Invariant closure proposals for the interface tracking in two-phase turbulent flows

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Abstract. The present work focuses on the formulation of new modelling approaches to ensemble-averaged equations describing multiphase flows, based on the symmetries admitted by these equations. Particular attention will be given to the proper treatment of the unclosed terms in the equation for the interface tracking which represent the influence of unresolved part of the surface. Modelling of those terms is crucial in flows with heat and mass transfer. In the work, two approaches to track the interface will be considered: the level-set function and sharp-step indicator function method. The differences between the two approaches in terms of turbulence-interface interactions modelling will be outlined.

1. Introduction

The phenomenon of turbulence and its interaction with the surface in two-phase flows is particularly interesting from the physical point of view and is important in a variety of industrial and geophysical applications. Examples of turbulent flows with agitated surface include the wave breaking flows, relevant in the ocean and marine engineering (Brocchini & Peregrine 2001a), open channel flows with the surface disrupted by the action of turbulence as well as flows where heat and mass transfer is considerably enhanced due to the deformation of the surface (Smolentsev & Miraghaie 2005). In spite of an increasing research effort oriented towards investigation and modelling of such flows some authors claim that there is still a lack of fundamental physics based modelling approaches, cf. Prosperetti & Tryggvason (2007), and that there is considerable room for improvements in this field.

To find a closure, a given term should be written in terms of known variables, hence, it is necessary to derive the most general, consistent form of such closures and decide which flow variables can be used in the model. Such basic rules for the modelling approaches can be provided by the group theory. Lie group analysis of the original, closed system of equations will lead to its symmetries. The main idea is that the modelled system should reflect the same symmetries as the original one. Otherwise, a turbulence model may fail to properly describe the physics of the flow. With the use of the group theory one may identify which terms can be present in a model for unclosed terms, so that all symmetries are satisfied. For interface problem in the context of premixed combustion this has been done for the first time by Oberlack et al. (2001).

The aim of this wok is, first, to apply the Lie group analysis to equations describing the multiphase flows. A possible outcome of such analysis are guidelines for modelling approaches. Moreover, new ideas will also be developed, as far as tracking of the interface in turbulent flow is concerned. The indicator function, smoothed as a result of averaging or filtering process will be interpreted as a probability of finding the k-th phase in the considered point of the flow. We will investigate an equation for this quantity and aim to model an evolution of the whole layer where the probability of finding the surface is non-zero.

The paper is structured as follows. In the next section, a short review of the existing approaches to turbulent two-phase flows modelling is presented. In Section 3 we perform group analysis of the equations governing two-phase flows, first for the level-set and then for the indicator function formulation. The closure proposals to the averaged indicator function equation are proposed in Section 4. This is followed by the conclusions and perspectives for the further work.

2. State of the art

We consider a two-phase flow with clearly defined interface where one or both phases exhibit turbulence characteristics. If the turbulent eddies are present in the bulk flow they may reach and deform the interface between the phases, as well as influence its motion. On the other hand, the disturbances generated at the surface may contribute to the turbulent production in the bulk flow. Brocchini & Peregrine (2001)a provide a comprehensive empirical study of the turbulent air-water flows. The authors classify different regimes of free-surface deformations and parameterize them using two turbulence-related quantities: the typical length scale of the turbulent "blobs" reaching the surface - L and the intensity of the turbulent fluctuations q. To investigate the stabilizing effect of the surface tension and gravity Brocchini & Peregrine consider three criterial numbers the Reynolds number: $Re = qL/\nu$, the Froude number: $Fr = q/\sqrt{(2gL)}$ and the Webber number: $We = q^2 L\varrho/(2\gamma)$, where ν is the kinematic viscosity of the liquid phase, g stands for the acceleration due to the gravity and γ is the surface tension coefficient. The rough estimate of their critical values divide the $L - q$ diagram into various flow regions, cf. Fig. (2). In the region 0 on the diagram one deals with the flat surface where both the gravity and the surface tension stabilizes it (small We and /or Fr). In Region 1, where the Froude number is large and the Webber number small, we observe small-scale structures on the surface, the surface tension prevents the surface from being disintegrated. Next, in region 2 neither gravity nor surface tension can prevent the surface breakage (both Fr and We are large). Finally, in Region 3 we have $Fr << 1$ and $We >> 1$ which means that the gravity effects plays a dominant stabilizing role.

When the averaging or filtering procedure is applied to transport equations describing multiphase flows, a number of unclosed terms appear. Some of them are connected with jump conditions at the interface and hence, they are very specific to multiphase flows. Labourasse et al. (2007) classify the unclosed terms in the evolution equations in the one-fluid approach and estimate their subgrid-scale contribution using *apriori* study. Moreover, Toutant et al. (2008) propose to use a scale similarity models to approximate those terms and estimate the error of such modelling attempt by performing a DNS of an interaction between a deformable bubble and spatially decaying turbulence. All the above-mentioned works concern the LES context. The Reynolds averaged (RANS) approach is discussed in Brocchini & Peregrine (2001)b. Those authors present the averaged equations for the liquid phase with appropriate boundary conditions to be applied on the surface (the gas phase is neglected). They also discuss a closure proposals, mainly referring to the intermittency models used in classical turbulence modelling. Contrary to the latter contribution we consider here the motion of both phases and concentrate on the Reynolds-averaged equation describing motion of the interface.

