Memo

SIMCOFLOW basic concepts and multiphase flow solver algorithm

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Figure 1 Oil boom operated by two vessels in calm sea

Abstract

In SIMCOFLOW the predictiosn of oil spill, waves, sea current and atmospheric wind are all involved. A Cartesian cut cell method will be applied to solid interfaces such as external solid boundaries and internal solid boundaries.
Instead of the original plan to use cut-cells for the fluid-fluid boundaries, it is now suggested to use the multi fluid description for all internal fluid-fluid interfaces.
Numerically, all the continuous fluids will be discretized using a VOF-type method.
Detailed external boundary conditions, as well as the method to define the interfacial friction in volumes containing large scale interfaces has not been given at this stage.
Implementation of the method may use simplified closures as a first step.
The proposed method will be able to handle any number of continuous fluids sharing the same control volume.

Contents

1 Introduction

The present proposal is, when it comes to handling interfaces cutting a Cartesian grid, similar to the FAVOR method of Tony Hirt [1]. However, we will start with the formal volume averaging technique.

2 Single phase flow

2.1 Scalar transport

In order to familiarize ourselves with cut cell related issued we start with investigation the evolution of enthalpy in a cut-cell domain. We investigate the conservation of enthalpy h and where only conduction, convection and simple energy sources S_h are allowed to change the enthalpy field.

It is assumed that the relation between enthalpy and temperature is known. Currently we assume that $h = C_p T$. Using the generic formalism ([2], [3] and [4]), the conservation of enthalpy on a Cartesian grid cell is given by:

$$\frac{\partial}{\partial t}\int_{V_f}\rho_f h dV = -\int_{S_f}\rho_f h\mathbf{u}_f\cdot\mathbf{n}_f dS - \int_{A_w}\rho_f h\left(\mathbf{u}_f-\mathbf{u}_I\right)\cdot\mathbf{n}_{f,w}dS - \\ -\int_{S_f}\mathbf{q}\cdot\mathbf{n}_f dS - \int_{A_w}\mathbf{q}\cdot\mathbf{n}_f dS + \int_{V_f}\rho_f S_h dV \tag{2.1}$$

Here $\int_{S_f}\rho_f h\mathbf{u}_f\cdot\mathbf{n}_f dS$ express the convection of enthalpy across cell faces, $\int_{A_w}\rho_f h\left(\mathbf{u}_f-\mathbf{u}_I\right)\cdot\mathbf{n}_{f,w}dS$ is the mass transfer between wall and fluid, $\int_{S_f}\mathbf{q}\cdot\mathbf{n}_f dS$ is the conduction across the open to fluid conduction cell boundary, and $\int_{A_w}\mathbf{q}\cdot\mathbf{n}_f dS$ is the heat flow (by conduction) to the solid wall.

The discrete enthalpy equations becomes:

$$\Delta V\frac{\rho_f\alpha_f h-\left(\rho_f\alpha_f h\right)^0}{\Delta t} = -\sum_{\substack{live\\ cellfaces}}\left(\alpha_f\rho_f h\mathbf{u}_f\cdot\mathbf{n}_f\Delta A\right)_{cellface} \\ -\sum_{\substack{live\\ cellfaces}}\left(\alpha_f\mathbf{q}\cdot\mathbf{n}_f\Delta A\right)_{cellface} \tag{2.2}$$
$$-\sum_{wall}\left(\mathbf{q}\cdot\mathbf{n}_f\Delta A\right)_{wall} + \int_{V_f}\rho_f S_h dV$$

In eq. (2.2) the wall mass transfer term is absorbed into the generic source term. It is assumed that a mass conserving velocity field is existing and is available. We will now discuss the implications of equation (2.2) when it comes to handling of the cut cells.

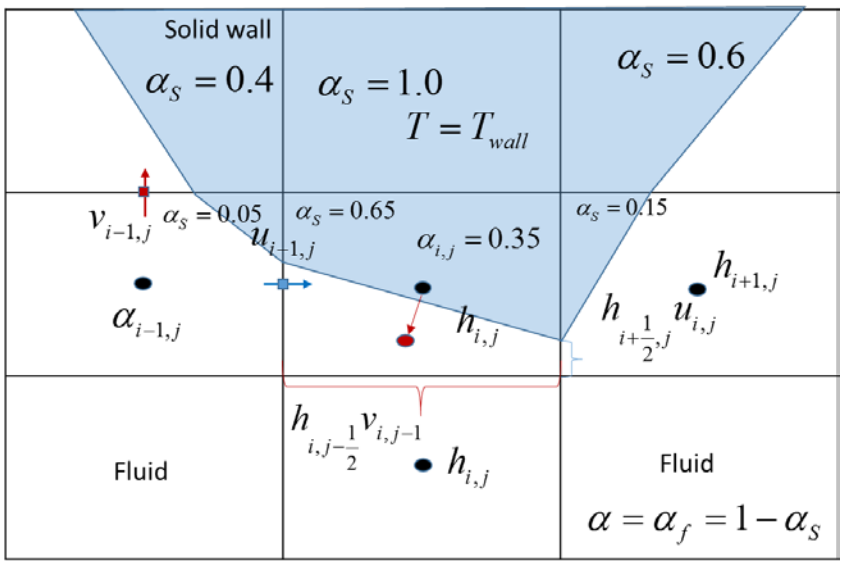

Figure 2 Cartesian cut cell domain with solid walls (blue) and enthalpy in cell i,j is $h_{i,j}$.

