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Analytic expressions for interface terms in general dispersed two–phase flow laden with arbitrary–shaped dispersed elements

Expresiones análiticas para los términos interfaciales en flujos bifásicos dispersos generales cargados con elementos dispersos de forma arbitraria

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Se aceptan comentarios y/o discusiones al artículo

Abstract
This paper presents the methodology of the indicator function–discrete elements probability density function statistical average applied to Two–phase flow modelling. This formulation allows to consider particles of arbitrary shape and size and it can be applied to any laminar or turbulent flow. In the case of equal sized spherical dispersed elements, the most common case found in the literature, the final expression for the interaction terms (contributions that describe the effect of the second phase on the continuous one) are obtained without great difficulties due to the high isotropy of the spherical shape. This task, in the general case of non–spherical non–equal particles is no longer straightforward and the derivation of the appropriate general interaction terms is presented in §4. In the case that the dispersed elements are small enough, some simplifications can be further introduced leading to a final presentation

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that remembers that obtained for the simplest case of spherical particles, but where some of the quantities must be adequately redefined.

Key words: Dispersed Two–phase Flow, arbitrary shaped elements, probability density function, indicator function.

Resumen

Este artículo presenta la aplicación al modelado de flujos bifásicos de la metodología de promediado estadístico utilizando la combinación de la función indicadora de fase y la función densidad de probabilidad de los elementos dispersos. Esta formulación permite considerar partículas de forma y tamaño arbitrarios y puede aplicarse a flujo laminar o turbulento. En el caso de elementos dispersos esféricos de igual tamaño, el más frecuente reportado en la literatura, la expresión final de los términos de interacción (contribuciones que describen el efecto de la segunda fase sobre la fase continua) se obtiene sin mayores dificultades debido a la isotropía de la forma esférica. En el caso general, sin embargo, la tarea es más complicada por lo que la derivación de los términos de interacción generales se aborda en §4. Si los elementos dispersos son suficientemente pequeños se pueden introducir simplificaciones adicionales permitiendo obtener una expresión final que recuerda la obtenida para el caso más simple de partículas no esféricas, aunque algunas cantidades deben redefinirse adecuadamente.

Palabras claves: flujo bifásico disperso, elementos de forma arbitraria, función densidad de probabilidad, función indicadora.

1 Introduction

In the theoretical deduction of Two–phase flow equations, extensive use has been made of volume, temporal or ensemble averages and double/mixed averaging operators. Besides, conditioned averaging formalisms based on a phase indicator function, I, and Reynolds transport theorem are widely found in Two–phase Flow literature [1, 2, 3, 4, 5, 6].

Despite the consolidation of some of the above mentioned approaches, the appropriate theoretical technique to generate useful exact continuous phase Eulerian equations to deal with general Two–Phase Flow is nowadays far from being a closed subject. In fact, a lot of work has been done on developing semi–empirical formulations for engineering purposes.

It is well known that for any systematic conditioned averaging procedure the mean value of any scalar derivative appearing in an instantaneous Eulerian equation is transformed into a derivative of the scalar averaged mean value, plus an extra interface source term. This term introduces information about the presence of the other phase into the equations.

In Lundgren (1972) and Hercynski & Pienkowska (1980) [1, 4] a promising alternative point of view is found following the usual conditioning technique based on a phase indicator function and properly defining a simple probability density function (PDF) for a suspension of spherical solid particles. Within the context of PDF–indicator function, Prosperetti & Zhang (1994) [7] have developed another kind of PDF approach for spheres in a hydrodynamic potential flow and obtained Eulerian transport equations in the framework of the two–fluid engineering modelling with application to bubbly flows. However, the extension of the conditioning average procedure for disperse elements other than spherical ones in general flows was not a trivial task. In Aliod & Dopazo (1990) [8] and Laín & Aliod (2000) [9] the main relationships for arbitrary shaped particles was immediately applied to establish a $k-\epsilon$ extended model for gas–solid turbulent two–phase jet flows. Nevertheless, up to now no detailed foundation or proof of these essential relationships and related properties has been available in the literature. The detailed presentation of the derivation of the fundamental relationships of conditioned average for Two–Phase Flow laden with discrete elements of arbitrary size and shape, which can be applied to any laminar of turbulent flow, constitutes the objective of this paper. Additionally, in order to illustrate the capabilities of the introduced approach, the essential relationships are employed to present a detailed derivation of the statistically averaged exact continuity and momentum equations for Two–Phase Flow, including examples of closure of interaction terms.

2 Description of the Two–Phase system

The disperse phase is treated as a cloud of N different material elements, σ^j, identified by index, $j = 1, ..., N$, each of them with a volume V^{dj} and limited by a closed surface S^j that defines the interface (Fig. 1). $\boldsymbol{y}^j$ will denote the

σ^j position, defined, for instance, by its geometrical center

$$\boldsymbol{y}^j = \frac{1}{V^{dj}} \int\limits_{V^{dj}} \boldsymbol{x} d\boldsymbol{x}; \qquad d\boldsymbol{x} = dx_1 dx_2 dx_3 \;\; \forall\, \sigma^j \,.$$

Each disperse element dynamic and geometrical configuration will be characterized by a set of variables, denoted by $\boldsymbol{z}^j$, which will describe the shape, size and thermo–mechanical state (e.g., velocity $\boldsymbol{v}^j$, temperature T^j, density ρ^{dj}, etc.) of σ^j located at $\boldsymbol{y}^j$.

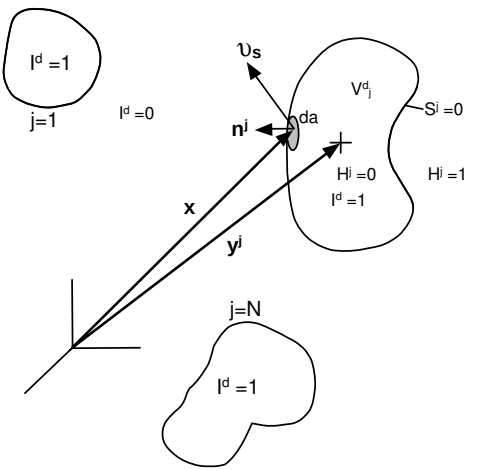

Figure 1: Example of disperse phase elements. It is necessary to distinguish between the disperse element geometrical center, $\boldsymbol{y}$, and the space point, $\boldsymbol{x}$, in which disperse element boundary is present