2.1. Governing equations

In the following, we consider a flow of incompressible, non-miscible fluids, separated from each other by an interface. The position of the interface can be described by the level-set function $f^k(\mathbf{x}, t)$ as follows; $\mathbf{x}$ is a point placed at the interface if and only if $f^k(\mathbf{x}, t) = f_0$ where f_0 is a selected level of the function f^k. Moreover, it is assumed that the k-th phase is placed at a given point $\mathbf{x}$ if $f^k(\mathbf{x}, t) > f_0$. Based on the level-set function one can define a sharp indicator function as

$$\chi^k(\mathbf{x}, t) = H(f^k(\mathbf{x}, t) - f_0) \tag{1}$$

where H is the Heaviside function.

A part of the surface at a given time t is sketched in Fig. 1. The surface is parametrized using a two-dimensional, local coordinate system (λ, μ). A unit vector normal to the point $\mathbf{x}_s(\lambda, \mu, t)$ of the surface is denoted by $\mathbf{n}^k(\lambda, \mu, t)$ and is directed towards the phase $i \neq k$. It is important to note that the parametrization of the surface is arbitrary and does not influence its properties.

The gradient of the indicator function is zero everywhere except at the surface and it reads, cf. Juric and Tryggvason (1998)

$$\nabla \chi^k = -\iint \mathbf{n}^k(\lambda, \mu, t) \delta\left(\mathbf{x} - \mathbf{x}_s(\lambda, \mu, t)\right) A \mathrm{d}\lambda \mathrm{d}\mu \tag{2}$$

where the volume integral has been transformed into the integral over the surface and $A \, \mathrm{d}\lambda \mathrm{d}\mu$ describes the infinitesimal area of the surface with A given by the formula

$$A = \left| \frac{\partial \mathbf{x}_s}{\partial \lambda} \times \frac{\partial \mathbf{x}_s}{\partial \mu} \right|. \tag{3}$$

In the most general formulation, the flow of k phases can be described by a set of conservation equations, separately for each phase. These equations are complemented by jump conditions at the interface. Alternatively, a one-fluid formulation can be considered where one set of equations is solved in the entire flow region and the interface is tracked directly by a kinematic equation for the level-set function or for the indicator function. The one-fluid variables are written as $\phi = \sum_k \chi^k \phi^k$. The one-fluid mass and momentum conservation equations have the following form, cf. Labourasse et al. (2007)

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \mathbf{u}) = 0, \tag{4}$$

$$\frac{\partial \varrho \mathbf{u}}{\partial t} + \nabla \cdot (\varrho \mathbf{u}\mathbf{u}) + \nabla p - \varrho f - \nabla \cdot \tau = -\gamma \left(\nabla_s \cdot \mathbf{n}^1 \right) \nabla \chi^1. \tag{5}$$

where $\nabla_s \cdot \mathbf{n}^k = \kappa^k$ is the surface curvature, equal to the surface divergence of the normal vector $\kappa^k = \nabla_s \cdot \mathbf{n}^k = (\mathrm{Id} - \mathbf{n}^k \mathbf{n}^k) : \nabla \mathbf{n}^k$. In the absence of mass transfer the deviatoric part of the stress tensor can be written as $\tau = \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T \right)$. The flow variables and material properties of the fluid are computed with the use of the indicator function, $\varrho = \chi^1 \varrho^1 + \chi^2 \varrho^2$, $\mu = \chi^1 \mu^1 + \chi^2 \mu^2$. The system (4)–(5) is supplemented by an equation for the motion of the interface which can be described either in terms of the level-set function, cf. Osher & Sethian (1998)

$$\frac{\partial f^k}{\partial t} + \mathbf{u} \cdot \nabla f^k = \dot{m}^k \left(\frac{1}{\varrho^1} + \frac{1}{\varrho^2} - \frac{\varrho}{\varrho^1 \varrho^2} \right) |\nabla f^k|. \tag{6}$$

or the sharp-step indicator function, cf. Labourasse et al. (2007)

$$\frac{\partial \chi^k}{\partial t} + \mathbf{u} \cdot \nabla \chi^k = -\iint \dot{m}^k \left(\frac{1}{\varrho^1} + \frac{1}{\varrho^2} - \frac{\varrho}{\varrho^1 \varrho^2} \right) \delta\left(\mathbf{x} - \mathbf{x}_s\right) A \mathrm{d}\lambda \mathrm{d}\mu. \tag{7}$$

Although both approaches are mathematically equivalent the mass transfer terms in Eq. (7) and (6) have different forms. The further analysis will show that this difference is of large significance for the issues of statistical averaging or filtering of the governing equations and modelling approaches.