The transient term in equation (2.2) is allowing for a change in geometry (α_s is changing between time steps).

For the convective term $\left(\alpha_f \rho_f h \mathbf{u}_f \cdot \mathbf{n}_f \Delta A\right)_{cellface}$ it becomes important that we have good estimates of the fluid fraction at cell boundaries. At the interface between cell i,j and i,j+1 the solid fraction in the drawing is clearly 1.0. If we compute the cell interface fraction by simple averaging, we have a situation where energy will flow between the two cells by fluid convection. This is not acceptable. To avoid this we have to introduce the flowing rule for cell interface fractions:

Rule I.
A cell which is fully loaded by one phase will have that all the cell-face fractions of that phase is 1.0.

Rule II
A cell which have one, or more, but not all of the cell-faces dictated by Rule I will have a special method available to compute cell fractions for the remaining cell faces.

The value of the density and enthalpy at the cell-face [$\left(\alpha_f \rho_f h \mathbf{u}_f \cdot \mathbf{n}_f \Delta A\right)_{cellface}$] is interpolated using the preferred interpolation method. We note that the flux $\left(\alpha_f \rho_f h \mathbf{u}_f \cdot \mathbf{n}_f \Delta A\right)_{cellface}$ is to be understood as the time averaged flux over the time step.

Wall treatment:
The wall flux $\left(\alpha_f \mathbf{q} \cdot \mathbf{n}_f \Delta A\right)_{wall}$ is the generic transfer of heat between the fluid in the cell and the wall. The flux is generally treated as:

$$\left(\mathbf{q} \cdot \mathbf{n}_f \Delta A\right)_{wall} = -\lambda \frac{\partial T}{\partial n} \Delta A_{wall} = -\lambda \frac{T_{wall,i,j} - T_{i,j}}{\delta_n} \Delta A_{wall} \qquad (2.3)$$

In equation (2.3) ΔA_{wall} is the true surface area of the wall inside the cell.
Equation (2.3) can be replaced by wall functions in the case of turbulent flows.

Here ΔA_{wall} is the actual area (see Figure 3) (Rule III) of the wall cutting through the cell and δ_n is the distance between the wall and the mass centre of the cell (Rule IV).

Rule III.
The heat transfer area ΔA_{wall} of a cell cut by a wall is computed by a specific method.

Rule IV.
The distance between a wall and the cell centre inside the fluid part of the cell is computed by a specific method. The first version of the method is based on computation of the mass centre in the fluid part of the cell and computation of the normal distance δ_n between this point and the cell-face.

The fluid non-wall conduction fluxes $\left(\alpha_f \mathbf{q}\cdot\mathbf{n}_f \Delta A\right)_{cellface} = -\left(\alpha_f \lambda \nabla T\cdot\mathbf{n}_f \Delta A\right)_{cellface}$ can be treated in the same manner as for the convective fluxes. An example for the x-direction flux at the positive x-cell-face is:

$$\left(\alpha_f q_x \cdot n_{f,x}\Delta A\right)_{cellface}^{x^+} = -\alpha_f \Delta A \lambda^{x^+} \frac{T_{i+i,j} - T_{i,j}}{\Delta x} \tag{2.4}$$

The computations and application of the cell interface fractions α_f are identical for conduction and convection. However, we note that due to Rule IV, the location point for the temperature and enthalpy is moved from the cell centre to a new position (red circle in Figure 2). The movement of the point will impact the conductive fluxes across the neighbouring cell faces. It is therefor suggested that the offset of points in the cut cells are accounted for in the conductive flux calculations.

Rule V.
The offset of cell centre points for a fluid in a cut cell is used to correct the diffusive exchange fluxes with neighbouring fluid cells.

2.2 Single phase mass equations

According to the formalism ([2], [3] and [4]), the transport equation for the mass is:

$$\frac{\partial}{\partial t}\int_{V_f} \rho_f dV = -\int_{S_f} \rho_f \mathbf{u}_f \cdot \mathbf{n}_f dS - \int_{A_w} \rho_k \left(\mathbf{u}_f - \mathbf{u}_I\right)\cdot \mathbf{n}_{f,w} dS \tag{2.5}$$

Here areas, volumes and vectors and explained in Figure 3. When we integrate over the fluid volume V_f we find the intrinsic average of the density. Using α as fluid fraction of the control volume the fluid mass per volume in the complete control volume is $\hat{\rho} = \alpha\rho_f = \left(1-\alpha_S\right)\rho_f$. Here α_S is the solids fraction (solid wall fraction) and $\alpha = 1-\alpha_S$, and where $\rho(p,T)$ is the intrinsic density of the fluid phase.