Even for small values of N it is neither possible nor necessary to describe the element dynamics in a deterministic way. Consequently, a probability density function (PDF) denoted by $P^N\left(t, \boldsymbol{y}^1, \boldsymbol{z}^1, \boldsymbol{y}^2, \boldsymbol{z}^2, ..., \boldsymbol{y}^N, \boldsymbol{z}^N\right)$ is introduced, which represents the probability of having, at instant t, the σ^1 element located around point $\boldsymbol{y}^1$, with state $\boldsymbol{z}^1$ while the σ^2 element is around $\boldsymbol{y}^2$ with state $\boldsymbol{z}^2$, ..., and so on. For the sake of simplicity the following notation is adopted:

$$\left\{C^N\right\} = \left\{\boldsymbol{Y}^N, \boldsymbol{Z}^N\right\} = \left\{\boldsymbol{y}^1, \boldsymbol{z}^1, \boldsymbol{y}^2, \boldsymbol{z}^2, ..., \boldsymbol{y}^N, \boldsymbol{z}^N\right\},$$

$$P^N\left(t, C^N\right) = P^N\left(t, \boldsymbol{Y}^N, \boldsymbol{Z}^N\right) \,.$$

The P^N particle indifference principle, or full P^N symmetry, is a well known and essential property of any discrete elements distribution that will be assumed. It stands that the interchange of position ($\boldsymbol{y}$), shape and dynamic states ($\boldsymbol{z}$) between whatever two disperse elements i, j provides the same value for the P^N function. Therefore, if $\boldsymbol{C}^j = \{\boldsymbol{y}^j, \boldsymbol{z}^j\}$, this symmetry property means

$$P^N(t, \boldsymbol{C}^1, ..., \boldsymbol{C}^i, ..., \boldsymbol{C}^j, ..., \boldsymbol{C}^N) = P^N(t, \boldsymbol{C}^1, ..., \boldsymbol{C}^j, ..., \boldsymbol{C}^i, ..., \boldsymbol{C}^N)\,.$$

In order to apply the conditioning formalism, phase indicator functions for the continous phase, I, and the disperse phase, I^d, are defined in terms of the Heaviside function $H^j(S^j)$:

$$I^d(\boldsymbol{x}, t, C^N) = \sum_{j=1}^{N} \left[1 - H^j\left(S^j\right)\right], \qquad I(\boldsymbol{x}, t, C^N) = 1 - I^d(\boldsymbol{x}, t, C^N)\,,$$

where $H^j(S^j)$, equals 1 if $(\boldsymbol{x}, t)$ is in the continuous phase ($S^j > 0$) and equal 0 otherwise.

The average value of any flow quantity $\phi(\boldsymbol{x}, t, C^N)$ is defined as

$$\langle\phi\rangle\,(\boldsymbol{x}, t) = \frac{1}{N!}\int \phi(\boldsymbol{x}, t, C^N) P^N(t, C^N) dC^N\,. \tag{1}$$

3 Conditional average derivatives

Due to the discontinuity of I in the interfaces, the conmutativity between the conditioned averaging and derivative operators is lost. This is an essential feature because, when conditioning continuous phase instantaneous equations (i.e., Navier–Stokes–Fourier equations), the conditioned average of spatial and time derivatives systematically appears. Therefore, it is necessary to find an expression for the derivative of the conditional average of the generic variable ϕ. It is not difficult to show that

$$(\alpha\overline{\phi})_{,\lambda} = \langle I\phi\rangle_{,\lambda} = \langle (I\phi)_{,\lambda}\rangle = \langle I\ \phi_{,\lambda}\rangle + \langle I_{,\lambda}\ \ \phi\rangle\,, \tag{2}$$

where α is the continuous phase void fraction, $\alpha = \langle I\rangle$, $\overline{\phi} = \langle \phi / I = 1\rangle$, is the conditioned average of ϕ to the presence of continuous phase and λ subscript

after a comma denotes either spatial or time derivatives. The expression (2) shows that the derivative of the conditioned average of ϕ, left hand side (LHS), is split in two parts, right hand side (RHS): the first one is the conditioned average of the derivative of ϕ, and the second, named interaction term, includes the contribution of the interfaces of dispersed elements and is related to the derivatives of the indicator function.

The derivative of I, in the sense of distributions, can be computed in terms of the derivatives of the Heaviside step function as

$$I_{,\lambda} = \sum_{j=1}^{N} \frac{dH^j}{dS^j} S^j{}_{,\lambda} = \sum_{j=1}^{N} \delta^j(S^j) S^j{}_{,\lambda} \ , \tag{3}$$

where $\delta(S)$ is the Dirac's delta whose value is ∞ when $S = 0$ (i.e., in the interface) and equals to zero anywhere else.

If $S^j(\boldsymbol{x} - \boldsymbol{y}^j) = 0$ is the implicit equation of σ^j interface, its derivatives can be computed as

$$\begin{array}{l} S^j{}_{,t} = -|\nabla_x S^j| \ \boldsymbol{v}_s \cdot \boldsymbol{n}^j \\ S^j{}_{,i} = |\nabla_x S^j| \ n_i^j \end{array} \Rightarrow S^j{}_{,\lambda} = |\nabla_x S^j| \, n_\lambda^j; \quad n_\lambda^j = \left\{ \begin{array}{ll} -\boldsymbol{v}_s \cdot \boldsymbol{n}^j & if \ \lambda \equiv t \\ n_i^j & if \ \lambda = i \end{array} \right. . \tag{4}$$

Then, from (3), (4) and average definition (1)

$$\langle I_{,\lambda} \, \phi \rangle = \frac{1}{N!} \int \left[\sum_{j=1}^{N} \delta^j(S^j) \mid \nabla_x S^j \mid n_\lambda^j \phi \right] P^N dC^N = \alpha_s \, \langle \phi \mid \nabla_x S \mid n_\lambda / S = 0 \rangle \tag{5}$$

where α_s represents the expected value of having interface at $(\boldsymbol{x}, t)$

$$\alpha_s(\boldsymbol{x}, t) = \frac{1}{N!} \int \left[\sum_{j=1}^{N} \delta^j(S^j) \right] P^N dC^N = \int \delta(S) P^*(t, \boldsymbol{y}) d\boldsymbol{y} \, . \tag{6}$$

P^* is the reduced probability function of one particule obtained by integration on the other $N-1$ particles configuration. In the second equality of (6) the P^N particle indifference principle has been applied, resulting in the equivalence of all the addends under the summatory symbol.

