AVERAGED TOPOLOGICAL EQUATIONS FOR DISPERSED TWO-PHASE FLOWS

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Abstract—A general relationship between the volume fraction and the specific interfacial area for averaged dispersed two-phase flows is proposed. This relationship, expressed as a basic set of two scalar evolution equations and two vectorial non-uniformity state equations, is an analytical result obtained by a systematic approach using the derivatives of some generalized functions and a local volume-averaging technique. The proposed set of equations was expressed for measurable macroscopic parameters of the system and has the same generality as the averaged transport equations of two-phase flows. By combination of the basic set of equations, called the averaged topological equations (ATEs), second-order ATEs for the volume fraction were found. The second-order ATEs were expressed both by a Lagrangian formulation and by a Eulerian formulation. The importance and physical meaning of the ATEs developed in this study were clarified within the framework of the theory of kinematic waves.

Key Words: topological laws, kinematic waves, void fraction waves, volume averaging, interfacial area, two-phase flow

1. INTRODUCTION

The Sauter mean diameter is a very useful geometric parameter. It accounts for the relationship between the volume of a polydispersed phase and its interfacial area. Expressions for the volume fraction " ϵ_a " of a given phase "a" [a = d for the dispersed phase and a = c for the connected (or continuous) phase] as a function of the specific interfacial area " a_{cd} " are commonly used to account for the macroscopic geometric structure of the dispersed phase. These expressions are commonly used for the modeling and design of fixed-bed chemical reactors and packed separation columns. Algebraic functions of the type " $\epsilon_d = f(a_{cd})$ " are frequently proposed. However, when the dispersed phases are in motion, it seems natural to think that the relationship between the volume fraction of a given dispersed phase (denoted as the volume fraction, for short) and its specific interfacial area should be dependent on the velocity of such a dispersed phase. The relevant velocity to be considered should, in general, be the local-instantaneous interfacial velocity " w^{i} ", which together with the mean curvature, accounts for the distorting and dispersive effects, as well as for the distribution of sizes and shapes. Moreover, as the dispersed phase travels through the bulk of the connected phase, different states of agglomeration of the particles could be found surrounding a given point as the time elapses. In other words, the topological relationship between the volume fraction and the specific interfacial area for fluid or fluidized dispersed phases should be established as a set of evolution equations and non-uniformity state equations, in which the interfacial velocity and the mean curvature of the interface are relevant parameters. Despite its importance for transient modeling and for the study of flow pattern transitions, a general relationship between the volume fraction and the specific interfacial area for dispersed two-phase flows has not been found in previous studies.

Geometric—or topological—relationships, known as topological laws (Bouré 1978), are fundamental in two-phase flow modeling because the introduction of the volume fraction and the specific interfacial area as additional unknowns in the averaged transport equations contributes to the appearance of a problem known as the *closure issue* (Bouré 1987). In fact, introduction of these additional unknowns makes imperative the establishment of additional equations in order to look for particular solutions of the governing transport equations.

Studies on volume fraction closure equations can be divided in two kinds: algebraic topological laws and differential topological laws (Bouré 1987). Algebraic topological laws focus mainly on correlations considering operation parameters, such as the superficial velocities of both phases. Topological laws of this kind are mostly appropriate for stationary operation and for the system as a whole. One of the more widely used studies of this kind is the drift-flux model closure procedure (Wallis 1969). Differential topological laws are more recent. The first differential topological law is a non-homogeneous one-dimensional first-order wave equation for the volume fraction (Bouré 1978). Two parameters are involved in such an equation: the volume fraction wave speed and a characteristic relaxation time. A first-order differential topological law with the same structure was also proposed for the drift flux (Bouré 1987). While this closure is an extension of the classical drift-flux procedures, resulting in the obtention of differential closures, its underlying physical sense is based on the fact that inertial effects could be represented by topological laws which allow ϵ_d to change as a function of time, probably within a second-order PDE (Bouré 1987). In a further development of this approach, Bouré (1988) postulates a differential closure which, combined with the one-dimensional continuity equations, leads to a second-order one-dimensional PDE as a topological law for $\epsilon_{\rm d}$.

On the other hand, the interfacial area closure issue has also been considered by a number of researchers. Some semi-empirical correlations fitting experimental results based on photographic or chemical techniques have been summarized, with the aim of generating a more structured method considering several flow patterns (Ishii *et al.* 1982; Ishii 1987). Thus, a set of algebraic relationships for the interfacial areas as a function of the volume fraction, the Sauter mean diameter and the drag radius, for different flow patterns is proposed. The specific interfacial area at the local-instantaneous level of description under transient conditions has been formulated as a so-called equation of "conservation of interfacial area concentration", postulated by Kataoka (1985). Generalized functions are used as a convenient way of representing the phases and interfaces. Kataoka's equation is used for the obtention of a more compact expression of the local-instantaneous energy transport equation has not been performed nor used for the obtention of averaged topological laws, since no fundamental advantages over other postulated equations are apparent from such an averaging procedure.

Averaging techniques developed by a number of contributions over the years (Birkhoff 1964; Anderson & Jackson 1967; Slattery 1967; Whitaker 1967; Panton 1968; Drew 1971; Slattery 1972; Whitaker 1973; Gray 1975; Ishii 1975; Delhaye 1976; Delhaye & Achard 1976; Gray & Lee 1977; Hassanizadeh & Gray 1979; Nigmatulin 1979; Gough 1980; Delhaye 1981; Marle 1982; Drew 1983; Soria 1985; Kataoka 1985, 1986; Gray & Hassanizadeh 1989; Ishii 1990; Wallis 1990; Joseph et al. 1990; Soria 1991; Soria & de Lasa 1991) can be extended for the obtention of additional geometric relationships for the volume fraction and the specific interfacial area. It is also important to remark that, while a method of obtaining topological laws using averaging techniques should be more general than one postulating some closure equations, it has not been systematically explored to date. Nevertheless, some averaged geometric relationships have been found. Thus, substitution of unit functions in the spatial and time-averaging theorems for a local time-averaging operator led Ishii (1975) and Delhaye (1981) to the obtention of local time-averaged differential relationships between the void fraction and the time-specific interfacial area. Further volume averaging of the above-mentioned relationships, as well as their combination, led to a one-dimensional wave equation for the volume fraction (Bouré 1987). The parameters involved in such an equation are the averaged interfacial speed and the normalized averaged projection of the interfacial area on the cross section of the pipe. Both parameters are not explicitly present in the transport equations and this fact precluded the use of the above-mentioned relationships as topological laws, in spite of their exactness in an average sense.

Thus, at the present state-of-the-art, topological laws for the volume fraction are imposed by algebraic or differential postulational approaches. However, the averaging method has been proved capable of providing geometric relationships with the same rank of generality as the averaged transport equations. Those geometric relationships have not been considered relevant because of the appearance of averaged geometric parameters whose connections with the macroscopic parameters usually considered by other topological equations remain unexplored. On the other hand, the only available topological laws for the specific interfacial area are algebraic correlations which involve a few relevant parameters.

A general relationship between the volume fraction and the specific interfacial area for an averaged dispersed two-phase flow system is established in the present study. This relationship is expressed as a set of four PDEs, with two first-order PDEs for ϵ_d that relate to the spatial- and time-derivatives of the volume fraction with the specific interfacial area, using the propagation speed, the propagation unit normal vector and the dimensionless strength of the volume fraction waves as relevant geometric parameters. The other two PDEs involve first-order spatial- and time-derivatives of a_{cd} and second-order spatial derivatives of ϵ_d . The propagation speed, the propagation unit normal vector and the dimensionless strength of the specific interfacial area waves, together with the averaged mean curvature of the interfaces, appear in these equations as relevant parameters. The spatial- and time-derivatives of both ϵ_d and a_{cd} give rise to a set of new averaged topological equations (ATEs), which are an analytical result obtained by a systematic approach using generalized functions and a local volume-averaging operator. Since no restrictions were set, other than those inherent to the averaging region (Whitaker 1969; Carbonell & Whitaker 1984; Bachmat & Bear 1987; Celmiņš 1988), the equations obtained here have the same generality as the averaged transport equations for multiphase systems (Soria 1985, 1991; Soria & de Lasa 1991).