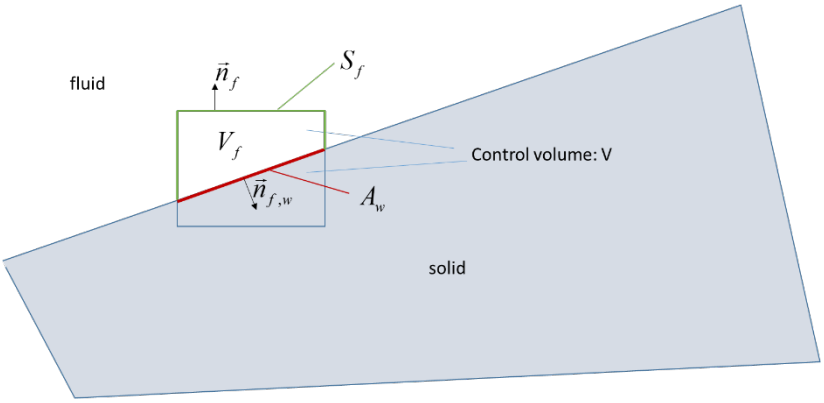

Figure 3 Control volume cut by solid

The mass equation can for a control volume ΔV be

$$\frac{\partial}{\partial t}\left(\hat{\rho}\right)+\nabla\cdot\left(\hat{\rho}\mathbf{u}\right)=-\rho\left(\mathbf{u}-\mathbf{u}_I\right)\cdot\mathbf{n}_{f,w}\frac{A_w}{\Delta V} \tag{2.6}$$

Note that the term $\left(\mathbf{u}-\mathbf{u}_I\right)\cdot\mathbf{n}_{f,w}A_w$ may represent both a flow (mass source) coming through the wall, or any combination with a moving interface with velocity $\mathbf{u}_I$.

Here the effective (extensive) density $\hat{\rho}$ is represented by:

$$\hat{\rho}=\alpha\rho(p,T)=\left(1-\alpha_S\right)\rho(p,T) \tag{2.7}$$

Here α_S is the solids fraction (solid wall fraction) and $\alpha=1-\alpha_S$, and where $\rho(p,T)$ is the intrinsic density of the fluid phase.

If the solid (walls, external domain) is stationary the mass equation will simplify to:

$$\alpha\frac{\partial\rho}{\partial t}+\nabla\cdot\left(\alpha\rho u\right)=S \tag{2.8}$$

In Figure 4 we see a typical staggered grid layout in 2D. The fluid fractions at the cell face where the $u_{i,j}=U_{x;i,j}$ velocity is located is denoted $\alpha_{u;i,j}$. Similarly for the vertical velocity component $v_{i,j}=U_{y;i,j}$, the fluid volume fraction on this cell face is $\alpha_{v;i,j}$.

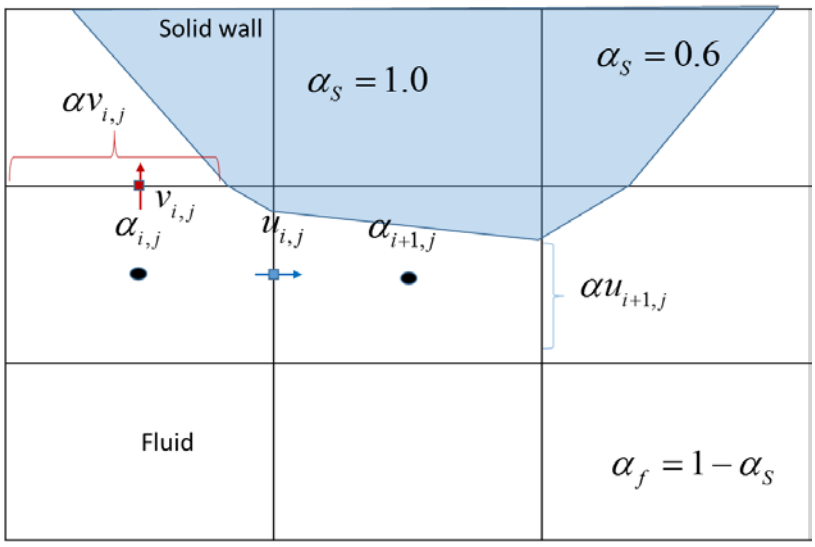

Figure 4 Staggered grid layout in 2D

The discrete mass equation can now be represented by:

$$\alpha_{i,j}\Delta V_{i,j}\frac{\rho_{i,j}-\rho^{0}{}_{i,j}}{\partial t}+A_x\left(\alpha_u\right)_{i,j}\rho_{i+\frac{1}{2},j}u_{i,j}-A_x\left(\alpha_u\right)_{i-1,j}\rho_{i-\frac{1}{2},j}u_{i-1,j}$$
$$+A_y\left(\alpha_v\right)_{i,j}\rho_{i,j+\frac{1}{2}}v_{i,j}-A_y\left(\alpha_v\right)_{i-1,j}\rho_{i,j-\frac{1}{2}}v_{i-1,j}=S \qquad (2.9)$$