Nevertheless, in spite of the straightforward deduction of the formulae (5), this presentation lacks direct physical interpretation and useful properties for disperse Two–Phase Flow practical modelling. Neither the expected value of interface presence, α_s, nor the apparently spurious factor $\mid \nabla_x S \mid$ are evident and measurable properties of the flow.

4 Interaction term general expression

Expression (5) can be integrated firstly on the disperse element position variables keeping the rest of the dynamic variables and other particles frozen

$$\langle I,_\lambda \phi \rangle = \frac{1}{N!} \sum_{j=1}^{N} \int d\boldsymbol{z}^j \int dC^{N-1} \int d\boldsymbol{y}^j \delta^j(S^j) \mid \nabla_x S^j \mid n_\lambda^j \phi P^N. \qquad (7)$$

$\delta^j(S^j)$ only captures events in which some element, whose center is located at $\boldsymbol{y}^j$, presents part of its boundary $S^j(\boldsymbol{x} - \boldsymbol{y}^j)$ at $\boldsymbol{x}$ (see Fig. 2). For any function $f(t, \boldsymbol{x}, \boldsymbol{y})$, in the Appendix is shown that

$$\int d\boldsymbol{y} \delta(S(\boldsymbol{x} - \boldsymbol{y})) f(t, \boldsymbol{x}, \boldsymbol{y}) = \int_{S'} da_{\boldsymbol{y}_s} \frac{f(t, \boldsymbol{x}, \boldsymbol{y}_s)}{\mid \nabla_y S \mid_{\boldsymbol{y}=\boldsymbol{y}_s}}, \qquad (8)$$

where points $\boldsymbol{y}_s$ verify $S(\boldsymbol{x} - \boldsymbol{y}_s) = 0$ and $\mid \nabla_y S \mid_{\boldsymbol{y}=\boldsymbol{y}_s} \neq 0$ (i.e., $\boldsymbol{y}_s$ are regular points on the surface S).

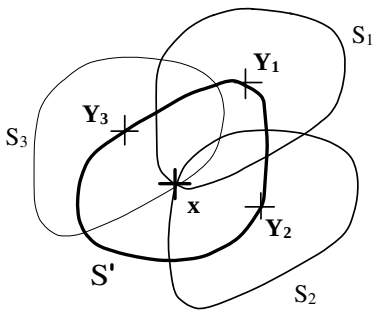

Figure 2: Three different realizations of a frozen shape disperse element, whose volume center $\boldsymbol{y}_i$ is located over S', producing interface presence at $\boldsymbol{x}$

The volume integral of LHS of (8), capturing only disperse element center position $\boldsymbol{y}$ values making $S^j(\boldsymbol{x}-\boldsymbol{y}^j)=0$, is transformed into the RHS surface integral extended along a surface denoted by S' and called the *homologous surface of S with reference to $\boldsymbol{x}$*. S' is defined by the set of points $\boldsymbol{y}_s$ which have the property that, when locating the center of a given disperse element (whose boundary is S) at $\boldsymbol{y}_s$, some part of the particle boundary passes by the fixed point $\boldsymbol{x}$. Figure 2 illustrates the S' concept. A certain disperse element with state $\boldsymbol{z}$ is visualized for three different realizations over S', offering at the same point $\boldsymbol{x}$ different parts of its boundary. Other locations of disperse element center $\boldsymbol{y}$ apart from those located over $S'(\boldsymbol{y}_s)$ will not produce interface presence at $\boldsymbol{x}$ and will not contribute to (7) LHS integral.

In fact S' is obtained from S by making a symmetry of center $(\boldsymbol{x}-\boldsymbol{y})/2$. Therefore, S and S' have identical local geometries for respective $\boldsymbol{y}_s$, $\boldsymbol{x}$ points.

Applying (8) to (7), denoting $\boldsymbol{C}_s^j=\{\boldsymbol{y}_s^j,\boldsymbol{z}^j\}$, it is possible to write

$$\langle I,_\lambda\,\phi\rangle=\frac{1}{N!}\sum_{j=1}^{N}\int d\boldsymbol{z}^j\int dC^{N-1}\times$$

$$\int\limits_{S'} da_{\boldsymbol{y}_s^j}\phi(t,\boldsymbol{x},\boldsymbol{C}_s^j,C^{N-1})P^N(t,\boldsymbol{C}_s^j,C^{N-1})\frac{\mid\nabla_x S^j\mid}{\mid\nabla_y S^j\mid_{\boldsymbol{y}=\boldsymbol{y}_s^j}}n_\lambda^j(t,\boldsymbol{x},\boldsymbol{C}_s^j)\,.$$

Integration on C^{N-1} configuration and taking into account the P^N particle indifference, it results

$$\langle I,_\lambda\,\phi\rangle=\int d\boldsymbol{z}\int\limits_{S'} da_{\boldsymbol{y}_s}\phi_s\frac{\mid\nabla_x S\mid}{\mid\nabla_y S\mid_{\boldsymbol{y}=\boldsymbol{y}_s}}n_\lambda P^*(t,\boldsymbol{y}_s,\boldsymbol{z})\,, \tag{9}$$

where $\phi_s=\phi(t,\boldsymbol{x},\boldsymbol{y}_s,\boldsymbol{z})$ does only depend on its own disperse element parameters.

Due to the relationship between the geometries of S and S' (Fig. 3) it is not difficult to demonstrate that the quotient between both gradients appearing in (9) is just one. Therefore, the general expression for the interaction term is found

$$\langle I,_\lambda\,\phi\rangle=\int d\boldsymbol{z}\int\limits_{S'} da_{\boldsymbol{y}_s}\phi(t,\boldsymbol{x}',\boldsymbol{z})n_\lambda(\boldsymbol{x}',t,\boldsymbol{z})P^*(t,\boldsymbol{y}_s,\boldsymbol{z})\,, \tag{10}$$

where $\boldsymbol{x}$ is fixed, $\boldsymbol{y}_s \in S'$ and $\boldsymbol{x}' = \boldsymbol{x} - \boldsymbol{y}_s$. It is remarkable that for a given disperse element state $\boldsymbol{z}$, the ϕn_λ product depends only on relative vector position $\boldsymbol{x}'$ with respect to its geometrical centre, regardless of the absolute positions.