In the present study two different concepts are associated to the terms of *macroscopic geometry* and *averaged geometry*, respectively, and they should be clearly distinguished. The term "macroscopic geometry" refers here to the geometric structure of a dispersed flow, based on the volume fraction and the specific interfacial area functions, without reference to the detailed (local-instantaneous) configurations of the particles that constitute the dispersed system. On the other hand, the term "averaged geometry" is a result of averaging local-instantaneous geometric relationships of generalized functions. Such generalized functions represent the detailed configurations of the particles that constitute the dispersed phase. Moreover, the concept of the *phasic structure*, as distinct from the *interfacial structure*, is identified and defined in this contribution. In fact, while the interfacial structure is determined by the specific interfacial area dynamics, the phasic structure is determined by the volume fraction dynamics, being both geometric structures interrelated by the non-uniformity state ATEs.

The logic of the whole process followed for the obtention of the ATEs is visualized in figure 1. The well-established geometric theory of surfaces embedded in space (e.g. Aris 1962; Flügge 1972) is used for the description of both macroscopic isoconcentration surfaces and interfaces. The macroscopic level is studied in section 2. It is assumed that the volume fraction and the specific interfacial area are well-defined concentration functions. Then, the geometric study of isoconcentration surfaces of ϵ_d and a_{cd} gives expressions for the spatial- and time-derivatives of both parameters. Section 3 is devoted to the derivation of spatial- and time-derivatives of the interface function, as well as a review of the derivatives of the phase function. In section 4 averaging of the phase function and the interface function is performed. Section 5 is a one-to-one comparison of the averaged derivatives with their analogous macroscopic derivatives in section 2. This process is called linkage and equations resulting from that comparison are called linking equations. In section 6 application of the linking equations gives a final set of averaged spatial- and time-derivatives of the volume fraction and the specific interfacial area (the basic set of ATEs). The parameters involved in such equations are measurable geometric parameters with a clear physical meaning. Combinations of the basic set of ATEs give Eulerian and Lagrangian second-order ATEs. Section 7 is a discussion of the physical meaning of the ATEs as well as of their role and importance in the solution of several issues concerning two-phase flow behavior.

1.1. Notation conventions

The following notation conventions are maintained throughout the work unless specified otherwise:

- 1. Two repeated indices, one a superscript and the other a subscript, imply a summation upon such indices. For example: $w^k n_k$ means $\sum_k w^k n_k$.
- 2. Indices i, j and k, refer to the three-dimensional generalized coordinate system. Summations on these indices go from 1 to 3.



Figure 1. Flow diagram for obtaining the ATEs.

- 3. Greek indices refer to two-dimensional intrinsic surface coordinate systems. Summations on these indices go from 1 to 2.
- 4. Subscript "a" refers to either the connected (a = c) or the dispersed (a = d) phase. Subscript "cd" refers to the interface between the connected and dispersed phases. No summation convention for subscript "a" is allowed.
- 5. Bold-face characters denote vectors.
- The symbol "∇" (the nabla operator) can represent the following differential operators: V = gradient, V · = divergence and V² = Laplacian.

The Gibbs' (bold-face) vectorial notation is preferred for final results. Nevertheless, the use of a generalized coordinate reference frame enhances the presentation of some demonstrations in the initial sections of this study.

2. THE MACROSCOPIC GEOMETRY OF DISPERSED FLOWS

A two-phase dispersed flow resembles some aspects of the behavior of single-phase flows. Thus, at a macroscopic level, both phases might be considered as *components* or *constituents* of a homogeneous mixture. Extension of the classical theory of mixtures (Bowen 1976), based on the Superimposed Continua Hypothesis, to these heterogeneous mixtures has provided some models [reviewed by Bedford & Drumheller (1983)]. In these models the presence of the dispersed phase is considered by the introduction of a concentration function, the volume fraction of the dispersed phase $\epsilon_d(\mathbf{x}, t)$. Extension of this concept to the interfaces facilitates the understanding of the specific interfacial area as a concentration function $a_{cd}(\mathbf{x}, t)$. Both functions are, at the same time, the most relevant geometric parameters of the dispersed system at the macroscopic level. Study of the behavior of such parameters should allow the establishment of the geometric structure of the two-phase flow at the macroscopic level of description.

Conservation or balance *principles* such as those governing the mass, momentum and energy transports in the system are not available for the transport of geometric quantities, such as the volume fraction or the specific interfacial area. Therefore, a geometric study of these functions, as proposed here, is a better alternative than the one considering conservation or balance *postulates* on the volume fraction and/or on the specific interfacial area (Kataoka 1985), since such postulates could not be subject to general application.

2.1. The geometry of isoconcentration surfaces

Consider a three-dimensional Euclidean space provided with a generalized coordinate system x^{j} (j = 1, 2, 3) and metrics such that $ds^{2} = g_{ij} dx^{i} dx^{j}$, where g_{ij} are the covariant components of the metric tensor. The geometric description of any sufficiently smooth surface embedded in a volume (Aris 1962; Flügge 1972) can be applied, in particular, to *isoconcentration surfaces of volume fraction* and *isoconcentration surfaces of specific interfacial area*, which can be defined by

$$\epsilon_{d}(x^{1}, x^{2}, x^{3}, t) = k$$
 [1a]

and

$$a_{cd}(x^1, x^2, x^3, t) = K,$$
 [1b]

respectively, where k and K are constants. A point on these isoconcentration surfaces can also be given by the parametric equations

$$x^{i} = \chi^{i}(U^{1}, U^{2}, t; k)$$
 [2a]

and

$$x^{i} = v^{i}(V^{1}, V^{2}, t; K)$$
 [2b]

for the volume fraction and the specific interfacial area, respectively. U^{α} and V^{α} ($\alpha = 1, 2$) are independent parameters on the surfaces, that can be taken as intrinsic surface coordinates for the volume fraction isoconcentration surfaces and the specific interfacial area isoconcentration surfaces, respectively.

From [1a, b] and [2a, b] the complete geometric structure of the volume fraction and the specific interfacial area can be developed. The most relevant parameters of the volume fraction geometry are summarized below:

• A unit tangential mixed tensor T_{α}^{i} can be found by deriving [2a] with respect to U^{α} (Aris 1962):

$$T^{j}_{\alpha} = \frac{\partial \chi^{j}}{\partial U^{\alpha}}.$$
 [3]

• The covariant derivative is represented by a subscript prime (Aris 1962). In terms of such a derivative, the unit normal vector to the surface is found by means of the surface covariant derivative of [1a] (Truesdell & Toupin 1960; Thomas 1961):

$$\epsilon_{\mathbf{d}'\boldsymbol{\alpha}} = \epsilon_{\mathbf{d}'\boldsymbol{j}} T_{\boldsymbol{\alpha}}^{\boldsymbol{j}} = 0, \qquad [4]$$

where $\epsilon_{d'j}$ is orthogonal to T_{α}^{j} . Then it results that the covariant unit normal vector " ξ_{j} " can be defined by

$$\boldsymbol{\xi}_{j} = -\frac{\boldsymbol{\epsilon}_{\mathbf{d}'j}}{\sqrt{\boldsymbol{g}^{ij}\boldsymbol{\epsilon}_{\mathbf{d}'j}\boldsymbol{\epsilon}_{\mathbf{d}'}}}.$$
[5]

• The mean curvature H_v of the volume fraction isoconcentration surfaces is related to the contravariant unit normal vector ξ^i by

$$\boldsymbol{\xi}_{i}^{i} = -2H_{\mathbf{v}}.$$

• The velocity of a fixed point on the surface is called the *propagation wave velocity* and is defined from [2a], the parametric equations of the surface, as

$$C_{\rm v}^{i} = \left(\frac{\partial \chi^{i}}{\partial t}\right)_{\rm U}.$$
[7]

• The normal component of the propagation wave velocity is called the propagation speed C_{v} :

$$C_{\rm v} = \boldsymbol{\xi}_i C_{\rm v}^i. \tag{8}$$

The product $C_v \xi^k$ is known as the propagation normal wave velocity. Similar geometric parameters for the specific interfacial area are reported in table 1. Since both ϵ_d and a_{cd} do not change on the isoconcentration surfaces, the time-derivatives of ϵ_d and a_{cd} can be expressed by the following equations:

$$\frac{\partial \epsilon_{\rm d}}{\partial t} = -C_{\rm v} \boldsymbol{\xi}^k \epsilon_{\rm d'k} \tag{9}$$

and

$$\frac{\partial a_{\rm cd}}{\partial t} = -C_{\rm s} v^k a_{\rm cd'k}.$$
[10]

In [9] and [10], as well as in the whole study, the fact that the partial time-derivatives are taken at constant x is denoted simply by the derivation symbol $\partial/\partial t$, dropping, for notational simplicity, the symbol ()_x. It can be seen that " $C_v \xi^{k}$ ", used in [9], is the propagation normal velocity of volume fraction waves. Moreover, the propagation normal velocity of specific interfacial area waves " $C_s v^k$ ", as given by [T6], appears in [10]. Equations [9] and [10], together with [5] and [T2] will be used later in order to provide a linkage between the macroscopic and averaged description of dispersed flows.