The quantities $\alpha_{u;i,j}$ and $\alpha_{v;i,j}$ are computed from the volume fractions. The simplest and first approach is:

$$\alpha_{u;i,j}=\begin{cases}0 & ;\ \min(\alpha_{i,j},\alpha_{i+1,j})=0\\ \dfrac{\alpha_{i,j}+\alpha_{i+1,j}}{2} & ;\ \min(\alpha_{i,j},\alpha_{i+1,j})\neq 0\end{cases} \qquad (2.10)$$

$$\alpha_{v;i,j}=\begin{cases}0 & ;\ \min(\alpha_{i,j},\alpha_{i,j+1})=0\\ \dfrac{\alpha_{i,j}+\alpha_{i,j+1}}{2} & ;\ \min(\alpha_{i,j},\alpha_{i,j+1})\neq 0\end{cases} \qquad (2.11)$$

Later it will come clear that this may have to be refined. In the equations (2.10) and (2.11) it may be necessary to introduce a more complex averaging that should give $\alpha_{u;i,j}$ closer to $\min(\alpha_{i,j},\alpha_{i+1,j})$, when $\min(\alpha_{i,j},\alpha_{i+1,j})$ is small and closer to the larger value $\max(\alpha_{i,j},\alpha_{i+1,j})$ is large.

2.3 Single phase momentum equations

Similarly, the momentum equation reads:

$$\frac{\partial}{\partial t}\int_{V_f}\rho\mathbf{u}dV=\int_{V_f}\rho\mathbf{g}dV$$
$$+\int_{S_f}\left(-p\mathbf{I}+\boldsymbol{\tau}\right)\cdot\mathbf{n}_f dS+\int_{A_w}\left(-p\mathbf{I}+\boldsymbol{\tau}\right)\cdot\mathbf{n}_{f,w}dS \qquad (2.12)$$
$$-\int_{S_f}\rho\mathbf{u}\mathbf{u}\cdot\mathbf{n}_f dS-\int_{A_w}\rho\mathbf{u}\left(\mathbf{u}-\mathbf{u}_I\right)\cdot\mathbf{n}_{f,w}dS$$

The volume integrals are first evaluated, $\frac{\partial}{\partial t}\int_{V_f}\rho\mathbf{u}dV=\Delta V\frac{\partial}{\partial t}\hat{\rho}\mathbf{u}$, and $\int_{V_f}\rho\mathbf{g}dV=\Delta V\hat{\rho}\mathbf{g}$. Here the velocity and density are the volume averages, where $\hat{\rho}=\alpha\rho$ and $\mathbf{u}$ is the volume averaged velocity inside the fluid volume. Next we do the surface integrals:

$$\Delta V\frac{\partial}{\partial t}\rho\mathbf{u}=\Delta V\hat{\rho}\mathbf{g}$$
$$+\sum_{\text{all cell faces Sf}}\left(-p\mathbf{I}+\boldsymbol{\tau}\right)\cdot\mathbf{n}_{Sf}\alpha_{Sf}\Delta A+\left(-p\mathbf{I}+\boldsymbol{\tau}\right)\cdot\mathbf{n}_{f,w}A_w \qquad (2.13)$$
$$-\sum_{\text{all cell faces Sf}}\rho\mathbf{u}\mathbf{u}\cdot\mathbf{n}_{Sf}\alpha_{Sf}\Delta A-\int_{A_w}\rho\mathbf{u}\left(\mathbf{u}-\mathbf{u}_I\right)\cdot\mathbf{n}_{f,w}dS$$

From equation (2.13) we see several interesting consequences:

i) Pressures in term $\sum_{\text{all cell faces Sf}}\left(-p\mathbf{I}+\boldsymbol{\tau}\right)\cdot\mathbf{n}_{Sf}\alpha_{Sf}\Delta A$ are the surface averages, which can be approximated closely by the volume averages.

ii) In term $\sum_{\text{all cell faces Sf}}\left(-p\mathbf{I}+\boldsymbol{\tau}\right)\cdot\mathbf{n}_{Sf}\alpha_{Sf}\Delta A$, some cell faces have a zero fluid fraction ($\alpha_{Sf}=0$). The contribution from these cell faces will disappear for the pressure and the shear stress.

iii) The wall effect is reintroduced by the term $\left(-p\mathbf{I}+\boldsymbol{\tau}\right)\cdot\mathbf{n}_{f,w}A_w$. The stress contribution will have to be computed based on the surrounding velocities and volume fractions and linearized (to be evaluated at a later stage). In addition the pressure contribution here involves only the pressure internally in the fluid in the cell, not a pressure behind the interface. As a consequence of ii) and iii) there will be no fluid pressure (and no need for it) in a cell which is fully solid.