3. Group analysis of transport equations for multiphase flows

The purpose of the symmetry analysis based on the Lie group theory is to analyse, simplify and find solutions of partial differential equations cf. Ibragimov (1993). The method gives a deep insight into the underlying physical problems described by PDE. By "symmetry transformation" we understand such transformation of variables which does not change the functional form of the considered equation. As an example, consider the equation written in terms of independent variables $\mathbf{x}$, t and dependent variables $\mathbf{u}$

$$F(\mathbf{x}, t, \mathbf{u}, \underset{1}{\mathbf{u}}, \underset{2}{\mathbf{u}}, \ldots, \underset{q}{\mathbf{u}}) = 0 \tag{8}$$

where $\underset{k}{\mathbf{u}}$ denote the k-th derivatives of the function $\mathbf{u}$ with respect to any possible combination of independent variables and q is the highest order of derivative present in the above equation. Functional form of (8) is invariant under the transformation of variables $\mathbf{x} \rightarrow \mathbf{x}^*$, $t \rightarrow t^*$ $\mathbf{u} \rightarrow \mathbf{u}^*$ if the following equality also holds $F(\mathbf{x}^*, t^*, \mathbf{u}^*, \underset{1}{\mathbf{u}^*}, \underset{2}{\mathbf{u}^*}, \ldots, \underset{q}{\mathbf{u}^*}) = 0$. Using a strictly determined mathematical procedure the one-parameter Lie group method provides the infinitesimal transformations η_i, ξ_t, χ_{xi} and, further, by solving the equations

$$\frac{\mathrm{d}u_i^*}{\mathrm{d}\epsilon} = \eta_i, \quad \frac{\mathrm{d}t^*}{\mathrm{d}\epsilon} = \xi_t, \quad \frac{\mathrm{d}x_i^*}{\mathrm{d}\epsilon} = \xi_{xi} \tag{9}$$

with the boundary conditions $\epsilon = 0$, $\mathbf{u}^* = \mathbf{u}$, $t^* = t$, $\mathbf{x}^* = \mathbf{x}$ leads to the final form of the finite transformations $\mathbf{u}^*$, t^*, $\mathbf{x}^*$. Different, independent group transformations can be presented using a set of independent differential operators

$$X_k = \xi_t \frac{\partial}{\partial t} + \sum_{i=1}^{3} \xi_{xi} \frac{\partial}{\partial x_i}, + \sum_{j=1}^{J} \eta_j \frac{\partial}{\partial u_j} + \quad k = 1, \ldots, N \tag{10}$$

where N is the total number of independent group transformations admitted by the considered equation.

3.1. Level-set formulation
The symmetry analysis of the system of equations with additional assumptions of the inviscid fluid without the surface tension and in the absence of the gravity was performed using the Maple program with the GeM (General Module) software developed by A. Cheviakov. The following infinitesimal transformations were found for the one-fluid system of equations (4)–(5) and (6) .

$$X_1 = \frac{\partial}{\partial t}, \quad X_{2-4} = \frac{\partial}{\partial x_i}, \quad X_{5/6} = t\frac{\partial}{\partial t} + \sum_{i=1}^{3} \left(x_i \frac{\partial}{\partial x_i} \right) \tag{11}$$

$$X_{7-9} = x_i \frac{\partial}{\partial x_j} - x_j \frac{\partial}{\partial x_i} + u_i \frac{\partial}{\partial u_j} - u_j \frac{\partial}{\partial u_i} \quad i < j, \tag{12}$$

$$X_{10-12} = t\frac{\partial}{\partial x_i} + \frac{\partial}{\partial u_i}, \quad X_{13} = F_1(t)\frac{\partial}{\partial p}, \tag{13}$$

$$X_{14} = \mathcal{F}(f^1)\frac{\partial}{\partial f^1} \tag{14}$$

The infinitesimal transformations X_1 and X_{2-4} represent the fact that the system of equations is invariant under the time and space translations, respectively. $X_{5/6}$ is a scaling group of space and time. This symmetry is broken for the non-zero viscosity and/or surface tension. The rotational invariance is determined by X_{7-9} and the Galilean invariance by X_{10-12}. The infinitesimal transformation X_{13} stands for the pressure translation. The presence of gravity does not break any symmetries. Instead, the scaling and rotation groups are appropriately modified. The transformations $X_1 - X_{13}$ are identical to those of the Euler equations of the single phase. Hence, the presence of the interface between two fluids of different densities and a possible jump of variables that follows from the boundary conditions do not break any symmetries. This would mean that, after the averaging procedure, basically the same approaches could be used to model unclosed terms in the continuity and momentum equations for two-phase flows.