The fact that the geometric structure of the specific interfacial area (the *interfacial structure*) and the geometric structure of the volume fraction (the *phasic structure*) are mutually independent, has been discussed by Soria (1991). Such independence can also be assessed by considering, for instance,

Table 1. Macroscopic geometric parameters of the specific interfacial area isoconcentration surfaces

	cf. Equation eter name equation Definition No.			
Parameter name	cf. equation	Definition	Equation No.	
Unit tangential mixed tensor	[3]	$P^{j}_{\alpha} = \frac{\partial v^{j}}{\partial V^{\alpha}}$	[T1]	
Unit normal vector	[5]	$\mathbf{v}_k = -\frac{a_{\mathrm{cd}'k}}{ \nabla a_{\mathrm{cd}} }$	[T2]	
Mean curvature	[6]	$H_{\rm s}=-\frac{1}{2}{\bf v}_{i}^{i}$	[T3]	
Propagation wave velocity	[7]	$C_{s}^{j} = \left(\frac{\partial v^{j}}{\partial t}\right)_{v}$	[T4]	
Propagation speed	[8]	$C_{\rm s} = v_j C_{\rm s}^j$	[T5]	
Propagation normal wave velocity		Csv ^k	[T6]	

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a "flow I" of small spherical bubbles in a liquid on one side and a "flow II" of big spherical bubbles in a liquid on the other side. Consider, in particular, that the flow rates are adjusted in order to get same volume fraction of gas $\epsilon_{\rm G}$ in both flows: $\epsilon_{\rm G}|_{\rm I} = \epsilon_{\rm G}|_{\rm II}$. In this situation the specific interfacial area $a_{\rm GL}$ is bigger for flow I than for flow II: $a_{\rm GL}|_{\rm I} > a_{\rm GL}|_{\rm II}$. Furthermore, consider that additional processes of deformation, coalescence and breakage modify $\epsilon_{\rm G}$ and $a_{\rm GL}$ in many different ways. Therefore, $a_{\rm cd}$ and $\epsilon_{\rm d}$ are assumed to be, in general, geometrically independent of each other. This assumption of geometric independence is extended to the specific interfacial length, $\gamma_{\rm d}$, defined in section 5 by [40]. The geometric independence assumption preserves the generality of the present approach, since the geometric parameters $\epsilon_{\rm d}$, $a_{\rm cd}$ and $\gamma_{\rm d}$, which determine the macroscopic configurations of the particles, are assumed free to change independently of each other. Therefore, the set of all possible macroscopic geometric configurations can be represented by appropriate sets of topological equations.

However, it should be clear that the governing transport equations are also needed for a general description of two-phase flows, since the ATEs are only a mathematical description of the geometric configurations and evolutions of the dispersed system.

3. THE LOCAL-INSTANTANEOUS GEOMETRY OF MOVING INTERFACES

In the present study an interface is defined as a thin film located between the connected phase and the dispersed phase. While the *Continuum Hypothesis* can be applied to each one of these phases, the thermodynamic properties and the mechanistic behavior of the material in the interface may be specified or not, according to the relevance of the interfacial processes to the global behavior of the system (Soria 1985). An interface can be described by considering it as a *dividing surface*, which is closely related to the actual three-dimensional geometric interfacial configuration (Gibbs 1928).

Under such an assumption, a dividing surface is a two-dimensional region S(t) embedded in a three-dimensional Euclidean space. In the present study, this Euclidean space is supposed to be expressed in terms of a generalized coordinate system x^{j} , coincident with the macroscopic coordinate system used in the foregoing section. It is possible to express the equation of a point in the dividing surface by the implicit form

$$f(x^1, x^2, x^3, t) = 0.$$
 [11]

Equation [11] implies that the function $f(\mathbf{x}, t)$ does not change on the dividing surfaces. Therefore $f(\mathbf{x}, t)$, the dividing surface equation, can be considered as belonging to a general kind of isoconcentration functions whose properties were studied previously by Soria (1991). A point on the dividing surface S(t) can also be given by the parametric equations

$$x^{i} = x^{i}(u^{1}, u^{2}, t), \quad i = 1, 2, 3,$$
 [12]

where u^{α} ($\alpha = 1, 2$) are independent parameters on the dividing surface, taken as intrinsic surface coordinates. From [11] and [12] a set of geometric parameters for the dividing surfaces can be established, as shown in table 2, following a similar mathematical procedure to that used for the study of volume fraction and specific interfacial area isoconcentration surfaces. A degree of freedom should be noticed in [11], as compared with [1a, b], since the values of the function $f(\mathbf{x}, t)$ surrounding the dividing surfaces have not been specified. This fact affects the definition of the unit normal vector n_j , given by [T8], and allows the possibility of establishing the existence of two unit normal vectors on the surface, each of them pointing to the other one in the opposite direction. The unit normal vector pointing towards the outside of the phase "a" is denoted by the symbol " n_{al} ", then

$$n_{\rm cj} = -n_{\rm dj}.\tag{13}$$

Further equations considering unit normal vectors are expressed with reference to a particular phase "a" as n_{aj} . Important orthogonality relationships involving derivatives of the unit normal vector n_{aj} are given by Truesdell & Toupin (1960), Estrada & Kanwal (1980) and Soria & de Lasa

Parameter name	cf. equation	Definition	Equation No.
Unit tangential mixed tensor	[3]	$t^{j}_{\alpha} = \frac{\partial x^{j}}{\partial u^{\alpha}}$	[T7]
Unit normal vector	[5]	$n_k = -\frac{f_k}{ \nabla f }$	[T8]
Mean curvature	[6]	$h_a = -\frac{1}{2}n^i_{a'i}$	[T9]
Velocity of displacement	[7]	$w^{j} = \left(\frac{\partial x^{j}}{\partial t}\right)_{\mathbf{u}}$	[T10]
Speed of displacement	[8]	$w_a = n_{aj} w^j$	[T 11]
Normal velocity of displacement		w _a n ^k _a	[T12]

Table 2. Geometric parameters of the dividing surfaces

(1991). Moreover, the interfacial velocity can be split into its normal and tangential components (Truesdell & Toupin 1960):

$$w^i = t^i_a w^a + w_a n^i_a.$$
 [14]

Finally, a relationship between the constant x and constant u partial time-derivatives for a general objective field ψ defined on the surface can be expressed, according to Soria & de Lasa (1991), by

$$\frac{\partial \psi}{\partial t} = \left(\frac{\partial \psi}{\partial t}\right)_{\mathbf{u}} - w^{\alpha} \psi_{\alpha} - w_{\alpha} n_{\alpha}^{k} \psi_{k}.$$
[15]

Equation [15] establishes that the time-derivative following the motion of a fixed point on the surface, corrected by the convective motion of the surface, is equal to the time-derivative at a fixed point in the volume reference frame.