iv) The transfer term $\int_{A_w}\rho\mathbf{u}\left(\mathbf{u}-\mathbf{u}_I\right)\cdot\mathbf{n}_{f,w}dS$ will only have values for the case where mass is entering/leaving through the wall face. In the case of an inert wall surface, moving through space, we will have zero contribution from this term. This applies to typical fluid-structure interaction cases. The only term that need special attention, assuming implicit treatment of pressure and stresses, is the advection terms. The advection term is generally represented by:

$$\frac{\partial}{\partial t}\left(\hat{\rho}\mathbf{u}\right)+\nabla\cdot\left(\hat{\rho}\mathbf{u}\mathbf{u}\right)\equiv\frac{d}{dt}\left(\hat{\rho}\mathbf{u}\right)+\hat{\rho}\mathbf{u}\left(\nabla\cdot\mathbf{u}\right)$$

Where $\frac{d}{dt}(\hat{\rho}\mathbf{u})$ is the Lagrangian time derivative and $\hat{\rho}\mathbf{u}(\nabla\cdot\mathbf{u})$ is an Eulerian term which express the effect of expansion or compression of the flow along a streamline.

If we wish to use the Lagrangian version of the momentum equation, it will read like:

$$\Delta V\frac{d}{dt}\hat{\rho}\mathbf{u} = \Delta V\hat{\rho}\mathbf{g} - \Delta V\hat{\rho}\mathbf{u}(\nabla\cdot\mathbf{u})$$
$$+\sum_{\text{all cell faces Sf}}(-p\mathbf{I}+\boldsymbol{\tau})\cdot\mathbf{n}_{Sf}\alpha_{Sf}\Delta A+(-p\mathbf{I}+\boldsymbol{\tau})\cdot\mathbf{n}_{f,w}A_w \qquad (2.14)$$
$$-\sum_{\text{all cell faces Sf}}\rho\mathbf{u}\mathbf{u}\cdot\mathbf{n}_{Sf}\alpha_{Sf}\Delta A-\int_{A_w}\rho\mathbf{u}(\mathbf{u}-\mathbf{u}_I)\cdot\mathbf{n}_{f,w}dS$$

2.3.1 Treatment of wall boundary conditions

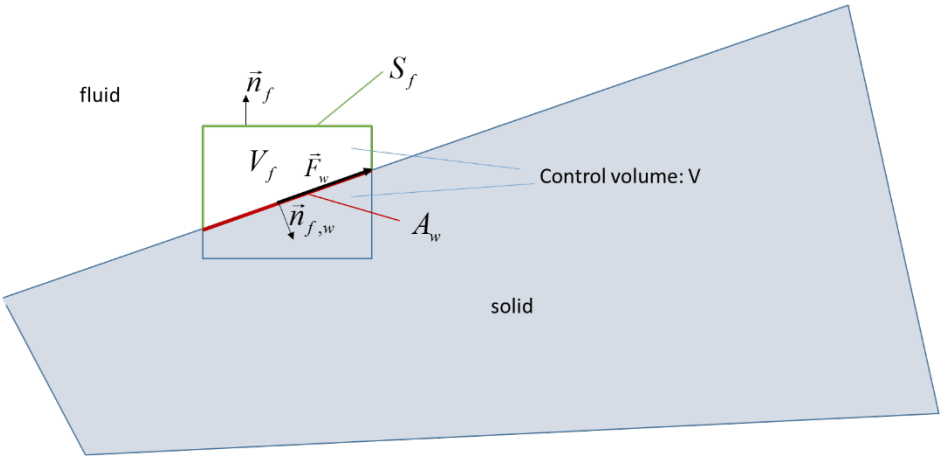

Figure 5 The force $\vec{F}_w$, acting on the fluid from the wall.

In Figure 5 we see the wall shear force $\vec{F}_w$ acting on the fluid in the volume V_f . The shear force acts in the direction of the fluid velocity , tangential to the wall. The wall may have any velocity $\vec{U}_w$. First we need the relative velocity between the fluid and the wall, tangential to the wall. The relative velocity between fluid and wall is represented by:

$$\Delta\mathbf{U} = \mathbf{u} - \mathbf{U}_\mathbf{w} \qquad (2.15)$$

The relative velocity normal to the wall is:

$$\Delta\mathbf{U}_n = \left[(\mathbf{u}-\mathbf{U}_\mathbf{w})\cdot\mathbf{n}\right]\mathbf{n} \qquad (2.16)$$

The relative velocity tangential to the wall is then:

$$\Delta\mathbf{U}_t = \Delta\mathbf{U} - \Delta\mathbf{U}_n = \Delta\mathbf{U} - \left[\Delta\mathbf{U}\cdot\mathbf{n}\right]\mathbf{n} \qquad (2.17)$$

The unit normal vector for the relative flow, parallel to the wall is now:

$$\mathbf{n_t} = \frac{\Delta \mathbf{U}_t}{\left|\Delta \mathbf{U}_t\right|} = \frac{\Delta \mathbf{U} - \left[\Delta \mathbf{U} \cdot \mathbf{n}\right]\mathbf{n}}{\left|\Delta \mathbf{U} - \left[\Delta \mathbf{U} \cdot \mathbf{n}\right]\mathbf{n}\right|} \tag{2.18}$$

