2$) and continuous liquid ($f0$, or CL) as shown in Fig. 2.

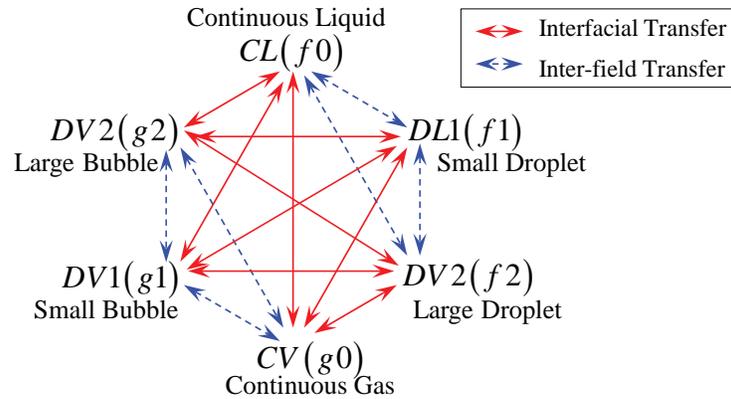


Fig. 2 Fluid fields and interfacial area groups in the six-field two-fluid model.

The first two gas fields ($g1/DV1$, $g2/DV2$) have the same definitions as those in the two group approach developed for cap-turbulent and churn-turbulent flows[8]. The continuous gas (CV) only exists beyond the transition to annular flow. The dispersed liquids are classified into two fields: group-1 droplets ($DV1$) and group-2 droplets ($DV2$) compared to only one field in the four-field two-fluid model [6]. This classification is based on the consideration of the following differences between small and large droplets. First, their significance in the total void fraction and interfacial area concentration are different because the surface area of a large droplet is much less than that of smaller droplets of equivalent volume. Second, the terminal velocity of large and small droplets can vary over an order of magnitude, which results in very different drag coefficients. Similar to that on bubbles, the lift force on droplets also changes its direction when the droplet Reynolds number exceeds a certain limit, according to the study by Sugioka and Komori [13]. In terms of droplet entrainment and deposition, large and small droplets show different characteristics. Due to their small inertia, small droplets tend to follow the gas turbulence more closely and present a turbulent diffusion like deposition mechanism. Large droplets can directly deposit on the wall or liquid film due to high initial momentum imparted to them at the time of their generation [14]. In the transition to annular flow, there are many “semi-dispersed” liquids such as bridges shown in Fig. 1, ligaments typically found in annular flow, and possibly other complicated liquid forms existing in wispy annular flow. These semi-dispersed liquids behave neither like a film, nor small droplets. Therefore, it is more reasonable to have a separate dispersed liquid field to describe large droplets and semi-dispersed liquids. This classification also allows for an accurate modeling of the liquid slugs that could appear in a post-Critical Heat Flux (CHF) regime.

With the above classification of the flow fields, a total of nine interfacial area groups can be identified; for example, interfacial area between group-1 bubbles and continuous liquid ($DV1-CL$), $a_{i, f0-g1}$, that between group-2 bubbles and continuous liquid ($DV2-CL$), $a_{i, f0-g2}$, and so on. Theoretically, each red line in Fig. 2 indicates a potential interfacial area group. Depending on the flow condition, certain interfacial area concentration groups and/or interfacial transfer terms may be negligible. For example, the small bubbles in the large droplets ($DV1-DL2$) may not be important in annular flow. However, such omission will not be made in this work until sufficient experimental justification becomes available.

2.6 Types of Constitutive Relations

In general, three types of inter- and intra-phase transfer terms are identified in the six-field two-fluid model based on the involved phases and fields: interfacial transfer terms, inter-field transfer terms, and

turbulence terms. Table 1 summarizes the required closures for these terms in a matrix, where the term in element (i, j) represents the interactions between the field of the i^{th} row and the field of the j^{th} column. The upper right triangle is left blank as this matrix is symmetric. The terms in the red dashed box consists of the major interfacial transfer closures. Interfacial mass, momentum, and energy transfers (also see the solid red line in Fig. 2) take place at the interface between a gas and a liquid field. Therefore, these terms have a strong dependence on the interfacial area concentration. Similar to the two-group IATE, the interfacial area transport equation and various source and sink models must be developed for the dispersed liquid fields and the continuous interface. The generalized drag term is probably the most important interfacial transfer term and will be discussed in a later section.