3.1. Definition of the phase distribution function

The phase distribution function $X_a(\mathbf{x}, t)$ is defined for the phase "a" (a = c, d) by

$$X_a(\mathbf{x}, t) = \begin{cases} 1 & \text{if phase "a" is present at point } \mathbf{x} \text{ and time } t \\ 0 & \text{otherwise } . \end{cases}$$
[16]

The function X_a satisfies the relationship

$$X_{\rm c} + X_{\rm d} = 1.$$
 [17]

3.2. Covariant distributional derivatives and the interface function

The distributional derivatives of the phase distribution function are normal to the interface (Estrada & Kanwal 1980). This fact can be shown for the first covariant derivative of X_a adopting the approach of Thomas (1961) once more, as was done for the establishment of [5]. The computation of the rate of change of X_a on the surface, following the coordinate u^{α} , gives

$$X_{a'\bar{a}} = t^i_{\alpha} X_{a'\bar{l}}, \qquad [18]$$

where the bar above the index of the covariant derivative makes clear the distributional character of such a derivative, extending the notation introduced by Estrada & Kanwal (1980). By the definition of X_a , [16], it can be noticed that $X_{a'\bar{a}} = 0$ and since X_a is a constant outside the surface and t_a^i is tangent to it, $X_{a'\bar{t}}$ is normal to the dividing surface. Then,

$$X_{a'\bar{i}} = -n_{ai}\delta_{cd}, \qquad [19]$$

where the interface distribution function δ_{cd} is defined by

$$\delta_{\rm cd} = -n_a^j X_{a'\bar{J}}.$$
 [20]

This is a Dirac-delta generalized function with support in the set of dividing surfaces (the interfaces) between the connected and dispersed phases. The fact that δ_{cd} does not depend on the choice of the phase "a" selected in [20] can be shown by covariant derivation of [17] and substitution, together with [13], into [20], for both the connected and dispersed phases.

Furthermore, the covariant derivative of the δ_{cd} function is also important for the present development. Covariantly deriving [20], it is shown (Soria 1991) that $\delta_{cd'\bar{i}}$ is normal to the dividing surface in such a way that

$$\delta_{\mathrm{cd}'\bar{i}} = -n_{ai}\delta'_{a}, \qquad [21]$$

where

$$\delta'_{a} = -n^{k}_{a} \delta_{\mathrm{cd}'\bar{k}}$$
^[22a]

$$=g^{ij}X_{a'ij}-2h_a\delta_{cd}$$
 [22b]

is the normal derivative of the interface function (Estrada & Kanwal 1980; Soria 1991; Soria & de Lasa 1991). In [21] and [22a, b] the subscript "a", in the normal derivative, refers to the choice of the unit normal vector used in the definition of δ'_a . It can also be shown, by using [13] and [22a] for (a = c, d), that $\delta'_c = -\delta'_d$. While [20] and [22a, b] are definitions of the interface function δ_{cd} and the normal derivative of the interface function δ'_a , respectively, [19] is a fundamental relationship between the generalized functions X_a and δ_{cd} . Moreover, [19] might also be considered as a formal definition of the unit normal vector n_{ai} , such a definition would be consistent with [18] and [13]. Furthermore, both [19] and [21] are symbolic expressions for the local-instantaneous non-uniformity states of the dispersed system at a given time. While [19] gives a relationship between the gradient of the phasic volumes and while [19] gives a relationship between the gradient of the phasic volumes, the gradient of the interfaces, [21] gives a relationship between the Laplacian of the phasic volumes, the gradient of the interfaces and the mean curvature of the interfaces.

3.3. Time distributional derivatives

The partial time-derivatives for X_a , keeping x and u constant, are related by [15], considering it in the sense of distributional derivatives. The derivatives on the dividing surfaces vanish because X_a does not change on the surfaces. The following equation, obtained by Gray & Lee (1977) is then also found:

$$\frac{\partial X_a}{\partial t} = -w_a n_a^i X_{a'\bar{i}} = w_a \delta_{cd}.$$
[23]

On the other hand, the time-derivative of δ_{cd} is obtained from its definition in [20], together with [19]:

$$\frac{\overline{\partial}\delta_{\rm cd}}{\partial t} = \frac{\overline{\partial}}{\partial t} \left(-n_a^k X_{a'\overline{k}} \right) = n_{ak} \frac{\partial n_a^k}{\partial t} \delta_{\rm cd} - n_a^k \left\{ \frac{\overline{\partial}X_a}{\partial t} \right\}_{'\overline{k}},$$
[24]

where the commutative law for the partial derivatives of the generalized functions has been used in the last term (Estrada & Kanwal 1980). Furthermore, the first term on the RHS of [24] is zero because of an orthogonality property for the unit normal vector and its derivatives, as reported by Soria (1991). The second term in this relationship can be substituted using [23] and [T9] in order to obtain

$$\frac{\partial \delta_{\rm cd}}{\partial t} = -n_a^k (w_a \delta_{\rm cd})_{\bar{k}}$$
[25a]

$$= -(w_a n_a^k \delta_{cd})_{\bar{k}} - 2h_a w_a \delta_{cd}.$$
 [25b]

Equation [25b] has been proposed by Kataoka (1985) as a local-instantaneous "conservation of interfacial area concentration". Kataoka's equation is based on the postulation of a balance for the interfacial area. The resulting form of the "generation rate of specific interfacial area per unit interfacial area, Γ_s " that satisfies the postulated equation is then found using some geometric relationships. While *balance principles* are only available for mass, momentum and energy

transports (Truesdell & Toupin 1960), a transport phenomena approach for geometric quantities, such as the phasic volumes or the interfacial areas, should require the use of *balance postulates*, which cannot be considered as general as the present derivation of [25a, b]. The present development, based only on general geometric relationships for generalized functions, provides the only available derivation of Kataoka's equation and also gives a simple form of the " Γ_s " term, which is equivalent to the factor $(-2h_aw_a)$ in the second term of [25b]. It is also interesting to point out that the generation rate of interfacial area can be accounted for by a surface metric tensor which is time-dependent. Then, the time-derivative of the determinant of the surface metric tensor is equal to the square of the factor $(-2h_aw_a)$ mentioned above (Moeckel 1975).

4. THE AVERAGED GEOMETRY OF DISPERSED FLOWS

4.1. Local volume-averaging operator

Averaging of the covariant and time distributional derivatives of the phase distribution function, [16], and the interface distribution function, [20], is necessary in order to obtain averaged equations of such derivatives at the macroscopic level. A definition of an averaging operator is required for obtaining these expressions. In order to clarify the procedure, a local volume-averaging operator is selected in this study, since the geometric meaning of the averaged equations becomes more apparent when using the volume-averaging technique. However, other averaging operators, different from those considered in this study, may have some advantages for a number of applications (Arnold *et al.* 1990; Joseph *et al.* 1990). It is also convenient to point out that the use of different averaging operators provides averaged expressions which, under a set of equivalent assumptions, are formally similar to each other. The meaning of the averaged quantities is what makes the main difference between the choice of averaging operators (Nigmatulin 1979; Bedford & Drumheller 1983).

In the present study the volume-averaging is defined as

$$\langle \cdot \rangle(\mathbf{x}, t) = \frac{1}{V} \iiint_{V(\mathbf{x})} \cdot \mathbf{d}V,$$
 [26]

where the averaging volume V is such that

$$V = \iiint_{V(\mathbf{x})} dV = \text{const}$$
[27]

and $\mathbb{V}(\mathbf{x}) \subset \mathbb{R}^3$ is fixed region inside the system, whose centroid is located at point \mathbf{x} .

There are important conditions for the proper application of the averaging method. The analysis of such conditions has been considered by Whitaker (1969), Carbonell & Whitaker (1984), Bachmat & Bear (1987) and Celmiņš (1988), among others.