The force acting on the fluid in a wall cell is now given by:

$$\vec{F}_w = -\left|\tau_w\right| A_w \mathbf{n_t} \tag{2.19}$$

The wall force decomposed into each direction follows:

$$\begin{aligned} F_{w,x} &= -\left|\tau_w\right| A_w \mathbf{n_t} \cdot \mathbf{e_x} \\ F_{w,y} &= -\left|\tau_w\right| A_w \mathbf{n_t} \cdot \mathbf{e}_y \\ F_{w,z} &= -\left|\tau_w\right| A_w \mathbf{n_t} \cdot \mathbf{e}_z \end{aligned} \tag{2.20}$$

For the stability of a numerical implementation without having to excessively limit the time step size, it is critical to linearize the wall stress in velocity for use in an implicit scheme for the viscous terms. This is done in the following (example for Cartesian x-direction). The wall stress is Taylor-expanded in the required direction, here x-direction:

$$\left|\tau_w\right| \approx \left|\tau_w\right|^0 + \frac{\partial\left|\tau_w\right|}{\partial\left|\Delta \mathbf{U}_t\right|} \frac{\partial\left|\Delta \mathbf{U}_t\right|}{\partial \Delta U_{t,x}} \left(\Delta U_{t,x} - \Delta U_{t,x}^0\right) \tag{2.21}$$

We use the wall function concept, stating that:

$$\left|\Delta \mathbf{U}_t(y)\right| = u_\tau u^+(y^+) \tag{2.22}$$

This is equivalent with:

$$\left|\tau_w\right| = \rho u_\tau^{\,2} = \rho \left(\frac{\left|\Delta \mathbf{U}_t(y)\right|}{u^+(y^+)} \right)^2 \tag{2.23}$$

Using (2.23) in (2.21) we have:

$$\left|\tau_w\right| \approx \left|\tau_w\right|^0 + \left\{ \frac{2\left|\tau_w\right|}{\left|\Delta \mathbf{U}_t\right|} \frac{\Delta U_{t,x}}{\left|\Delta \mathbf{U}_t\right|} \right\}^0 \left(\Delta U_{t,x} - \Delta U_{t,x}^0\right) \tag{2.24}$$

For the stress in the x-direction the force on the fluid becomes:

$$|\tau_w| \approx \underbrace{|\tau_w|^0 - \left\{\frac{2|\tau_w|}{|\Delta\mathbf{U}_t|}\frac{\Delta U_{t,x}}{|\Delta\mathbf{U}_t|}\right\}^0 \Delta U_{t,x}^0}_{\tau_A} + \underbrace{\left\{\frac{2|\tau_w|}{|\Delta\mathbf{U}_t|}\frac{\Delta U_{t,x}}{|\Delta\mathbf{U}_t|}\right\}^0}_{\chi}\left(u_x - U_{w,x}\right) \tag{2.25}$$

$$= \tau_A + \chi\left(u_x - U_{w,x}\right)$$

The x-direction force is now:

$$F_{w,x} = -\tau_{Aw} n_{t,x} - \chi_w n_{t,x}\left(u_x - U_{w,x}\right) \tag{2.26}$$

Test: Flow parallel to wall. N_y=1, N_{tx}=1, U_w=0.0 m/s:

$$|\tau_w| \approx -\underbrace{|\tau_w|^0}_{\tau_A} + \underbrace{\left\{\frac{2|\tau_w|}{|\Delta\mathbf{U}_t|}\right\}^0}_{\chi} u_x \tag{2.27}$$

Resulting force is:

$$F_{w,x} = |\tau_w|^0 - \frac{2|\tau_w|^0}{|\Delta\mathbf{U}_t|^0}u_x \tag{2.28}$$

This result is as expected. Due to properties of equation (2.23) the linearization factor becomes $\frac{2|\tau_w|^0}{|\Delta\mathbf{U}_t|^0}$ and not $\frac{|\tau_w|^0}{|\Delta\mathbf{U}_t|^0}$!!

3 Numerical implementation (single phase)

The implementation can follow the general method for doing multiphase flows. However, for simplicity we start with single phase compressible flows.

The semi discretized momentum equation for momentum in Cartesian direction i reads:

$$\Delta V\hat{\rho}^0\frac{U_i - U_i^0}{\Delta t} + \sum_{\substack{\text{all directions j containing}\\ \text{active flow cell face Ff}}}\left\{\left(\rho U_j^0 n_j\right)\alpha_{Ff}\Delta A_j U_i^0\right\}_{Ff}$$

$$= \sum_{\substack{\text{all directions j containing}\\ \text{active flow cell face Ff}}}\left\{\left(-p\delta_{ij} + \tau_{ij}\right)n_j\alpha_{Ff}\Delta A\right\}_{Ff} - \widehat{p}A_w n_{f,w,i} - |\tau_w|A_w n_{t,i} + \Delta V G_i^0 \tag{3.1}$$

$$-\left(\rho U_j^0 n_{f,w,j}\right)\left(U_i - U_{w,i}\right)^0 A_w$$

Equation (5.3) has several important properties:

1) Convection term (here fully explicit), can be based on any interpolation method. Important is the cell-face fluid fractions (α_{Ff}). As we use staggered grid, a first estimate is to use the fluid fractions which is valid for the given pressure cell. If the boundary is moving we need to handle the geometry

at the new time step. Then we always use the new geometry α_{Ff}, even in the explicit terms. The accuracy for moving outer boundaries is for now limited to CFL below 1. This may however be extended, using the semi-Lagrangian approach.