The terms in the green and blue dashed boxes are the intra-phase transfer terms within the gas and liquid phase, respectively. The intra-phase transfer terms can be further divided into two types: turbulence terms which are the result of fluctuations within each field (the diagonal elements in Table 1), and the inter-field transfer terms which stand for the interexchange among different fields of the same phase (also see the dashed blue lines in Fig. 2).

It has been assumed that two fields of the same phase do not contact directly. This assumption leads to zero contact area between two fields of the same phase, and precludes any inter-field exchanges other than via a direct mass transfer. Therefore, the most important inter-field closures are the inter-field mass transfer rates, which must be modeled by considering various source and sink mechanisms such as those developed for group-1 and group-2 bubbles for gas-dispersed flows [7]. In an annular flow, the mass transfer between the liquid film and droplets is usually characterized by entrainment and deposition rates. These are particularly important in terms of predicting the film dryout and peak cladding temperature in reactor safety analysis. The entrainment and deposition rate correlations should be treated under the bigger umbrella of the interfacial area transport modeling as they are just two of the many droplet-droplet and droplet-film interaction mechanisms.

Table 1 Inter- and intra-phase transfer terms in the six-field two-fluid model.

	$g0/cv$	$g1/dv1$	$g2/dv2$	$f0/cl$	$f1/dl1$	$f2/dv2$
$g0/cv$	$\underline{\underline{\tau}}_{g0}^r$ $\underline{\underline{q}}_{g0}^r$					
$g1/dv1$	$\dot{m}_{g0 \rightarrow g1}$ $\dot{m}_{g1 \rightarrow g0}$	$\underline{\underline{\tau}}_{g1}^r$ $\underline{\underline{q}}_{g1}^r$				
$g2/dv2$	$\dot{m}_{g0 \rightarrow g2}$ $\dot{m}_{g2 \rightarrow g0}$	$\dot{m}_{g1 \rightarrow g2}$ $\dot{m}_{g2 \rightarrow g1}$	$\underline{\underline{\tau}}_{g2}^r$ $\underline{\underline{q}}_{g2}^r$			
$f0/cl$	$\bar{a}_{i,f0-g0}$ $\bar{M}_{i,f0-g0}$ $\bar{q}_{i,f0-g0}$	$\bar{a}_{i,f0-g1}$ $\bar{M}_{i,f0-g1}$ $\bar{q}_{i,f0-g1}$	$\bar{a}_{i,f0-g2}$ $\bar{M}_{i,f0-g2}$ $\bar{q}_{i,f0-g2}$	$\underline{\underline{\tau}}_{f0}^r$ $\underline{\underline{q}}_{f0}^r$		
$f1/dl1$	$\bar{a}_{i,f1-g0}$ $\bar{M}_{i,f1-g0}$ $\bar{q}_{i,f1-g0}$	$\bar{a}_{i,f1-g1}$ $\bar{M}_{i,f1-g1}$ $\bar{q}_{i,f1-g1}$	$\bar{a}_{i,f1-g2}$ $\bar{M}_{i,f1-g2}$ $\bar{q}_{i,f1-g2}$	$\dot{m}_{f0 \rightarrow f1}$ $\dot{m}_{f1 \rightarrow f0}$	$\underline{\underline{\tau}}_{f1}^r$ $\underline{\underline{q}}_{f1}^r$	
$f2/dv2$	$\bar{a}_{i,f2-g0}$ $\bar{M}_{i,f2-g0}$ $\bar{q}_{i,f2-g0}$	$\bar{a}_{i,f2-g1}$ $\bar{M}_{i,f2-g1}$ $\bar{q}_{i,f2-g1}$	$\bar{a}_{i,f2-g2}$ $\bar{M}_{i,f2-g2}$ $\bar{q}_{i,f2-g2}$	$\dot{m}_{f0 \rightarrow f2}$ $\dot{m}_{f2 \rightarrow f0}$	$\dot{m}_{f1 \rightarrow f2}$ $\dot{m}_{f2 \rightarrow f1}$	$\underline{\underline{\tau}}_{f2}^r$ $\underline{\underline{q}}_{f2}^r$
	Interphase Transfer			Intra-phase Transfer (liquid)		

2.7 The Generalized Drag Force

The two-fluid model is based on the Eulerian formulation of the local instant mass, momentum, and energy conservation equations. The interfacial momentum transfer terms in the two-fluid model are often related to drag, lift and other forces acting on fluid particles. These particle forces depict the integral

effect of the pressure and shear stress over a particle surface imparted by the surrounding fluid. They appear in the equation of motion for particles in a moving fluid, and hence are based on the Lagrangian frame of reference. The interfacial momentum transfer terms in the Eulerian two-fluid model should be compatible with the particle force terms arising in the equation of motion. However, the relation between these two approaches has not been adequately addressed in the past, which led to various forms of momentum interfacial transfer terms. In this section, a brief discussion will be presented on this topic.