4.2. Intrinsic averaging operators and averaged variables

Weighted averaging operators are also important for the present approach, thus the *intrinsic* interfacial area average for a variable ψ is, after Ishii (1975):

$$\langle \psi \rangle_{\rm cd}(\mathbf{x},t) = \frac{\langle \delta_{\rm cd} \psi \rangle}{\langle \delta_{\rm cd} \rangle};$$
 [28]

and the intrinsic interfacial length average is defined by

$$\langle \psi \rangle_a^*(\mathbf{x}, t) = \frac{\langle \delta'_a \psi \rangle}{\langle \delta'_a \rangle}.$$
 [29]

It is assumed that the averaging volume is such that the intrinsic interfacial area average satisfies the property

$$\langle \varphi(\langle \psi \rangle_{\rm cd} + \mu) \rangle_{\rm cd} = \langle \varphi \rangle_{\rm cd} \langle \psi \rangle_{\rm cd} + \langle \varphi \rangle_{\rm cd} \langle \mu \rangle_{\rm cd} + \langle \tilde{\varphi} \tilde{\mu} \rangle_{\rm cd}, \qquad [30]$$

for φ , ψ and μ variables defined on the surface. The variables with a z in [30] are the fluctuations around the averaged values, according to the equation

$$\tilde{\psi} = \psi - \langle \psi \rangle_{\rm cd}.$$
[31]

It can be shown that $\langle \tilde{\psi} \rangle_{cd} = 0$ by averaging [31] and using [30] for particular values of φ and μ ($\varphi = 1$ and $\mu = 0$). This result, extended in general to arbitrary functions ψ , φ and μ , allows us also to conclude that

$$\langle \tilde{\varphi} \tilde{\mu} \rangle_{cd} = \langle \varphi \tilde{\mu} \rangle_{cd} = \langle \tilde{\varphi} \tilde{\mu} \rangle_{cd}.$$
 [32]

4.3. Averaging of distributional derivatives

Since the averaging region $\mathbb{V}(\mathbf{x})$ is fixed and its volume is constant, the derivative operators can be interchanged with the averaging operators if the derivatives are defined over the complete region $\mathbb{V}(\mathbf{x})$. This requirement is satisfied by the distributional derivatives in the two-phase system. Thus, the averaging of Eqs. [23], [25a, b], [19] and [21] gives, respectively:

• averaged distributional time-derivatives,

$$\frac{\partial \langle X_a \rangle}{\partial t} = \langle w_a \rangle_{\rm cd} \langle \delta_{\rm cd} \rangle$$
[33]

and

$$\frac{\partial \langle \delta_{\rm cd} \rangle}{\partial t} + \{ \langle w_a n_a^k \rangle_{\rm cd} \langle \delta_{\rm cd} \rangle \}_{k} = -2 \langle h_a w_a \rangle_{\rm cd} \langle \delta_{\rm cd} \rangle;$$
[34]

and

• averaged distributional covariant derivatives,

$$\langle X_a \rangle_{k} = -\langle n_{ak} \rangle_{cd} \langle \delta_{cd} \rangle$$
^[35]

and

$$\langle \delta_{\rm cd} \rangle_{k} = -\langle n_{ak} \rangle_{a}^{*} \langle \delta_{a}' \rangle, \qquad [36]$$

where, from [22a, b],

$$\langle \delta'_a \rangle = \langle g^{ij} X_{a' \overline{i}} \rangle - 2 \langle h_a \rangle_{cd} \langle \delta_{cd} \rangle.$$
^[37]

Equations [33]-[37] can be considered as the more general geometric relationships between $\langle X_a \rangle$ and $\langle \delta_{cd} \rangle$ within an averaging approach for dispersed two-phase flows. Higher-order derivatives of the interface function should give further PDEs as geometric relationships involving the derivatives of other geometric parameters, such as the averaged normal derivative of the interface function δ'_a . While [33] and [35] are already known, [34], [36] and [37] are new contributions to the theory of dispersed two-phase flows by averaging methods. In fact, [33] together with a one-dimensional version of [35], using a composite volume-time-averaging procedure, was presented by Bouré (1987). Limiting forms of the Gauss theorem and Leibniz rule, as derived by Delhaye (1981), can be applied to unit scalar and vectorial functions, giving equations closely related to the projection of [35] onto the axial coordinate of a pipe, and with [33], respectively. A one-dimensional combination of [33] and the referred projection of [35] onto the axial coordinate allows the expression for a topological equation presented by Bouré (1987).

5. LINKAGE BETWEEN THE MACROSCOPIC AND AVERAGED GEOMETRIES

A volume-averaging operator should be selected in such a way that the measurable macroscopic geometric parameters are equivalent to the averaged distribution functions. Thus, the averaged phase function should be equal to the volume fraction, as was established by Joseph *et al.* (1990) and frequently taken as a definition of the volume fraction of the dispersed phase or the void fraction (e.g. Drew 1971, 1983; Whitaker 1973; Ishii 1975; Gray 1975; Delhaye & Achard 1976;

Gray & Lee 1977; Delhaye 1981; Soria 1985; Soria & de Lasa 1991):

$$\langle X_a \rangle = \epsilon_a.$$
 [38]

Also the averaged interface function should be equal to the *specific interfacial area* " a_{cd} " (cf. Ishii 1975; Delhaye 1976; Drew 1983; Kataoka 1986; Gray & Hassanizadeh 1989; Soria & de Lasa 1991):

$$\langle \delta_{\rm cd} \rangle = a_{\rm cd}.$$
 [39]

Furthermore, the averaged normal derivative of the interface function should be equivalent to the specific interfacial length " γ_a ", defined here by

$$\langle \delta'_a \rangle = \gamma_a.$$
 [40]

The averaged covariant and time-derivatives of X_d and δ_{cd} , given by [33]–[36], can be compared one-to-one with the correlative macroscopic covariant and time-derivatives of the functions ϵ_d and a_{cd} , given by [9], [10], [5] and [T2]. From the comparisons of [5] with [35] and [T2] with [36], considering the fundamental linking equations [38]–[40], it results, respectively, that

$$\langle n_{\rm dk} \rangle_{\rm cd} = \Xi \boldsymbol{\xi}_k$$
 [41]

and

$$\langle n_{\rm dk} \rangle_{\rm d}^* = N \mathbf{v}_k,$$
 [42]

where the scalar Ξ , the dimensionless strength of the volume fraction waves, is defined by

$$\Xi = \frac{|\nabla \epsilon_{\rm d}|}{a_{\rm cd}}$$
[43]

and the scalar N, the dimensionless strength of the specific interfacial area waves, is defined by

$$N = \frac{|\nabla a_{\rm cd}|}{\gamma_{\rm d}}.$$
 [44]

Moreover, [41] and [42] can be substituted into [35] and [36], respectively, for the dispersed phase and the correlative scalar products in the normal directions can be taken in order to obtain

$$\boldsymbol{\xi}^{k}\boldsymbol{\epsilon}_{d'k}=-\boldsymbol{\Xi}\boldsymbol{a}_{\mathrm{cd}}$$

$$[45]$$

and

$$\mathbf{v}^k a_{\mathrm{cd}'k} = -N\gamma_{\mathrm{d}}.$$

Then, [45] and [46] can be further substituted into [9] and [10], respectively. The resulting equations are

$$\frac{\partial \epsilon_{\rm d}}{\partial t} = \Xi C_{\rm v} a_{\rm cd}$$
^[47]

and

$$\frac{\partial a_{\rm cd}}{\partial t} = NC_{\rm s} \,\gamma_{\rm d} \,. \tag{48}$$

Comparison of [47] with [33], considering [38] and [39], gives the linkage between the averaged speed of displacement of the interface and the propagation speed of the volume fraction waves:

$$\langle w_{\rm d} \rangle_{\rm cd} = \Xi C_{\rm v}.$$
 [49]

On the other hand, the linkage of [48] with the averaged time-derivative of the interface function, [34], requires an additional development. Relationships for the averaged and the local values of both the contravariant metric tensor g^{ij} and the contravariant unit vector ξ^i are relevant for that purpose and are elaborated on in the next section.

5.1. Averaging the averaged geometric structure of dispersed media

Averaging of the normal vector ξ^i deserves careful attention. Consider an arbitrary point x in the system and a point y in the vicinity of x. It is assumed that the unit normal vector $\xi^i|_y$ can be expanded into a Taylor series around point x:

$$\boldsymbol{\xi}^{i}|_{\mathbf{y}} = \boldsymbol{\xi}^{i}|_{\mathbf{x}} + (y^{j} - x^{j})\boldsymbol{\xi}^{i}_{j}|_{\mathbf{x}} + \frac{1}{2}(y^{j} - x^{j})(y^{k} - x^{k})\boldsymbol{\xi}^{i}_{jk}|_{\mathbf{x}} + \cdots$$
[50]

Truncation of this series to the first term gives

$$\boldsymbol{\xi}^{i}|_{\mathbf{y}} = \boldsymbol{\xi}^{i}|_{\mathbf{x}} + o^{i}\{|\mathbf{y} - \mathbf{x}|| 2H_{\mathbf{y}}|\},$$
[51]

where the approximation order is related to both the distance between the points and the mean curvature of the volume fraction waves. Averaging of [51] with the centroid at point x gives

$$\langle \boldsymbol{\xi}^{i} \rangle (\mathbf{x}, t) = \boldsymbol{\xi}^{i} (\mathbf{x}, t) + \langle o^{i} \{ V^{1/3} | H_{\mathbf{y}} | \} \rangle.$$
^[52]

Equation [52] can be simplified if the approximation order term is negligible. Under such an assumption

$$\langle \boldsymbol{\xi}^i \rangle \approx \boldsymbol{\xi}^i \quad \text{for } V^{1/3} \ll |1/H_v|.$$
 [53]

The condition of validity for application of [53] is satisfied without restriction for the averaging volume size, by plane volume fraction waves because $H_v = 0$ for plane waves. If the volume fraction waves are not planar a careful adjustment of the averaging volume must be made in order to apply [53]. This condition, however, is equivalent to one of the conditions to be satisfied by any averaging volume, say that the averaging volume should be much smaller than the size of the flow structure to be investigated (Celminš 1988).