2) Here n_j is the j component of the unit vector pointing out of a cell-face.
3) $n_{f,w,i}$ is the i-component of the normal vector, at a wall, pointing out of the fluid.
4) The pressure $\widehat{p}A_w n_{f,w,i}$ is a surface averaged value inside a cell. A first estimate will, for the case of flow in Cartesian x-direction (i=1), will be that $\widehat{p} = \frac{p_{i+1} + p_i}{2}$; i= x direction cell index .
5) The wall stress is represented by eq. (2.23) and linearized (x-direction example) by eq. (2.26).
6) The last term can readily be extended to handle mass transfer. Now, it only includes blowing and suction ($U_i \neq U_{w,i}$, at the wall face). We note that if the geometry is moving we still have $U_i = U_{w,i}$, giving a zero contribution here. The term must be handles explicitly, as it does not depend on the unknown velocity, but only through the formalistic write-up. The treatment here will be fully consistent with the explicit treatment of the convection terms.
7) G_i^0 represents body forces and other explicit momentum sources, taken at the previous time step.
8) We note that in the transient term, and in the stress terms, we use the fluid fractions and density at the old time step.
9) Note that in $\hat{\rho}^0$ we have the product of fluid fraction (due to cut cells) and fluid density, using definition $\hat{\rho} = \alpha_{Ff} \cdot \rho(p,T)$. As we use the current (new) fluid fraction, we have $\hat{\rho}^0 = \alpha_{Ff} \cdot \rho(p^0, T^0)$.

We next do the first fractional step for the momentum equation, solving for the temporary velocity U_i^*:

$$\Delta V \hat{\rho}^0 \frac{U_i^* - U_i^0}{\Delta t} + \sum_{\substack{\text{all directions j containing} \\ \text{active flow cell face Ff}}} \left\{ \left(\rho U_j^0 n_j \right) \alpha_{Ff} \Delta A_j U_i^0 \right\}_{Ff}$$

$$= \sum_{\substack{\text{all directions j containing} \\ \text{active flow cell face Ff}}} \left\{ \left(-p^0 \delta_{ij} + \tau_{ij}(\mathbf{U}^*) \right) n_j \alpha_{Ff} \Delta A \right\}_{Ff} - \widehat{p}^0 A_w n_{f,w,i} - \left| \tau_w(\mathbf{U}^*) \right| A_w n_{t,i} + \Delta V G_i^0 \qquad (3.2)$$

$$- \left(\rho U_j^0 n_{f,w,j} \right) \left(U_i - U_{w,i} \right)^0 A_w$$

In this first step we solved implicitly for the viscous stresses (turbulent stresses are straight forward, to be included later). In next step, by subtracting equation (5.5) from equation (5.3), we obtain:

$$\Delta V \hat{\rho}^0 \frac{U_i'}{\Delta t} = - \sum_{\substack{\text{all directions j containing} \\ \text{active flow cell face Ff}}} \left\{ p' \delta_{ij} n_j \alpha_{Ff} \Delta A \right\}_{Ff} - \widehat{p}' A_w n_{f,w,i}$$

$$- \left(\left| \tau_w \right| - \left| \tau_w(\mathbf{U}^*) \right| \right) A_w n_{t,i} + \sum_{\substack{\text{all directions j containing} \\ \text{active flow cell face Ff}}} \left\{ \left(\tau_{ij} \left(\mathbf{U}^* + \mathbf{U}' \right) - \tau_{ij}(\mathbf{U}^*) \right) n_j \alpha_{Ff} \Delta A \right\}_{Ff} \qquad (3.3)$$

$$\approx - \sum_{\substack{\text{all directions j containing} \\ \text{active flow cell face Ff}}} \left\{ p' \delta_{ij} n_j \alpha_{Ff} \Delta A \right\}_{Ff} - \widehat{p}' A_w n_{f,w,i}$$

In equation (3.3) we have an equation for the implicit correction of the velocity. It is here assumed that errors in the stresses, due to fractional step are negligible. If this is proven to be an issue we may have to iterate on the solution. However, iterations are last resort.
We note from equation (3.3) that if the fluid cell face fraction is zero, the contribution from $\left\{p'\delta_{ij}n_j\alpha_{Ff}\Delta A\right\}_{Ff}$ is zero, while the term $\widehat{p}'A_w n_{f,w,i}$ may still contribute.