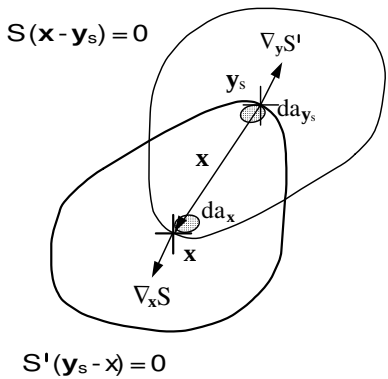

Figure 3: Geometrical similarity between points of S, disperse element boundary, and S', its *homologous surface*

It should be stressed that (10) constitutes a quite general expression for the interaction term for multiphase disperse flows and no restrictions are required apart from the finite volume of the disperse elements. The physical meaning of the interaction term is straightforward. It tells us that the interaction term at one point $\boldsymbol{x}$ is just the statistical average of all interfacial fluxes of the ϕ volumetric property, obtained in each realization in which any interface element is present at $\boldsymbol{x}$. The statistical average is performed in two steps. Inner integral over S' represents the grouping of all those realizations for a *frozen* geometrical–dynamic state while the outer integral accounts for all possible states.

5 The case of small disperse discrete elements

In the case in which the dispersed elements are small enough, the interaction term (10) can be further simplified providing an equivalent expression with a clear interpretation and analitically fruitful for Two–Phase Flow modelling.

Let l^d be the characteristic size of disperse elements and L be the characteristic length of the region where the disperse phase flow develops. If $l^d \ll L$ (a condition quite usual for disperse Two–Phase Flow) the interaction term (10) can be split in two terms

$$\langle I_{,\lambda}\, \phi \rangle = I_{\phi\lambda} + \epsilon_{\phi\lambda}\,, \tag{11}$$

where $I_{\phi\lambda}$ is called *main contribution* and $\epsilon_{\phi\lambda}$ is named *residue*. Both are evaluated as:

$$I_{\phi\lambda}(\boldsymbol{x},t) = \frac{\alpha^d}{\overline{V^d}^*} \overline{\oint_{S_p} \phi n_\lambda da}^{\,*}\ ;\ \epsilon_{\phi\lambda}(\boldsymbol{x},t) = -\left[\frac{\alpha^d}{\overline{V^d}^*} \overline{\oint_{S_p} \phi x'_i n_\lambda da}^{\,*}\right]_{,i} + \sigma\left(\left(\frac{l^d}{L}\right)^2\right). \tag{12}$$

$\overline{V^d}^*$ is the average disperse phase volume conditioned to the presence of the disperse phase centered at $(\boldsymbol{x},t)$ and the integration surface, S_p, is the disperse element interface centered at $\boldsymbol{x}$ (see Fig. 4).

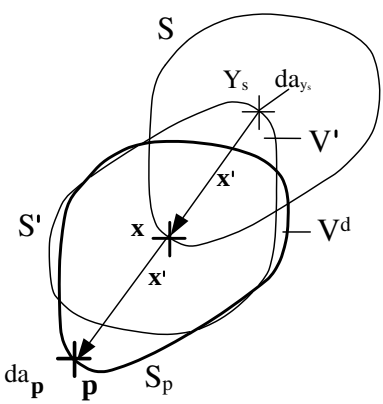

Figure 4: Equivalence between points of S, disperse element boundary, and S_p, boundary of the disperse element whose volume center is displaced to $\boldsymbol{x}$

Moreover, if $I_{\phi\lambda}$ is not identically null and

$$\sigma\left(\oint_{S_p} \boldsymbol{x}'\phi n_\lambda da\right) \leq l^d \sigma\left(\oint_{S_p} \phi n_\lambda da\right), \tag{13}$$

where $\sigma()$ denotes order of magnitude, the magnitude order of $\epsilon_{\phi\lambda}$ is much smaller than the $I_{\phi\lambda}$ one, $\sigma(\epsilon_{\phi\lambda}) \ll \sigma(I_{\phi\lambda})$.

Hereafter, (11) and (12) will be derived starting from (10). The first objective is to transform (10) into an integral over the real disperse element surface S_p centered at $\boldsymbol{x}$ instead of the mathematical S' surface. For this purpose, it should be noted first that if the σ^d center is displaced from $\boldsymbol{y}_s$ to the $\boldsymbol{x}$ point (Fig. 4), the relation $\boldsymbol{x}' = \boldsymbol{p} - \boldsymbol{x}$ will define some relative interfacial position and taking into account the geometrical similarity between S_p and S', the integral on (10) over the homologous surface with reference to $\boldsymbol{x}$ can be written as an integral over the boundary of the disperse element S_p centered at $\boldsymbol{x}$

$$\langle I_{,\lambda}\, \phi\rangle = \int d\boldsymbol{z} \oint_{S_p} da\phi(\boldsymbol{x}', t, \boldsymbol{z}) n_\lambda(\boldsymbol{x}', t, \boldsymbol{z}) P^*(\boldsymbol{x} - \boldsymbol{x}', t, \boldsymbol{z}), \tag{14}$$

with $S_p \equiv S(\boldsymbol{p} - \boldsymbol{x}) = 0$ and da is the surface element on S_p.

If $l^d \ll L$, P^* can be expanded in Taylor series around $\boldsymbol{x}$. To the first order

$$P^*(t, \boldsymbol{x} - \boldsymbol{x}', \boldsymbol{z}) = P^*(t, \boldsymbol{x}, \boldsymbol{z}) - P^*{}_{,i}\,(t, \boldsymbol{x}, \boldsymbol{z}) x_i' + \sigma\left(\left(\frac{l^d}{L}\right)^2\right).$$

$\sigma((\frac{l^d}{L})^2)$ is a residue or order $(l^d/L)^2$. Thus, within this approximation order (14) can be evaluated as

$$\begin{aligned}\langle I_{,\lambda}\, \phi\rangle = &\int d\boldsymbol{z} P^*(t, \boldsymbol{x}, \boldsymbol{z}) \left[\oint_{S_p} da\phi(\boldsymbol{x}', t, \boldsymbol{z}) n_\lambda(\boldsymbol{x}', t, \boldsymbol{z})\right] - \\ &- \int d\boldsymbol{z}\left[\oint_{S_p} da P^*{}_{,i}\,(t, \boldsymbol{x}, \boldsymbol{z}) x_i' \phi(\boldsymbol{x}', t, \boldsymbol{z}) n_\lambda(\boldsymbol{x}', t, \boldsymbol{z})\right] + \sigma\left(\left(\frac{l^d}{L}\right)^2\right)\end{aligned} \tag{15}$$

In such a case, the first addend in (15) is expressed as

$$I_{\phi\lambda} = \int d\boldsymbol{z} P^* \left[\oint\limits_{S_p} da \phi n_\lambda \right] = \mathcal{N} \overline{\oint\limits_{S_p} \phi n_\lambda da}^{*} ,$$

where $\mathcal{N}(\boldsymbol{x}, t) = \int d\boldsymbol{z} P^*(t, \boldsymbol{x}, \boldsymbol{z})$ is the local particle number density and the overbar followed by an asterisk denotes the average conditioned to the presence of disperse phase centered at $(\boldsymbol{x}, t)$.