The equation of motion for a small rigid sphere in a non-uniform flow has been rigorously derived by Maxey and Riley [15]. In this approach, the flow field is divided into two simpler ones: the undisturbed single-phase flow ($\underline{v}^{(0)}$), and the disturbance flow created by the rigid sphere moving in a stagnant liquid ($\underline{v}^{(1)}$), more generally speaking, in a uniform flow field. For particle Reynolds numbers much less than 1, they show that the solution is a linear superposition of the two flow fields. The equation of motion for the sphere is shown to be [15]:

$$\rho_p \frac{d\underline{v}_p}{dt} = \rho_p \underline{g} + \frac{1}{V_b} \sum \underline{F}_{-p} + \nabla \cdot (p^{(0)} \underline{I} - \underline{\tau}^{(0)}), \quad (37)$$

where, $\sum \underline{F}_{-p}$ contains all the normal particle forces such as drag, Basset, virtual mass and lift forces, *etc.* The last term in Eq. (37) represents a force due to the pressure and shear stress distribution in the undisturbed non-uniform flow field.

The connection between the Eulerian two-fluid model and the equation of motion of a single particle can be established by introducing the probability density function (pdf) of the dispersed particles and a statistical averaging [16]. The evolution equation of the pdf is given by:

$$\frac{\partial f}{\partial t} + \nabla \cdot (f \underline{v}_p) + \frac{\partial}{\partial \underline{v}_{p,j}} \left(f \frac{d\underline{v}_{p,j}}{dt} \right) = 0. \quad (38)$$

Here $f(\underline{x}, t, \underline{v}_p)$ is defined such that $f(\underline{x}, t, \underline{v}_p) \delta \underline{x} \delta \underline{v}$ is the probable number of particles located in the volume $[\underline{x}, \underline{x} + \delta \underline{x}]$ with a velocity in $[\underline{v}_p, \underline{v}_p + \delta \underline{v}_p]$ at time t . One can weight Eq. (38) with the particle velocity and take the integral over the entire particle velocity range. Substituting the equation of motion of a single particle, *i.e.*, Eq. (37), into Eq. (38), one can obtain the momentum equation for the dispersed phase based on a statistical averaging [16]. The equation is similar to the momentum equation obtained from an Eulerian approach, *i.e.*, Eq. (33) except that it contains the particle force terms $\sum \underline{F}_{-p}$ instead of the averaged surface stress terms. The interfacial force terms originated from these two different approaches should be consistent. By comparison, one has:

$$\begin{aligned} & \underbrace{-\nabla(\alpha_{kj} \bar{p}_{kj}) + \nabla \cdot \left[\alpha_{kj} \left(\overline{(\underline{\tau}^\mu)_{kj}} + \underline{\tau}_{kj}^T \right) \right]}_{\text{Eulerian approach}} + \nabla \chi_{kj} P - \nabla \chi_{kj} \cdot \underline{\tau}^\mu \\ & = \underbrace{-\alpha_{kj} \nabla \langle p^{(0)} \rangle + \alpha_{kj} \nabla \cdot \langle \underline{\tau}^{(0)} \rangle + \frac{\alpha_{kj}}{\langle V_b \rangle} \sum \langle \underline{F}_{-p} \rangle}_{\text{Statistical-averaging}}. \end{aligned} \quad (39)$$

Here, the angle bracket “ $\langle \rangle$ ” represents the statistical averaging.

In the two-fluid model, the pressures of the dispersed phase, the continuous phase and at the interface are assumed to be the same. The pressure related term in the two-fluid model can be simplified as $-\nabla(\alpha_{kj} \bar{p}_{kj}) + \bar{p}_{i,kj} \nabla \alpha_{kj} = -\alpha_{kj} \nabla \bar{p}_{kj}$. This assumption seems to be reasonable based on Eq. (39) as it yields similar pressure term as the statistical averaging approach. This also confirms that the averaged interfacial pressure should be separated from the generalized drag term as proposed by Ishii [3].

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