In the above system we additionally find the generalised scaling symmetry (14) for the level-set function. The new variables take a form:

$$f^{k*} = \mathcal{F}(f^k),\tag{15}$$

where $\mathcal{F}$ is an arbitrary monotonic function. It should be noted that the symmetries of the level-set equation have been first investigated in Oberlack et al. (2001) who found the generalised scaling for the level-set equation with mass transfer coupled with the Euler equations. Here we consider the system of conservation equations for the one-fluid variables and note that the Heaviside function $\chi = H(f^k - f_0^k)$ and, as a consequence, all one-fluid quantities are invariant under the generalised scaling symmetry of the f^k. Moreover, the presence of the surface tension in Eq. (5) does not break this symmetry. Hence, the considerations presented in Oberlack et al. (2001) concerning the consequences of the generalised scaling symmetry for the issues of averaging and modelling of interactions between turbulence and the flame will also apply to this case.

3.2. Indicator function formulation

Due to the presence of the integral form of the mass transfer term in Eq. (7) the group analysis of the conservation equations with this formula is more complicated. We recall that the quantity $\mathbf{x}_s(\lambda, \mu, t)$ denotes a point at the surface and, we argue that once the space variable $\mathbf{x}$ transforms to $\mathbf{x}^*$, $\mathbf{x}_s$ should transform in the same way. This leads to the following infinitesimals

$$X_1 = \frac{\partial}{\partial t}, \quad X_{2-4} = \frac{\partial}{\partial x_i} + \frac{\partial}{\partial x_{si}}, \quad X_{5/6} = t\frac{\partial}{\partial t} + \sum_{i=1}^{3}\left(x_i\frac{\partial}{\partial x_i} + x_{si}\frac{\partial}{\partial x_{si}}\right)\tag{16}$$

$$X_{7-9} = x_i\frac{\partial}{\partial x_j} - x_j\frac{\partial}{\partial x_i} + x_{si}\frac{\partial}{\partial x_{sj}} - x_{sj}\frac{\partial}{\partial x_{si}} + u_i\frac{\partial}{\partial u_j} - u_j\frac{\partial}{\partial u_i} \quad i < j,\tag{17}$$

$$X_{10-12} = t\frac{\partial}{\partial x_i} + t\frac{\partial}{\partial x_{si}} + \frac{\partial}{\partial u_i}, \quad X_{13} = F_1(t)\frac{\partial}{\partial p},\tag{18}$$

$$\tag{19}$$

In particular, with such a choice the space-time scaling invariance $X_{5/6}$ of Eq. (7) is satisfied. To see that this is true we first note that the delta distribution (as present in the RHS of Eq. (7)) transforms according to the following relation cf. Ibragimov (1993)

$$\delta^*(\mathbf{x}^*) = \left[\det\left(\frac{\partial x_i^*}{\partial x_j}\right)\right]_{\mathbf{x}=0}^{-1} \delta(\mathbf{x}).\tag{20}$$

For the scaling invariance $X_{5/6}$ with $t^* = a_1 t$, $\mathbf{x}^* = a_1\mathbf{x}$ and $\mathbf{x}_s^* = a_1\mathbf{x}_s$ the integral on the RHS of Eq. (7) transforms as

$$\iint \delta\left(\mathbf{x}^* - \mathbf{x}_s^*\right)\left|\frac{\partial \mathbf{x}_s^*}{\partial \lambda} \times \frac{\partial \mathbf{x}_s^*}{\partial \mu}\right|\mathrm{d}\lambda\mathrm{d}\mu = \iint \frac{1}{a_1^3}\delta\left(\mathbf{x} - \mathbf{x}_s\right)a_1^2\left|\frac{\partial \mathbf{x}_s}{\partial \lambda} \times \frac{\partial \mathbf{x}_s}{\partial \mu}\right|\mathrm{d}\lambda\mathrm{d}\mu.\tag{21}$$

As the LHS of Eq. (7) transforms in the same way we finally find that Eq. (7) is invariant under the scaling transformation $X_{5/6}$. Another important issue is that the generalised scaling invariance (14) is broken for the indicator function. The difference between symmetries for χ^k and f^k is crucial for the further modelling proposals, discussed in detail in Section 4.

4. Modelling of interface position

4.1. Averages
A direct solution of the system of conservation equations for multiphase flows is, at present, beyond our reach for most of the technically relevant cases. Hence, a reduced description, based on the averaged or spatially-filtered quantities is sought for. Due to the presence of the two-dimensional moving surface special attention should be given to the issues of averaging and interface tracking in the averaged field.