Averaging the modulus of the unit normal vector $\boldsymbol{\xi}^{i}$ and considering [53] allows one to conclude, after several steps (Soria 1991), that

$$\langle n_{\rm d}^i \rangle_{\rm cd} = \langle g^{ik} n_{\rm dk} \rangle_{\rm cd} = g^{ik} \Xi \boldsymbol{\xi}_k = \Xi \boldsymbol{\xi}^i$$
 [54]

and also that

$$\langle g^{ij} X_{a'\bar{i}\bar{i}} \rangle = g^{ij} \langle X_a \rangle_{ij} = g^{ij} \epsilon_{a'ij}.$$
[55]

5.2. Linking equations for the time-derivative of the specific interfacial area

The covariant derivative of the second term in [34] gives, after substitution of [39]:

$$\frac{\partial a_{\rm cd}}{\partial t} + \langle w_{\rm d} n_{\rm d}^k \rangle_{\rm cd} a_{\rm cd'k} + \langle w_{\rm d} n_{\rm d}^k \rangle_{\rm cd'k} a_{\rm cd} = -2 \langle h_{\rm d} w_{\rm d} \rangle_{\rm cd} a_{\rm cd}.$$
^[56]

Moreover, substitution of [36], [42] and [48] gives, after rearrangement of the terms, the following relationship:

$$N(C_{\rm s} - \langle w_{\rm d} n_{\rm d}^k \rangle_{\rm cd} v_k) \gamma_{\rm d} + (\langle w_{\rm d} n_{\rm d}^k \rangle_{\rm cd'k} + 2 \langle h_{\rm d} w_{\rm d} \rangle_{\rm cd}) a_{\rm cd} = 0.$$
^[57]

Because of the assumption of geometric independence, [57] is valid for arbitrary values of both γ_a and a_{cd} . This fact implies that both the coefficient of γ_d and the coefficient of a_{cd} are equal to zero. These equalities constitute the linkage between the macroscopic and averaged time-derivatives for a_{cd} . The first restriction established by the coefficient of γ_d is satisfied trivially when there are no interfacial area waves (N = 0). Otherwise, the propagation speed of specific interfacial area waves should satisfy the relationship

$$C_{\rm s} = \langle w_{\rm d} n_{\rm d}^k \rangle_{\rm cd} v_k, \qquad [58]$$

which implies the fact that the propagation normal velocity of specific interfacial area waves, given by [T6], is related to the averaged normal velocity of displacement of the interface by

$$\langle w_{\rm d} n_{\rm d}^k \rangle_{\rm cd} = C_{\rm s} v^k.$$
^[59]

Whatever the two-phase system satisfying [58] or (N = 0), the second restriction, coming from the coefficient of a_{cd} equated to zero in [57], can be expressed as

$$\langle w_{\rm d} n_{\rm d}^k \rangle_{\rm cd'k} + 2 \langle h_{\rm d} w_{\rm d} \rangle_{\rm cd} = 0.$$
^[60]

Equations [59] and [60] are useful expressions that, together with [38]-[42] and [49], constitute a link between the averaged and macroscopic geometric descriptions of dispersed two-phase flows.

6. AVERAGED TOPOLOGICAL EQUATIONS (ATEs)

6.1. A basic set of ATEs

Once the geometric structure of the two-phase system is determined and the link between the macroscopic and averaged descriptions established, the evolution equations [33] and [34], as well as the non-uniformity state equations [35] and [36], can be transformed into useful equivalent forms. Direct application of the set of linking relations, given by [38]–[42], [49], [59] and [60], into the set of averaged equations [33]–[37], gives the following *basic set of averaged topological equations*:

$$\frac{\partial \epsilon_{\rm d}}{\partial t} = \Xi C_{\rm v} a_{\rm cd}, \qquad [61]$$

$$\frac{\partial a_{\rm cd}}{\partial t} + C_{\rm s} \mathbf{v} \cdot \nabla a_{\rm cd} = 0, \qquad [62]$$

$$\nabla \epsilon_{\rm d} = -\Xi \boldsymbol{\xi} a_{\rm cd} \tag{63}$$

and

$$\nabla a_{\rm cd} = -N \nu (\nabla^2 \epsilon_{\rm d} - 2 \langle h_{\rm d} \rangle_{\rm cd} a_{\rm cd}).$$
^[64]

The use of Gibbs' (bold-face) vectorial notation is preferred in this section for these equations, which can be considered as one of the most important results of the present study. While [61] and [62] are scalar evolution equations for the volume fraction and the specific interfacial area, [63] and [64] are vectorial expressions for the gradients of both geometric parameters and account for the non-uniformity states of the dispersed medium. The topological equations for the volume fraction are first-order PDEs and depend algebraically on the specific interfacial area. On the other hand, the topological equations for the specific interfacial area are also first-order PDEs with respect to a_{cd} . However, [64] depends on the Laplacian of the volume fraction. Combinations of the basic set of ATEs [61]–[64] can give further equivalent sets of first- or second-order ATEs.

On the other hand, an alternative to [62] can be developed from [34] using the properties of averaging of products. Considering [30] and [32], together with [41] and [49], it can be shown that

$$\langle w_{\rm d} n_{\rm d}^k \rangle_{\rm cd} = \Xi^2 C_{\rm v} \boldsymbol{\xi}^k + \langle \tilde{w}_{\rm d} n_{\rm d}^k \rangle_{\rm cd}$$
^[65]

and also that

$$\langle h_{\rm d} w_{\rm d} \rangle_{\rm cd} = \Xi C_{\rm v} \langle h_{\rm d} \rangle_{\rm cd} + \langle \tilde{h}_{\rm d} w_{\rm d} \rangle_{\rm cd}.$$
 [66]

Substitution of [65] and [66] into [34] gives an ATE that includes one vectorial covariance $\langle \tilde{w}_d n_d^k \rangle_{cd}$ and one scalar covariance $\langle \tilde{h}_d w_d \rangle_{cd}$:

$$\frac{\partial a_{\rm cd}}{\partial t} + (\Xi^2 C_{\rm v} \boldsymbol{\xi}^k a_{\rm cd})_k + (\langle \tilde{w}_{\rm d} n_{\rm d}^k \rangle_{\rm cd} a_{\rm cd})_k = -2(\Xi C_{\rm v} \langle h_{\rm d} \rangle_{\rm cd} + \langle \tilde{h}_{\rm d} w_{\rm d} \rangle_{\rm cd}) a_{\rm cd}.$$

$$[67]$$

The only parameters involved in [67] are those of the volume fraction geometry. This fact encourages further developments based on [67], in spite of the presence of the above-mentioned covariances.

6.2. Second-order ATEs for ϵ_d

Second-order topological equations for ϵ_d can be obtained by derivation of [61] and [63] and by further application of such derivatives into [62] or alternatively into [67]. A procedure based on [62] (Soria 1991) gives the following second-order ATE:

$$\Theta\left(\frac{\partial^2 \epsilon_{\rm d}}{\partial t^2} - \Pi \,\nabla^2 \epsilon_{\rm d}\right) + \frac{\partial \epsilon_{\rm d}}{\partial t} + C_{\epsilon} \boldsymbol{\xi} \cdot \nabla \epsilon_{\rm d} = 0, \tag{68}$$

where

$$\Pi = \frac{C_{\rm v}C_{\rm s}}{\boldsymbol{\xi}\cdot\boldsymbol{v}},\tag{69}$$

$$\Theta = \left[-\frac{\partial}{\partial t} \ln(\Xi C_{v}) \right]^{-1}$$
[70]

and

$$C_{\epsilon} = \Theta \Pi \left(\boldsymbol{\xi} \cdot \nabla \ln \boldsymbol{\Xi} - 2H_{\nu} \right).$$
^[71]

Equation [68] represents a second-order wave with a relaxation time Θ . This equation, expressed in partial time-derivatives, will be referred as the *Eulerian form* of the second-order ATEs. The notation for parameters involved in [68] was taken from Bouré (1988).