In the second addend in (15) the derivative can be commuted with the integrals since there is no other dependence on $\boldsymbol{x}$ except in P^*, which is also extracted from the surface integral

$$\epsilon_{\phi\lambda} = - \left[\mathcal{N} \overline{\oint\limits_{S_p} \phi x_i' n_\lambda da}^{*} \right]_{,i} + \sigma \left(\left(\frac{l^d}{L} \right)^2 \right) .$$

The next step is to calculate the particle number density $\mathcal{N}(t, \boldsymbol{x})$. In order to do this, the phase indicator function I^d expectation value is evaluated as

$$\alpha^d = \left\langle I^d \right\rangle (\boldsymbol{x}, t) = \frac{1}{N!} \int dC^N P^N(t, C^N) \sum_{j=1}^{N} \left[1 - H^j(S^j(\boldsymbol{x} - \boldsymbol{y}^j) \right] .$$

Applying the distributive property, integrating C^{N-1} and taking into account the P^N particle indifference again, the following is obtained

$$\alpha^d = \int d\boldsymbol{z} \int\limits_{V'} d\boldsymbol{y} P^*(t, \boldsymbol{y}, \boldsymbol{z}) ,$$

where the spatial integration domain of this expression is reduced to the set of points $\boldsymbol{y}$ producing the presence of disperse elements at $(\boldsymbol{x}, t)$. In the same way as the reasoning followed previously, this region is V', the volume enclosed by the homologous surface S'.

Introducing again the first order expansion of $P^*(\boldsymbol{y})$ around $\boldsymbol{x}$

$$\alpha^d = \int d\boldsymbol{z} \left\{ P^* V^d + P^*{}_{,i} \int\limits_{V'} d\boldsymbol{y} (y_i - x_i) \right\} + \sigma \left(\left(\frac{l^d}{L} \right)^2 \right) .$$

But V' is a symmetry of a σ^d element with its center at $\boldsymbol{x}$, so the second addend is null. Thus, to the first order

$$\alpha^d = \int d\boldsymbol{z} V^d P^* + \sigma\left(\left(\frac{l^d}{L}\right)^2\right) = \overline{V^d}^* \int P^* d\boldsymbol{z} + \sigma\left(\left(\frac{l^d}{L}\right)^2\right)$$
$$= \overline{V^d}^* \mathcal{N} + \sigma\left(\left(\frac{l^d}{L}\right)^2\right).$$

This result supplies a straightforward interpretation of the expectation value of the I^d indicator function, α^d: it tells us that α^d is the average disperse elements' volume fraction and therefore the local particle number density is expressed as

$$\mathcal{N} = \int P^* d\boldsymbol{z} \approx \frac{\alpha^d}{\overline{V^d}^*},$$

which is accurate up to the first order.

To summarize, the expression of $\langle I_{,\lambda}\, \phi\rangle$ estimated to the first order in the series expansion of P^* around $\boldsymbol{x}$ is

$$\langle I_{,\lambda}\, \phi\rangle = \frac{\alpha^d}{\overline{V^d}^*} \overline{\oint_{S_p} \phi n_\lambda da}^* - \left[\frac{\alpha^d}{\overline{V^d}^*} \overline{\oint_{S_p} x_i' \phi n_\lambda da}^*\right]_{,i} + \sigma\left(\left(\frac{l^d}{L}\right)^2\right) = I_{\phi\lambda} + \epsilon_{\phi\lambda}. \tag{16}$$

With this result, (11) and (12) are proven.

To finish, it remains to demonstrate that if the *main contribution* is different from zero and condition (13) is satisfied, the order of magnitude or the *residue* $\epsilon_{\phi\lambda}$ is much smaller than the order of magnitude of $I_{\phi\lambda}$. In order to show this, note that the order of magnitude of residue can be estimated as

$$\sigma\left(\epsilon_{\phi\lambda}\right) \approx \frac{1}{L} \frac{\alpha^d}{\overline{V^d}^*} \sigma\left(\overline{\oint_{S_p} x_i' \phi n_\lambda da}^*\right). \tag{17}$$

Therefore, from (13) and (17)

$$\sigma\left(\epsilon_{\phi\lambda}\right) \approx \frac{1}{L}\frac{\alpha^d}{\overline{V^d}^*}\,\sigma\left(\overline{\oint_{S_p} x_i'\phi n_\lambda da}^*\right) \leq \frac{l^d}{L}\frac{\alpha^d}{\overline{V^d}^*}\,\sigma\left(\overline{\oint_{S_p} \phi n_\lambda da}^*\right) \approx \frac{l^d}{L}\sigma\left(I_{\phi\lambda}\right)\,;$$

consequently, as long as $l^d \ll L$ is satisfied, $\sigma\left(\epsilon_{\phi\lambda}\right) \ll \sigma\left(I_{\phi\lambda}\right)$.

In general, the hypothesis ($l^d \ll L$) and the condition (13) are frequently found in turbulent disperse Two–Phase Flow of industrial interest. As a consequence of the results stated in the previous section, provided that $I_{\phi\lambda} \neq 0$, the interaction term can be approximated as

$$\langle I\phi_{,\lambda}\rangle \approx (\alpha\overline{\phi})_{,\lambda} - \frac{\alpha^d}{\overline{V^d}^*}\overline{\oint_{S_p}\phi n_\lambda da}^*\,, \tag{18}$$

which constitutes the *essential relation for conditioned statistical average*. Presentation (18) is much more convenient than the first expression deduced for the interaction term, relation (10).

The interaction term appearing in (18) represents the *statistical average of the net flux over the entire boundary of a single disperse element, S_p, per unit average volume, times the disperse phase void fraction.* In the interaction term the net flux and the disperse phase volume statistical average values are computed as conditioned to particle centre presence at point $\boldsymbol{x}$. The statistically averaged variables α, $\overline{\phi}$ are truly local and time dependent. Moreover, volume filtering effects of small scales associated with conventional volume averages are absent.

Furthermore (18) resembles and is directly related to the relationships appearing in the context of volume average [10], but the present approach allows unnecesary complexities in the subsequent Two–Phase Flow modelling to be overcome because the introduction of complex space–time weighting functions or additional time averaging procedures is avoided.