First, the classical ensemble-averaged quantity $\langle\phi\rangle(\mathbf{x}, t)$ is defined as a mean over infinitely many independent realisations. Another type of average was introduced by Pope (1988) for the quantities averaged at the instantaneous surface. The surface-average of a quantity $Q(\mathbf{x}, t)$ reads

$$\langle Q(\mathbf{x},t)\rangle_s = \frac{1}{\Sigma}\iint \langle Q(\mathbf{x},t)\delta(\mathbf{x}-\mathbf{x}_s)A(\lambda,\mu,t)\rangle \mathrm{d}\mu\mathrm{d}\lambda. \tag{22}$$

where Σ is the so-called surface-to-volume ratio and describes the ratio of the mean infinitesimal area $\langle\delta\mathcal{A}\rangle$ to the infinitesimal volume δV containing $\delta\mathcal{A}$. The term Σ is computed as the following integral

$$\Sigma(\mathbf{x},t) = \iint \langle\delta\left(\mathbf{x}-\mathbf{x}_s(\lambda,\mu,t)\right)A(\lambda,\mu,t)\rangle\mathrm{d}\lambda\mathrm{d}\mu. \tag{23}$$

4.2. Level-set equation.
A special attention should be given to the issue of the interface tracking in the averaged/filtered field. As far as the level-set equation (6) is concerned, it was shown in Oberlack et al. (2001), with the use of group theory, that classical ensemble-averaging or filtering of the level-set equation leads to a contradiction. This is related to the generalised scaling symmetry of the level-set equation (14) and may also be interpreted as follows, the f^k-field has the physical meaning only at $f^k = f_0$. Outside the front its values are arbitrary, what is reflected in the invariance under transformation $f^{k*} = \mathcal{F}(f^k)$. When the ensemble averaging at a certain point in space $\mathbf{x}$ is performed different values of f^k contribute to the mean $\langle f^k\rangle$. Hence, the level $\langle f^k\rangle = f_0$ does not, in general, specify the position of the mean interface. Instead, a well-posed methodology would be to find a single surface that would describe the most probable position of the interface and track this surface by the use of the level-set method.

As it was discussed by Oberlack et al. (2001) the fundamental form of the level-set equation is solely determined by its symmetries. The symmetries of the system restrict and determine the possible, general form of the turbulence model to be used. In particular, due to the presence of the generalised scaling symmetry the level-set equation cannot contain the diffusion term $\nabla^2 f^k$. Hence the gradient diffusion hypothesis cannot be used as a turbulence closure in the level-set equation. Although such attempts exist in the literature, they were proven to be mathematically incorrect, cf. Peters (2000). Moreover, from the same scaling symmetry it follows that only the derivatives of f^k (and not f^k explicitly) can be present in the level-set equation.

Indicator function.   In this work we concentrate on the indicator function approach. In contrary to the level-set function approach, the system (4–5) and (7) does not reflect the generalised scaling symmetry. This has important consequences. First, and the most important is that

the transport equation for the level-set function can be averaged. As a result of averaging or filtering of the indicator function one obtains a smoothed function α^k, cf. Labourasse et al. (2007) , $\alpha^k = \langle \chi^k \rangle$ which can be interpreted as the probability of finding the phase k at point **x**. The evolution of the function α is described by the averaged/filtered Eq. (7)

$$\frac{\partial \alpha^k}{\partial t} + \langle \mathbf{u} \cdot \nabla \chi^k \rangle = - \iint \langle \dot{m}^k \left(\frac{1}{\varrho^1} + \frac{1}{\varrho^2} - \frac{\varrho}{\varrho^1 \varrho^2} \right) \delta \left(\mathbf{x} - \mathbf{x}_s \right) A \rangle \mathrm{d}\lambda \mathrm{d}\mu. \tag{24}$$

The unclosed term on the LHS is connected with the contribution of the instantaneous velocity on the interface shape and the interface position. The influence of turbulence on the interfacial mass and heat transfer is contained in the RHS of the above equation. In most of the works the unclosed LHS term in the kinematic equation for interface tracking is simply replaced by $\langle \mathbf{u} \rangle \cdot \nabla \alpha^k$ (or by a term with Favre-averaged velocity). The first work, where the closure for analogous term in a LES context was proposed is Toutant et al. (2008). The scale similarity hypothesis was used there to model the unclosed term in the equation for the interface tracking. A possible closure in the RANS context has recently been discussed by Wacławczyk & Oberlack (2011). The considerations presented therein will be shortly outlined below. Substituting Eq. (2) into the LHS of Eq. (24) leads to

$$\frac{\partial \alpha^k}{\partial t} - \iint \langle \mathbf{u} \cdot \mathbf{n}^k \delta(\mathbf{x} - \mathbf{x}_s) A \rangle \mathrm{d}\lambda \mathrm{d}\mu = RHS \tag{25}$$

If we use the definition of the surface mean (22) in the above equation we obtain

$$\frac{\partial \alpha^k}{\partial t} - \langle \mathbf{u} \rangle \cdot \langle \mathbf{n}^k \rangle_s - \langle \mathbf{u}' \cdot \mathbf{n}^k \rangle_s \Sigma = -\frac{1}{\varrho^k} \langle \dot{m}^k \rangle_s \Sigma \tag{26}$$

where the velocity has been decomposed into the mean $\langle \mathbf{u} \rangle$ and the fluctuation part $\mathbf{u}'$. Wacławczyk & Oberlack (20011) proposed to replace the correlation $\langle \mathbf{u}' \cdot \mathbf{n}^k \rangle_s$ by the eddy diffusivity hypothesis which, after further transformations led to the following formula

$$\frac{\partial \alpha^k}{\partial t} + \langle \mathbf{u} \rangle \cdot \nabla \alpha^k = D_t \nabla \cdot (\nabla \alpha^k) + D_t \langle \mathbf{n}^k \rangle_s \cdot \nabla \Sigma - \frac{1}{\varrho^k} \langle \dot{m}^k \rangle_s \Sigma. \tag{27}$$