Second-order ATEs based on [67] can also be developed. Some of these equations should contain parameters only from the volume fraction geometry. However, the inclusion of the covariances seems to be unavoidable. A second-order topological equation has been developed by Soria (1991), from the set [61], [63] and [67], together with the use of the geometric properties of the volume fraction function. The resulting equation is

$$\hat{\Theta}\left[\frac{\tilde{\mathbf{D}}}{\mathbf{D}t}\left(\frac{\partial\epsilon_{\mathsf{d}}}{\partial t}\right) - \hat{\Pi} \nabla^{2}\epsilon_{\mathsf{d}}\right] + \frac{\partial\epsilon_{\mathsf{d}}}{\partial t} + \hat{C}_{\epsilon}\boldsymbol{\xi}\cdot\nabla\epsilon_{\mathsf{d}} = 0,$$
[72]

where the introduction of a convected or substantial derivative operator, defined by

$$\frac{\tilde{\mathbf{D}}}{\mathbf{D}t} = \frac{\partial}{\partial t} + \langle \tilde{w}_{\mathrm{d}} \mathbf{n}_{\mathrm{d}} \rangle_{\mathrm{cd}} \cdot \nabla, \qquad [73]$$

was adopted. The parameters used in [72] were called $\hat{\Theta}$, $\hat{\Pi}$ and \hat{C}_{ϵ} , according to the notation introduced by Bouré (1988). However, the physical meaning of the parameters involved in [72], as given by [74]–[76], is different from the physical meaning of similar parameters in Bouré's void-drift closure equation. This difference is result of the different approaches followed in the respective derivations: while in Bouré's work it is assumed that \hat{C}_{ϵ} is the propagation speed of volume fraction waves (see [8]), evaluated in the basic state of the linearization method followed, in the present derivation of [72] \hat{C}_{ϵ} is a more sophisticated function given subsequently by [76]. The derivation of [72], as given by Soria (1991), is an analytical result of the geometric study, which does not involve specific assumptions on the set of parameters involved. These parameters result from the lumping of groups of primary macroscopic parameters, and are defined by

$$\hat{\Pi} = (\Xi C_v)^2, \tag{74}$$

$$\hat{\Theta} = \left[-\frac{\tilde{\mathbf{D}}}{\mathbf{D}t} \ln(\Xi C_{v}) \right]^{-1}$$
[75]

and

$$\hat{C}_{\epsilon} = \hat{\Theta} \hat{\Pi} (\boldsymbol{\xi} \cdot \nabla \ln \boldsymbol{\Xi} - 2H_{\mathrm{v}}).$$
^[76]

Equation [72] is a Lagrangian form of the second-order ATEs. Equation [72] apparently does not involve parameters for the specific interfacial area geometry. In fact this is not true, since considering [65] and [59], the substantial derivative \tilde{D}/Dt , given by [73], can also be written as

$$\frac{\tilde{\mathbf{D}}}{\mathbf{D}t} = \frac{\partial}{\partial t} + (C_{s}\mathbf{v} - \Xi^{2}C_{v}\boldsymbol{\xi})\cdot\nabla.$$
[77]

Thus, the propagation normal velocity of the specific interfacial area has also been introduced in this Lagrangian second-order ATE. While [77] clarifies the meaning of the velocity covariance, it should be stressed that the use of [72], as compared with the Eulerian formulation, may be advantageous only if the velocity covariance can be represented by a closure in which the geometric parameters of the specific interfacial area geometry are avoided. Thus, further explorations on closures of the velocity covariance, considering only the volume fraction geometric parameters, would be desirable since no experimental studies on the propagation velocity of specific interfacial area waves seem to be available. However, research on the geometric structure of the specific interfacial area is crucial for the application of the ATEs in highly distorting dispersed flows, such as that occurring at some flow pattern transitions and at the entrance of pipes and columns; especially for applications in distributed parameter models.

7. DISCUSSION

While one purpose of this paper is the systematic development of a second-order wave hierarchy of ATEs, the general procedure developed here is also capable of giving systems of ATEs of an arbitrary order, since the Dirac-delta distribution function is infinitely differentiable (Estrada & Kanwal 1980). However, third-order ATEs involve parameters related to the macroscopic geometric structure of the specific interfacial length " γ_d " and higher-order ATEs involve macroscopic geometric parameters associated with the geometric structure of other higher-order specific interfacial parameters, such as the *specific interfacial point* $\pi_{cd} = \langle \delta_{cd}^{"} \rangle = \langle -n_a^j \delta_{aj}' \rangle$. The present lack of experimental techniques to measure such parameters diminishes the practical interest in the ATEs of order greater than 2. Nevertheless, the theoretical importance of the higher-order topological equations remains unaffected, since a wide variety of high complex kinematical wave behaviors in dispersed systems can be, at least in principle, accurately modeled and explained by appropriate sets of ATEs.

7.1. The theory of kinematic waves and the ATEs

The ATEs developed in the present study constitute a novel approach within the theory of kinematic waves (Lighthill & Whitham 1955; Zuber 1964; Wallis 1969; Whitham 1974; Bouré 1988). Most theoretical studies on kinematic waves begin with the proposition of mass and momentum balances for two-fluid, two-phase flows. Then, rearrangement of the continuity and momentum equations, together with some considerations on the interfacial mass and momentum transfer terms, gives rise to *ad hoc* kinematic wave equations, under a set of simplifying assumptions (i.e. Foscolo & Gibilaro 1987; Biesheuvel & Gorissen 1990; Dankworth *et al.* 1990; Lahey 1991).

The present study does not follow the above approach, since no mass or momentum balances have been employed so far. The set of ATEs given by [61]-64] is valid for any kind of dispersed two-phase flow system under no additional restrictions other than those required by the averaging approach. It can be proposed that the ATEs, together with the transport equations, constitute a general averaged formulation for dispersed two-phase flows. The evolution equations and the non-uniformity state equations for ϵ_d and a_{cd} , given by [61]–[64] are independent of the continuity and momentum equations. Therefore, the wave hierarchy for ϵ_d is increased in two orders of derivation with respect to the classical approach of considering the transport equations as the only source of the evolution description. This fact can have significant consequences on the modeling of dispersed two-phase flows. Thus, stability studies on one-dimensional gas-liquid bubbling flows (i.e. Lyczkowski et al. 1982; Jones & Prosperetti 1985; Prosperetti & Jones 1987) should include two additional evolution equations considering one-dimensional combinations of the ATEs [61]-[64] in set of relevant averaged equations. The ATEs [61]-[64] provide geometric constraints for the set of transport equations in the same way as the continuity equations can be seen as mass constraints for the momentum balances. Thus, the solutions of the ATEs constitute the set of geometrically meaningful functions which are candidates to be solutions of the averaged model under particular conditions. It should also be noticed that the ATEs are coupled with the transport equations and therefore the simultaneous solution of the enlarged set of ATEs and the averaged transport equations is a requirement to obtain results with added confidence.