An additional aspect to be emphasised is related to the possible subsequent analytical transformations of the interaction term at (18), because the ϕn_λ flux extends over the closed surface defined by the disperse element boundary, S_p.

It must be noticed that the appearance of the residue contribution $\epsilon_{\phi\lambda}$ in (16) is a consequence of the different values of $\phi\, P^*$ in the neighbourhood of $\boldsymbol{x}$. $\phi\, P^*$ has been approximated by a linear expansion around $\boldsymbol{x}$ which is valid as far as $\sigma\left(|\boldsymbol{x}'|/L\right) \approx l^d/L \ll 1$. Therefore the residue is a contribution of order $\sigma(\frac{l^d}{L})$ regarding to the *main contribution*.

In many contexts, such as the ones associated with Two–Phase Flow turbulent modelling, it may be accurate enough to retain only the *main contribution* to the interaction term as long as strong uncertainties, coming from the approximate closures of the several transport and interaction contributions involved, are clearly superior to *residue contributions* of order $\left(\frac{l^d}{L}\right)$.

It should be noted that (13) establishes that the order of magnitude of $x_i'\phi$ flux over the particle boundary can be approximated by the order of magnitude of total ϕ flux through the interface multiplied by a characteristic length of the particle size. Although condition (13) will generally be satisfied by arbitrary functions ϕ over regular or irregular particle shapes it should be emphasized that $\epsilon_{\phi\lambda}$ should not be neglected without further considerations. For instance, when the main contribution exactly cancels, (i.e. ϕ or ϕn_λ is strictly constant over S_p) the interaction term reduces to the residue contribution, then, it should be kept or discarded in comparison with other flow terms. Moreover, theoretical limiting cases, where known exact analytical solutions are to be reconstructed or small correction terms are of interest, residue should be retained, otherwise inconsistencies or inaccurate results will appear.

6 Relevance for Two–Phase Flow modelling

Conditioned averaging to deduce continuous phase Eulerian equations in multiphase flows has been examined in detail in the literature. Nevertheless, in order to illustrate the most important characteristics of the present approach, we will derive the continuous phase continuity and momentum equations. Deduction of the general equations for continuous phase in Two–Phase Flow where relationship (18) applies can be achieved by the standard methodology used in the indicator function context.

The continuous phase instantaneous local Eulerian continuity, momentum equations are written down in a conservative presentation for convenience

$$\rho_{,t} + [\rho u_i]_{,i} = 0$$

$$[\rho u_j]_{,t} + [\rho u_i u_j]_{,i} = [-p\delta_{ij} + \tau_{ij}]_{,i} + \rho g_j \,, \tag{19}$$

u_i, p, ρ and τ_{ij} are the instantaneous velocity, pressure, density and viscous stress tensor respectively.

Since the system (19) is not valid everywhere but only at points $\boldsymbol{x}$, where at time t, a continuous phase exists, these events must be differentiated with the aid of the continuous phase indicator function.

Multiplying both equations on system (19) by I and taking the statistical average (1) afterwards

$$\langle I\rho_{,t} \rangle + \langle I\,[\rho u_i]_{,i} \rangle = 0$$

$$\langle I\,[\rho u_j]_{,t} \rangle + \langle I\,[\rho u_i u_j]_{,i} \rangle = \langle I\,[-p\delta_{ij} + \tau_{ij}]_{,i} \rangle + \langle I\rho g_j \rangle \,. \tag{20}$$

In (20), all contributions, except volume force $\langle I\rho g_j \rangle$, are conditioned averages of variable derivatives. The interaction terms in (20) for $\rho(u_i - v_{si})n_i$, $\rho u_j(u_i - v_{si})n_i$ and $\tau_{ij}n_j$ are defined at the disperse phase, continuous through the interface and expressed according to (18) Therefore, by systematically applying the essential relation for conditioned statistical average (18), recalling the n_λ definition depending on the kind of derivative, spatial or temporal, and locating all interaction terms on the right hand side of the respective equation, continuity yields to

$$[\alpha\rho]_{,t} + [\alpha\rho U_i]_{,i} = \frac{\alpha^d}{\overline{V^d}^*} \overline{\oint_{S_p} \rho\,[u_i - v_{si}]\,n_i da}^* + \epsilon_I$$

and momentum

$$[\alpha\rho U_j]_{,t} + [\alpha\rho U_i U_j]_{,i} = -[\alpha P]_{,j} + [\alpha\overline{\tau_{ij}}]_{,i} - \left[\alpha\rho\overline{u_i' u_j'}\right]_{,i} + \alpha\rho g_j -$$

$$-\frac{\alpha^d}{\overline{V^d}^*} \overline{\oint_{S_p} [-p\delta_{ij} + \tau_{ij}]\,n_i da}^* + \frac{\alpha^d}{\overline{V^d}^*} \overline{\oint_{S_p} \rho u_j\,[u_i - v_{si}]\,n_i da}^* + \epsilon_{pj} + \epsilon_{[\tau_{ij}]i} + \epsilon_{IM}.$$

The usual notation is assumed: $U_i = \overline{u_i}$, $P = \overline{p}$, $u_i' = u_i - U_i$. ϵ_I and ϵ_{IM} are the residues associated to the entrainment terms in the continuity and momentum equations respectively, ϵ_{pj} corresponds to the pressure gradient and $\epsilon_{[\tau_{ij}]i}$ to the stress tensor. Henceforth, for simplicity, ρ constant will be assumed.

The combination of interaction terms coming from temporal and convective contributions in any conservative equation generate a characteristic source term, the entrainment term, associated with interfacial mass transfer phenomena. When there is no local mass transfer across the interface $\boldsymbol{u} = \boldsymbol{v}_s$, all the entrainment source terms become zero (main contribution and residue).

For a Navier–Stokes viscous stress tensor in an incompressible flow

$$\alpha\overline{\tau_{ij}} = \langle I\mu \left[u_{i,j} + u_{j,i}\right]\rangle \,. \tag{21}$$

Since the conditioned averaged viscous tensor (21) contains further spatial derivatives, essential relationship (18) should be carefully applied again. Assuming a constant dynamic viscosity coefficient, μ

$$\alpha\overline{\tau_{ij}} = \mu \left[\left[\alpha U_i\right],_j + \left[\alpha U_j\right],_i\right] - \frac{\alpha^d}{\overline{V^d}^*}\overline{\oint_{S_p} \mu \left[u_i n_j + u_j n_i\right] da}^* + \mu \left[\epsilon_{u_i j} + \epsilon_{u_j i}\right] .$$

The second term in the right hand side is the so called "extradeformation term" [3], related to the viscous stress tensor and due to average local deformation introduced by disperse element boundaries. Let's take a closer look to this term.