It was argued that the first term on the RHS of Eq. (27) causes diffusion, i.e. spreading of the region where $0 < \alpha < 1$ due to the action of turbulence. The effect of the second RHS term is likely to be opposite, it describes the stabilization of the surface due to the action of gravity and surface tension which, after the ensemble averaging, is observed as the shrinking of the surface layer.

In this work we aim to derive a possible form of the closure for the "antidiffusion" term from the symmetries of the considered system of equations. We follow here the work of Oberlack et al. (2001) where the same procedure was used to derive the level-set equation from its symmetries. We will assume that the model equation will have the following, general functional form

$$F(t, \mathbf{x}, \hat{\mathbf{x}}_s, \alpha, \mathbf{u}, \alpha_t, \underset{1}{\alpha}, \underset{2}{\alpha}) = 0 \tag{28}$$

where $\hat{\mathbf{x}}_s$ denotes a point at the isosurface $\alpha = 0.5$ where the probability of finding both phases is equal, α_t denotes the derivative of α with respect to time, $\underset{1}{\alpha}$ and $\underset{2}{\alpha}$ denote, respectively, all possible first and second order space derivatives. As formula (28) should be invariant under the symmetries (16–18) the following condition should simultaneously be satisfied

$$X_1 F = 0, X_{2-4} F = 0, \quad \ldots \quad X_{10-12} F = 0. \tag{29}$$

where the point $\mathbf{x}_s$ is replaced by the point $\hat{\mathbf{x}}_s$. From $X_1 F = 0$ it follows that $\partial F/\partial t = 0$, hence, formula (28) does not explicitly contain time. For the space translations group X_{2-4} we have the relation

$$\frac{\partial F}{\partial x_i} + \frac{\partial F}{\partial \hat{x}_{si}} = 0, \quad i = 1, \ldots, 3, \tag{30}$$

hence, F can possibly depend on a difference $\mathbf{x} - \mathbf{x}_s$, i.e. a distance from a given point $\mathbf{x}$ to an arbitrary point at the isosurface $\alpha = 0.5$. Employing additionally the Galilean invariance X_{10-12}, cf. Eq. (18) as it was done by Oberlack et al. (2001) provides the following form of the model

$$F(\alpha_t - \mathbf{u} \cdot \nabla \alpha, \mathbf{x} - \hat{\mathbf{x}}_s, \alpha, \underset{1}{\alpha}, \underset{2}{\alpha}) = 0, \tag{31}$$

In order to investigate the rotational invariance we derived the so-called second prolongation of X_{7-9}, denoted as $X_{7-9}^{(2)}$. Details of this procedure are explained e.g. in Oberlack et al. (2001). The condition $X_{7-9}^{(2)} F = 0$ leads to a partial differential equation which can be solved by the method of characteristics. This leads to the following possible form of F

$$F(\alpha_t - \mathbf{u} \cdot \nabla \alpha, \alpha, \left|\mathbf{x} - \hat{\mathbf{x}}_s\right|, (\mathbf{x} - \hat{\mathbf{x}}_s) \cdot \nabla \alpha, \left|\nabla \alpha\right|, \nabla^2 \alpha, \nabla \cdot \hat{\mathbf{n}}) = 0. \tag{32}$$

where $\hat{\mathbf{n}} = -\nabla \alpha/|\nabla \alpha|$ is a vector normal to the isosurfaces of α. In contrary to the level-set approach described by in Oberlack et al. (2001) the functional F can depend explicitly on α and $\nabla^2 \alpha$. Moreover, an additional variable $\hat{\mathbf{x}}_s$ was introduced which leads to the term $(\mathbf{x} - \hat{\mathbf{x}}_s) \cdot \nabla \alpha$ in Eq. (32). An analogous term was considered in the previous work of the authors, cf. Waclawczyk & Oberlack (2011) as a closure for the antidiffusion term in Eq. (27), therein $\hat{\mathbf{x}}_s$ was defined as a point at the isosurface $\alpha = 0.5$ closest to $\mathbf{x}$. Therein it was shown that the stationary solution of the 1D equation

$$\frac{\partial \alpha}{\partial t} + \langle u \rangle \frac{\partial \alpha}{\partial x} = D_t \frac{\partial^2 \alpha}{\partial x^2} + \Omega \left(x - \hat{x}_s\right) \frac{\partial \alpha}{\partial x}. \tag{33}$$