The inclusion of the ATESs into the modeling of fluidized beds may also modify the results of some stability analyses made on the basis of the continuity and momentum equations. For instance, an equation for the fluctuations of ϵ_d around its steady state values was reported by Foscolo & Gibilaro (1987). Such an expression, developed from the continuity and momentum equations, is a second-order PDE with the same terms as the Eulerian description given by [68]. While Foscolo & Gibilaro's "particle bed model" is capable of reasonably predicting the transition between particulate and aggregative fluidization, it makes use of some simplifying assumptions and

empirical correlations as well. The meaning of their propagation speeds is not the same as the geometric meaning of the parameters C_{i} and $\Pi^{1/2}$ in [71] and [69]. However, the influence of the elastic modulus of the particulate medium on the parameters Π and Ξ should be the subject of further research. Moreover, it should be clarified that the assumptions used by Foscolo & Gibilaro (1987), in order to obtain the particle bed model, might be considered grosso modo as equivalent to certain similarity conditions on the mass and momentum balances that simulate the pure geometric behavior of the dispersed medium to a second-order wave hierarchy, represented accurately by the ATEs. Furthermore, it should be stressed that within the averaging approaches, the condition $|H_v| \ll R^{-1}$ for one-dimensional pipe flow should always be satisfied (Soria 1991); R is the pipe radius. This condition is strictly satisfied by flat volume fraction isoconcentration surfaces, for which $H_{\rm v} = 0$. In fluidized beds this condition is satisfied in the particulate fluidization regime, in which homogeneous contractions or expansions are driven by small changes in the flow rate. However, in the aggregative fluidization regime, each one of the bubbles (assumed spherical with diameter " d_b " for simplicity in this analysis) can be interpreted geometrically as a volume fraction wave with mean curvature $H_v = 2/d_b$. On the other hand, the appearance of gas or liquid bubbles inside the fluidized bed also satisfies the inequality $d_b < 2R$ and therefore it can be concluded that

$$|H_{\rm v}| = 2d_{\rm b}^{-1} > R^{-1}, \tag{78}$$

which clearly violates the condition given above for the appropriate application of the averaging technique in one-dimensional models.

On the basis of this analysis, it cannot be assured that the ATE [68] can predict the transition between the particulate and aggregative fluidization regimes. This conclusion is consistent with a comment by Joseph (1990) regarding the particle bed model, based on one-dimensional equations (Foscolo & Gibilaro 1987). What can only be hypothesized at this stage is that the instability conditions for [68] may be one of its validity limits, if [68] remains meaningful up to that point. However, it is quite possible that [68] is valid up to the instability conditions because of the observed appearance of horizontal non-homogeneities, the so-called "parvoids", in particulate liquid fluidized beds (Hasset 1961; Gibilaro *et al.* 1986). In fact, such parvoids can be considered as bubbles with almost zero mean curvature.

The behavior of dispersed gas-liquid flows is even more complex because of the growth, distortion, coalescence and break-up processes in the dispersed phase. Significant contributions on the behavior of bubbling flows and on the bubble-slug flow pattern transition have been made by Bouré and co-workers (Mercadier 1981; Micaelli 1982; Bouré & Mercadier 1982; Tournaire 1987; Matuszkiewicz *et al.* 1987; Bouré 1988, 1989; Saiz-Jabardo & Bouré 1989), both in the experimental and theoretical areas. While Bouré's theoretical contribution has been referred to in the introduction of the present study, some important experimental findings of the mentioned researchers are referred to in the following:

- There exist two kinematic propagation modes (called modes 3 and 4) with propagation speeds C_3 and C_4 .
- At low void fractions ($\epsilon_d < 0.20$) only mode 3 exists and it is always damped (bubble flow pattern).
- At intermediate void fractions $(0.25 < \epsilon_d < 0.30)$ modes 3 and 4 coexist and are damped.
- At large void fractions $(0.30 < \epsilon_d \le 0.41)$ mode 3 is still present and is damped, at least upstream in the test section. Mode 4 is amplified when periodic small perturbations on the gas flow rate are induced at a certain range of wavelengths which do not exceed a few Hz.
- C_3 is, except for data at $\epsilon_d = 0.047$, smaller than the average gas velocity but greater than the average liquid velocity and even greater than the velocity of the mixture at the center of the volume.
- When only mode 3 is present, the amplitude decay, expressed as the ratio of the amplitude measured at a given level divided by the amplitude measured at the upstream adjacent measuring level, follows an exponential law.

- C_4 is in the same order of magnitude as the slug velocity and greater than the average gas velocity. At large void fractions, slugs can be observed in the upper part of the test section.
- Mode 4 is amplified as the wavelength of the perturbations grows bigger. The mode 4 amplitude exhibits a clear dependence upon ϵ_d .

The phenomena associated with the existence of the above-mentioned two kinematic modes, considering the propagation speeds, amplification and damping, can be qualitatively represented by a one-dimensional second-order ATE developed from [68] or, alternatively from the ATE [72]. In fact, a differential closure approach proposed by Bouré (1988) leads to an equation mathematically similar to a one-dimensional version of the Lagrangian ATE [72], even though the physical meaning of Bouré's parameters are different from those of the parameters $\hat{\Theta}$, $\hat{\Pi}$ and \hat{C}_{r} in [72], as referred to above in the discussion of [72]. Bouré's approach is an extension of the void-drift closure techniques used in the drift-flux models (Wallis 1969). His second-order PDE for ϵ_d results from the combination of the continuity equations for both phases, under incompressibility and the absence of interfacial mass transfer restrictions, and the postulation of the most general first-order quasilinear differential closure equation for the void fraction and the drift flux. As a postulated expression, the differential void-drift closure lacks generality. It also needs to specify five functions. The present demonstration of Bouré's equation remedies these drawbacks since its generality has been established from first principles of geometry only, under some equivalence conditions between the macroscopic and the averaged descriptions, given by the linking equations [38]-[42], [49], [59] and [60]. Nevertheless, three independent functions (selected from Ξ , N, C_v, C_s and $\langle h_d \rangle_{ed}$) have to be known, in order to be able to proceed with computations using the ATE [72]. It has also to be pointed out that, when applying the one-dimensional ATEs to the bubble-slug transition, some limitations exist. The bubbles grow bigger inside the pipe when approaching the bubble-slug transition and their number diminishes in a given region, up to the point that the flow cannot be correctly referred to as "dispersed" two-phase flow, but as "intermittent" two-phase flow. In such circumstances, a requirement on the minimum number of bubbles inside the averaging region might not be fulfilled (Celminš 1988). Once more in this case, as in the stability studies of fluidized beds, the instability conditions impose a validity limit for the application of the volume-averaged one-dimensional ATEs, if these ATEs remain meaningful up to this limiting condition. The use of different averaging operators (Ishii 1975; Delhaye & Achard 1976; Drew 1983; Arnold et al. 1990) may be a remedy for this problem, illustrating a posteriori the generality of the geometric approach developed in this contribution. In fact, other averaging operators should not modify substantially the procedure and the set of ATEs, but only the meaning of the averaged parameters involved in the relevant ATEs (Nigmatulin 1979; Bedford & Drumheller 1983).

8. CONCLUSIONS

- 1. A set of ATEs, not previously found in the published literature, resulted from the development of a novel approach in order to establish general relationships between the geometric parameters of a dispersed two-phase flow both at the local-instantaneous level ([23], [25], [19] and [21]) and at the macroscopic level ([9], [10], [5] and [T2]). A volume-averaging technique and a link between both the macroscopic and averaged descriptions ([38]-[42], [49], [59] and [60]) gave rise to the ATEs presented in this study.
- 2. The averaged geometric structure of a general dispersed two-phase flow was represented by a basic set of ATEs, constituting an evolution equation for the volume fraction ϵ_d , [61], an evolution equation for the specific interfacial area a_{cd} , [62], and two non-uniformity state equations, one for ϵ_d , [63], and the other for a_{cd} , [64].
- 3. The ATEs have the same generality as the averaged transport equations for dispersed two-phase flows, since the validity of the ATEs is only limited by the constraints that appear in the development of general averaged transport equations for multiphase systems. The constraints establish limitations on the size of the averaging volume (the applicability restriction in [53] and the validity condition for application of [30]).

- 4. Since the ATEs are independent of the averaged transport equations for dispersed two-phase flows, the use of the evolution ATEs [61] and [62], combined with the non-uniformity state ATEs [63] and [64], increases the wave hierarchy in two orders on the derivatives of ϵ_d , with respect to the wave hierarchies used previously in the averaging approaches of dispersed two-phase flows.
- 5. A Eulerian second-order ATE, [68], and a Lagrangian second-order ATE, [72], for ϵ_d were obtained by combination of the basic set of ATEs.
- 6. For an homogeneous fluidized bed as well as for a bubbling pipe or column, the instability conditions for the second-order ATEs [68] and [72], in their one-dimensional forms, may represent one of their validity limits, unless [68] and [72] are not meaningful up to that point, due to the failure of the averaging region in the fulfillment of the restrictions on its volume size.

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