It is known that an approximation of the velocity around a point in the dispersed element σ^d is a function of the deformation velocity tensor $\mathcal{D}_{ij}$ and vorticity vector $\boldsymbol{\omega}$ evaluated at the element center, i.e.

$$v_i(\boldsymbol{x}') \approx v_{oi} + \left(\frac{1}{2}\epsilon_{ijk}\omega_j + \mathcal{D}_{ik}\right) x_k' = a_i + b_{ik}x_k' \,, \tag{22}$$

where ϵ_{ijk} is the alternator pseudo-tensor. (22) will be exact for spherical particles rotating with angular velocity $\Omega_j = \frac{1}{2}\omega_j$ and experiencing an isotropic deformation $\mathcal{D}_{ij} = \frac{\dot{r}}{r}\delta_{ij}$, r being the particle radius and $\dot{r}$ the radius expansion

rate per unit time (such a disperse element will be kinematically characterized by the set $\boldsymbol{v}_o$, $\boldsymbol{\Omega}$, r, $\dot{r}$). Applying the divergence theorem it is not difficult to obtain

$$\frac{\alpha^d}{\overline{V^d}^*}\overline{\oint_{S_p} v_i n_j da}^* = \alpha^d \left[\frac{1}{2}\epsilon_{ijk}\overline{\omega_k}^d + \overline{D_{ij}}^d\right]. \tag{23}$$

Taking into account the anti-symmetry properties of the alternator pseudo-tensor and the no-slip condition in the dispersed element surface, using (23), the 'extradeformation term' is written as:

$$-\frac{\alpha^d}{\overline{V^d}^*}\overline{\oint_{S_p} \mu\left[u_i n_j + u_j n_i\right] da}^* = -\alpha^d \mu\left(\overline{D_{ij}}^d + \overline{D_{ji}}^d\right). \tag{24}$$

When disperse elements of any shape move without deformation (translation and/or rigid rotation) (24) cancels. For a spherical particle ongoing isotropic expansion (24) is simply

$$-\alpha^d \mu\left(\overline{\mathcal{D}_{ij}^d} + \overline{\mathcal{D}_{ij}^d}\right) = -\alpha^d \frac{2}{3}\mu T_r\left[\overline{\mathcal{D}_{ij}^d}\right]\delta_{ij} = -\alpha^d \mu 2\frac{\dot{r}}{r}\delta_{ij}\,. \tag{25}$$

The expression (25) can be interpreted, if desired, as volumetric viscous stress related to disperse element volume changes, affected by a pseudo–volumetric viscosity $\alpha^d\frac{2}{3}\mu$. In any case, (24) allows the order of magnitude to be computed easily and the extradeformation term to be approximated for modelling purposes, making it clear that the term depends on the average of the deformation tensor inside the disperse elements. Depending on the relative order of magnitude of the shear rates on the mean flow, $\frac{U}{L}$, and on the disperse elements, $\frac{\dot{r}}{l^d}$, the 'extradeformation term' could be dominant or negligible.

In order to illustrate the analitycal capabilities of the presented approach, let us consider a generalisation of (22) for the generic variable ϕ. Let us suppose that ϕ can be expressed inside the disperse element as a polynomial of type (which can be accepted at some degree of accuracy for any variable if the disperse element is small enough)

$$\phi(\boldsymbol{x}') = a_0 + b_i x_i' + c_{ij} x_i' x_j' + d_{ijl} x_i' x_j' x_l'\,, \tag{26}$$

where $\boldsymbol{x}'$ is the position of one disperse element point regarding its center $\boldsymbol{x}$ and a_0, $\{b_i\}$, $\{c_{ij}\}$ and $\{d_{ijl}\}$ are coefficients which are functions only

of the disperse element dynamics. It is clear that at (26) the magnitude order of the ϕ polynomial expression terms are not $\left(\frac{l^d}{L}\right)$, $\left(\frac{l^d}{L}\right)^2$, $\left(\frac{l^d}{L}\right)^3$, since coefficients b_{ij}, c_{ij}, d_{ijl} are estimated in terms of the particle inner derivatives. Therefore, as many terms as necessary should be retained (26) to reconstruct the ϕ over the disperse element, without any contradiction with the limiting first order $\left(\frac{l^d}{L}\right)$ approach defined in (16). It is easy to show, applying Gauss theorem, that the interaction term for the spatial derivative in the k direction is calculated

$$\frac{\alpha^d}{\overline{V^d}^*}\overline{\oint_{S_p}\phi n_k da}^* = \alpha^d\left[\overline{b_k}^d + \overline{d_{kij}\mathcal{I}_{ij}}^d + \overline{d_{ikj}\mathcal{I}_{ij}}^d + \overline{d_{ijk}\mathcal{I}_{ij}}^d\right], \qquad (27)$$

where $\mathcal{I}_{ij}$ are the geometrical inertia tensor components of the disperse element which, of course, depend on its shape.

The structure and symmetry properties of the series expansion coefficients of Eq. (26) allow us to simplify (27) which will help to model different interaction terms.

7 Conclusion

Derivation of the conditioned average essential relationships for general (laminar or turbulent) Two–Phase Flow, based on joint probability density and phase indicator functions, is presented in detail. No restrictions on shape, size or concentration of the disperse elements are required.

Useful transformations and related results have been documented specifically for disperse Two–Phase Flow. The final expressions provide consistent and meaningful interaction terms similar to others found with other indicator function and volume average procedures, but the adopted approach overcomes some conceptual and practical problems arising in these approaches and supplies helpful simplificative properties.

When the characteristic length of disperse elements is much smaller than the integral flow scale, interaction terms transform into particularly simple analytical structure. The interaction term is then split in two: a main contribution and a residue. The first one shows a fairly meaningful structure

resembling the structure of the volume average interaction term; moreover, it has a precise mathematical definition and is computed as the average of the ϕ general property flux over the whole boundary of a single disperse element, conditioned to realizations where the disperse element volume center is located at the point in which the statistical average is evaluated. The remaining term, or residue, can be neglected regarding to the main contribution under specified conditions generally fulfilled at disperse Two–Phase Flow. In addition, the residue also shows a precise mathematical structure allowing it to be computed exactly or its order of magnitude to be approximated. As an illustrative example the presented expresions are used to derive the statistically averaged continuity and momentum equations for the continuous phase of a dispersed Two–Phase flow. The corresponding interaction terms, including the so–called 'extradeformation term', are in some cases calculated explicitely.