(where Ω is a model coefficient proportional to the reciprocal of the turbulence time scale) is a Gaussian error function

$$\alpha(x) = 0.5 \left[1 + \text{erf}\left(\sqrt{\sigma_s}(x - \hat{x}_s)/\sqrt{2}\right)\right] \tag{34}$$

where $\sigma_s = \sqrt{D_t/\Omega}$. Such solution is physically reasonable as it was observed experimentally in various flow regimes cf. Hong & Walker (2000), Freeze et al. (2003) and was also mentioned by Brocchini and Peregrine (2001b) as a profile observed experimentally in the splashing" flow regime. Brocchini and Peregrine (2001b) argued that the values $b = -3\sigma$ and $t = 3\sigma$ can be taken as the bottom and the top of the surface layer. Therein the shape of the surface and the surface layer thickness were quantified on the $L - q$ diagram. The authors also relate two quantities: the maximal "width" of the layer $t - b$ (distance from lowest troughs to the highest splashes) and the amount of water above the base of the layer d, to the length scale L of turbulent eddies $d = \int_b^t \alpha^k \mathrm{d}x = \mathcal{A}L(q)$, $t - b = \mathcal{B}L(q)$ where $\mathcal{A}$ and $\mathcal{B}$ are constants. The diagram from Brocchini and Peregrine (2001b), cf. Fig. 2, presents quantitative estimate of the constants $\mathcal{A}$ and $\mathcal{B}$ for different flow regimes.

Wacławczyk & Oberlack (2011) connected the model proposal with the experimental observations of Brocchini and Peregrine (2001b). The formulas for d and $t - b$, based on the 1D, stationary profile of α^k, cf. Eq. (34), with $b = -3\sigma$ and $t = 3\sigma$ taken as the limits of the surface layer, read

$$d = 3\sqrt{\frac{D_t}{\Omega}} = \mathcal{A}L(q), \quad t - b = 6\sqrt{\frac{D_t}{\Omega}} = \mathcal{B}L(q). \tag{35}$$
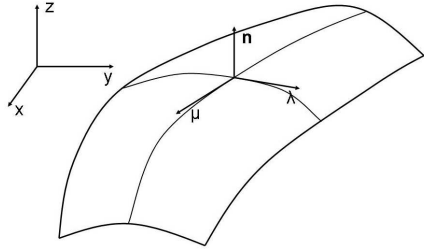
Figure 1. Coordinate system (x, y, z) and the local system (λ, μ) connected with the surface.
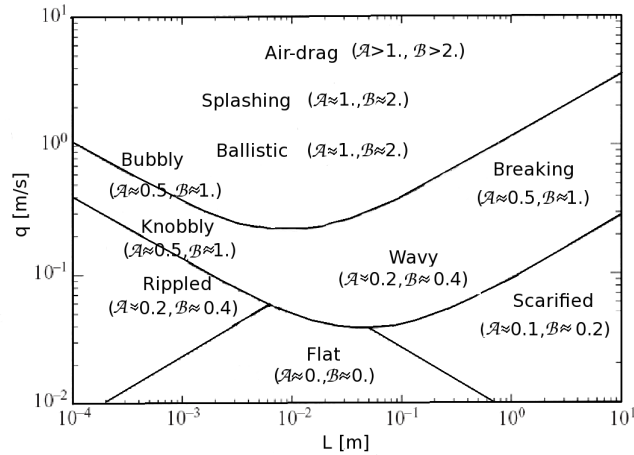

Figure 2. The L-q diagram from cf. Brocchini & Peregrine (2001a).

In the next step the values of modelling constants were estimated, based on Eqs (35). Assuming that $D_t = C_\mu k^2/(\epsilon S c_t)$ and $\Omega = C_\Omega \epsilon/k$ where k is the turbulent kinetic energy, ϵ is its mean dissipation rate, C_μ is the constant taken from the $k - \epsilon$ model and Sc_t is the turbulent Schmidt number, we obtain the value of the modelling constant C_Ω as a function of $\mathcal{A}$. This is an important point of the considerations, as it relates the newly derived, theoretical model with the constants in the experimental diagram from Brocchini and Peregrine (2001b) i.e. with the physics of the air-water flows.

In order to model dynamics of two-phase turbulent flows the model for the surface layer α should be coupled with the Navier-Stokes equation. The disadvantage of the proposal (33) is its non-conservative form. However, another closures for the antidiffusion term could be investigated, e.g. due to the explicit presence of α in Eq. (32) we can consider the form $\nabla(c\alpha(1 - \alpha)\hat{\mathbf{n}})$ where the coefficient c could be expressed as a product of the length scale L and Ω. Such closure would be analogous to those used in the equation for the progress variable in combustion, cf. Peters (2000). A stationary solution of the α equation with such a model will, probably, be close to the Gaussian error function. Hence, the values of modelling constants could also be estimated based on the data given in Brocchini and Peregrine (2001b).

A possible simple closure for the mass transfer term Eq. (27) was discussed by Wacławczyk & Oberlack (2011). Another forms of the model can also be proposed, possibly based on the models for the mass transfer term in combustion, cf. Peters (2000). Such closure could involve modelling of the surface-to-volume ratio Σ which can be done either by providing an algebraic relation or an additional model equation for this quantity. This task is left for further work.

5. Conclusions

In this work, the symmetry analysis of equations describing the flow of two incompressible, immiscible fluids in the one-fluid approach was performed. We considered two different descriptions for the interface tracking, namely, in terms of the the level-set function and the indicator function. The main difference between the two approaches was that the generalised scaling symmetry was found for the level-set function, while for the sharp-step indicator this scaling was broken. Moreover, due to the specific integral form of the mass transfer term in the indicator function approach an additional variable $\mathbf{x}_s$ was present in the symmetry

transformations. As it was shown by Oberlack et al. (2001), with the generalised scaling symmetry, the averaging of the level-set equation was not allowed. The lack of the generalised scaling symmetry for the χ function allows for some more freedom in choosing the modelling approach. The indicator equation can be averaged and an equation for the smoothed function α contained within the bounds $0 \leq \alpha \leq 1$ is obtained. In this work we put forward, based on the symmetry analysis, possible modelling closures for this equation. We have shown that values of modelling constant for the air-water flows can be estimated from the empirical observations given by Brocchini & Peregrine (2001b).

The perspective that follows from this theoretical study is to perform numerical RANS simulations of the turbulent two-phase flows in simple geometries using the proposed models. Another perspective is to consider turbulent two-phase flows with non-zero mass transfer between the phases and investigate possible closures for the mass transfer term in the equation for α.

References

[1] BROCCHINI M. & PEREGRINE D. H. 2001 The dynamics of strong turbulence at free surface. Part 1. Description. *J. Fluid Mech.* **449**, pp. 225–254.

[2] BROCCHINI M. & PEREGRINE D. H. 2001 The dynamics of strong turbulence at free surface. Part 2. Free-surface boundary conditions. *J. Fluid Mech.* **449**, 255–290.

[3] FREEZE B., SMOLENTSEV S., MORLEY N., & ABDOU M. 2003 Characterization of the effect of Froude number on surface waves and heat transfer in inclined turbulent open channel water flows *Int. J. Heat Mass Transf.* **46**, 3765–3775.

[4] HONG W.-L. & WALKER D. T. 2000 Reynolds-averaged equations for free-surface flows with application to high-Froude-number jet spreading. *J. Fluid Mech.* **417**, 183–209.

[5] IBRAGIMOV N. H. 1994 Handbook of Lie Group Analysis of Differential Equations. Vol.1: Symmetries, Exact Solutions and Conservation Laws. CRC Press, Boca Raton.

[6] JURIC D. & TRYGGVASON G. 1998 Computations of boiling flows. *Int. J. Multiphase Flows* **24**, 387–410.

[7] LABOURASSE E., LACANETTE D., TOUTANT A. LUBIN P., VINCENT S., LEBAIGUE O., CALTAGIRONE J.-P. & SAGAUT P. 2007 Towards large eddy simulation of isothermal two-phase flows: Governing equations and *a priori* tests. *Int. J. Multiphase Flow* **33**, 1-39.

[8] OBERLACK M., WENZEL H., PETERS N. 2001 On symmetries and averaging of the G-equation for premixed combustion *Comb. Theor. Model.* **5**, 363–383.

[9] OSHER S., SETHIAN J.A. 1988 Fronts propagating with curvature-dependent speed: algorithm based on Hamilton-Jacobi formulations *J. Comput. Phys.* **79**, 12–49.

[10] PETERS N. 2000 Turbulent combustion. Cambridge University Press, Cambridge.

[11] POPE S.B. 1988 The evolution of surfaces in turbulence. *Int. J. Engng Sci.* **26**, 445–469.

[12] PROSPERETTI A. & TRYGGVASON G. 2007 Computational methods for multiphase flows. Cambridge University Press, Cambridge.

[13] SAVELSBERG R. & VAN DE WATER W. 2009 Experiments on free-surface turbulence. *J. Fluid Mech.* **619**, 95–125.

[14] SMOLENTSEV S. & MIRAGHAIE R. 2005 Study of a free surface in open-channel water flows in the regime from "weak" to "strong" turbulence. *Int. J. Multiphase Flows* **31**, 921–939.

[15] TOUTANT A., LABOURASSE E., LEBAIGUE O. & SIMONIN O. 2008 DNS of the interaction between a deformable buoyant bubble and a spatially decaying turbulence. A priori test for LES two-phase flow modelling. *Comp. & Fluids* **37**, 877–886.

[16] WACŁAWCZYK M. & OBERLACK M. 2011 Closure proposals for the traking of turbulence-agitated gas-liquid interface in stratified flows. *Int. J. Multiphase Flows* in press