Appendix

Here, (8) is demonstrated. In order to achieve

$$\int d\boldsymbol{y}\delta(S(\boldsymbol{x}-\boldsymbol{y}))f(t,\boldsymbol{x},\boldsymbol{y}) = \int d\boldsymbol{y}_s \frac{f(t,\boldsymbol{x},\boldsymbol{y}_s)}{\mid \nabla_y S \mid_{\boldsymbol{y}=\boldsymbol{y}_s}}$$

let us recall the following property of the Dirac delta in one dimension [11]

$$\delta(g(y)) = \sum_{y_s} \frac{1}{\mid \frac{dg}{dy} \mid_{y=y_s}} \delta(y-y_s)\,,$$

where y_s are the zeros of the function g, i.e., the solutions of the equation $g(y)=0$. It is supposed that the derivative dg/dy is different from zero at y_s.

In the three–dimensional case, the zeros of the equation $g(\boldsymbol{y})=0$ are a continuous set and the appropriate generalization of the previous property will be

$$\delta(g(\boldsymbol{y})) = \int\limits_{\boldsymbol{y}_s} \frac{1}{\mid \nabla_y g \mid_{\boldsymbol{y}=\boldsymbol{y}_s}} \delta(\boldsymbol{y}-\boldsymbol{y}_s)d\boldsymbol{y}_s$$

supposing that $\mid \nabla_y g \mid_{\boldsymbol{y}=\boldsymbol{y}_s} \neq 0 \;\forall\; \boldsymbol{y}_s$ solution of $g(\boldsymbol{y})=0$. The integral is extended to the domain defined by the zeros of $g(\boldsymbol{y})$.

Here, the zeros, regarding $\boldsymbol{y}$, of the function $S(\boldsymbol{x}-\boldsymbol{y})=0$ define a surface and then

$$\int d\boldsymbol{y}\delta(S(\boldsymbol{x}-\boldsymbol{y}))f(t,\boldsymbol{x},\boldsymbol{y})=\int d\boldsymbol{y}f(t,\boldsymbol{x},\boldsymbol{y})\int\limits_{\boldsymbol{y}_s} da_{\boldsymbol{y}_s}\frac{1}{\mid\nabla_y S\mid_{\boldsymbol{y}=\boldsymbol{y}_s}}\delta(\boldsymbol{y}-\boldsymbol{y}_s)\,,$$

where $\boldsymbol{y}_s$ are the solution of $S(\boldsymbol{x}-\boldsymbol{y})=0$ for a given $\boldsymbol{x}$. Changing the integration sequence and performing the integration on $\boldsymbol{y}$ using the Dirac's delta

$$\int\limits_{\boldsymbol{y}_s} da_{\boldsymbol{y}_s}\frac{1}{\mid\nabla_y S\mid_{\boldsymbol{y}=\boldsymbol{y}_s}}\int d\boldsymbol{y}f(t,\boldsymbol{x},\boldsymbol{y})\delta(\boldsymbol{y}-\boldsymbol{y}_s)=\int\limits_{\boldsymbol{y}_s} da_{\boldsymbol{y}_s}f(t,\boldsymbol{x},\boldsymbol{y}_s)\frac{1}{\mid\nabla_y S\mid_{\boldsymbol{y}=\boldsymbol{y}_s}}$$

The $\boldsymbol{y}_s$ points constitute a surface given by $S'=S(-(\boldsymbol{y}_s-\boldsymbol{x}))$ as referred in the main text.

Nomenclature

Latin symbols

$\mathcal{D}_{ij}$ $[\frac{1}{s}]$	dispersed phase deformation tensor	R $[m]$	particle radius
f	generic function	S	surface
$\boldsymbol{g}$ $[\frac{m}{s^2}]$	acceleration of gravity	t $[s]$	time
H	Heaviside function	$\boldsymbol{u}$ $[\frac{m}{s}]$	instantaneous gas velocity
I	indicator function	$\boldsymbol{U}$ $[\frac{m}{s}]$	averaged gas velocity
$I_{\phi\lambda}$	main part interaction term	V^{sup} $[m^3]$	volume
I_{sub}	interaction term	$\boldsymbol{x}$ $[m]$	spatial point
L $[m]$	integral length scale	$\boldsymbol{x}'$ $[m]$	relative location to particle center
l^d $[m]$	characteristic particle size	$\boldsymbol{y}^{sup}$ $[m]$	particle center position
$\boldsymbol{n}$	normal vector	$\boldsymbol{Y}^N$	Center position vector N particles
p $[\frac{Kg}{m\cdot s^2}]$	instantaneous gas pressure	$\boldsymbol{z}^{sup}$	dynamic variable
P $[\frac{Kg}{m\cdot s^2}]$	mean gas pressure	$\boldsymbol{Z}^N$	Dynamic variable vector N particles
P^{sup}	probability density function	T $[K]$	Temperature

Greek symbols

α $[-]$	void fraction	$\boldsymbol{\tau}$ $[\frac{m^2}{s^2}]$	stress tensor
$\boldsymbol{\delta}$	Dirac's delta	$\boldsymbol{v}$ $[\frac{m}{s}]$	instantaneous particle velocity
ϵ_{ijk}	alternator pseudo-tensor	ϕ	generic variable
$\epsilon_{\phi\lambda}$	residue interaction term variable ϕ	ω $[\frac{1}{s}]$	vorticity
μ $[\frac{Kg}{m\cdot s}]$	dynamic viscosity	Ω $[\frac{1}{s}]$	angular velocity
ρ $[\frac{Kg}{m^3}]$	density		
$\sigma()$	order of magnitude	$\mathcal{I}_{ij}$ $[m^2]$	geometric inertia tensor
σ^j	discrete element j	$\mathcal{N}$	local particle number density

Subscripts

i	spatial component	λ	spatial or temporal component
s	surface	$\dot{}$	time rate change
sub	subscript		

Superscripts

$'$	fluctuating component	j	label of element
d	dispersed phase	sup	superscript

Other Symbols

$Tr[-]$	tensor trace
$\langle\,\rangle$	ensemble average
$\overline{}$	continuous phase conditioned average
$\overline{}^d$	dispersed phase conditioned average
$\overline{}^*$	centered disperse phase conditioned average

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