3.1 Obtaining a pressure equation

The pressure equation will be based on the mass equation. Multiphase flows is for now not included.

$$\frac{\hat{\rho}-\hat{\rho}^0}{\Delta t}+\nabla\left(\hat{\rho}^0\mathbf{u}\right)=S-\rho\left(\mathbf{u}-\mathbf{u}_I\right)\mathbf{n}_{f,w}\frac{A_w}{\Delta V}=S^* \tag{3.4}$$

Here the effective densities are represented by:

$$\hat{\rho}=\alpha_{Ff}\cdot\rho(p,T) \tag{3.5}$$

, where α_{Ff} always is the new geometry (represented by fluid fractions)

$$\Delta V\alpha_{Ff}\frac{\rho-\rho^0}{\Delta t}+\sum_{\substack{\text{all directions j containing}\\ \text{active flow cell face Ff}}}\left\{\left(\rho^0\left(U_j^*-U_j'\right)n_j\right)\alpha_{Ff}\Delta A_j\right\}_{Ff}=S^* \tag{3.6}$$

The fluid density may be linearized in pressure and temperature. Accounting only for the pressure, and inserting the velocity correction from equation (3.3), we have:

$$\begin{aligned}&\Delta V\alpha_{Ff}\left.\frac{\partial\rho}{\partial p}\right|_{p^0,T^0}\frac{p-p^0}{\Delta t}-\sum_{\substack{\text{all directions j containing}\\ \text{active flow cell face Ff}}}\left\{\left(\rho^0U_j'n_j\right)\alpha_{Ff}\Delta A_j\right\}_{Ff}\\&=S^*-\sum_{\substack{\text{all directions j containing}\\ \text{active flow cell face Ff}}}\left\{\left(\rho^0U_j^*n_j\right)\alpha_{Ff}\Delta A_j\right\}_{Ff}\end{aligned} \tag{3.7}$$

And where

$$U_j'=-\frac{\Delta t}{\Delta V\hat{\rho}^0}\sum_{\substack{\text{all directions j containing}\\ \text{active flow cell face Ff}}}\left\{p'\delta_{ij}n_i\alpha_{Ff}\Delta A\right\}_{Ff}-\frac{\Delta t}{\Delta V\hat{\rho}^0}\widehat{p}'A_w n_{f,w,j} \tag{3.8}$$

We take a two dimensional example, using equations (3.7) and (3.8), and having a wall at the upper boundary, as illustrated in pressure cell (i+1,j) in Figure 4. The pressure equation in a cell (i,j) with this wall configuration is represented by:

$$\begin{aligned}&\Delta V\alpha_{Ff}\left.\frac{\partial\rho}{\partial p}\right|_{p^0,T^0}\frac{p'_{i,j}-\cancel{p'^0_{i,j}}}{\Delta t}\\&-\left\{\rho^0U_x'\alpha_{Ff}\Delta A_x\right\}^{x+}+\left\{\rho^0U_x'\alpha_{Ff}\Delta A_x\right\}^{x-}-\left\{\rho^0U_y'\alpha_{Ff}\Delta A_y\right\}^{y+}-\left\{\rho^0U_y'\alpha_{Ff}\Delta A_y\right\}^{y-}\\&=S^*-\left\{\rho^0U_x^*\alpha_{Ff}\Delta A_x\right\}^{x+}+\left\{\rho^0U_x^*\alpha_{Ff}\Delta A_x\right\}^{x-}-\left\{\rho^0U_y^*\alpha_{Ff}\Delta A_y\right\}^{y+}-\left\{\rho^0U_y^*\alpha_{Ff}\Delta A_y\right\}^{y-}\end{aligned} \tag{3.9}$$

Here we have that:

$$U_x^{'+} = -\left\{\frac{\Delta t}{\Delta V \rho^0 \alpha_{Ff}}\right\}_{i+\frac{1}{2},j}\left[\left\{p'\alpha_{Ff}\Delta A_x\right\}_{i+1,j} - \left\{p'\alpha_{Ff}\Delta A_x\right\}_{i,j} + \frac{p'_{i,j}+p'_{i+1,j}}{2}A_{w_{i+\frac{1}{2},j}}n_{f,w,x;i+\frac{1}{2},j}\right]$$

$$U_x^{'-} = -\left\{\frac{\Delta t}{\Delta V \rho^0 \alpha_{Ff}}\right\}_{i-\frac{1}{2},j}\left[\left\{p'\alpha_{Ff}\Delta A_x\right\}_{i,j} - \left\{p'\alpha_{Ff}\Delta A_x\right\}_{i-1,j} + \frac{p'_{i-1,j}+p'_{i,j}}{2}A_{w_{i-\frac{1}{2},j}}n_{f,w,x;i-\frac{1}{2},j}\right] \qquad (3.10)$$

$$U_y^{'+} = -\left\{\frac{\Delta t}{\Delta V \rho^0 \alpha_{Ff}}\right\}_{i,j+\frac{1}{2}}\left[\left\{p'\alpha_{Ff}\Delta A_y\right\}_{i,j+1} - \left\{p'\alpha_{Ff}\Delta A_y\right\}_{i,j} + \frac{p'_{i,j}+p'_{i,j+1}}{2}A_{w_{i,j+\frac{1}{2}}}n_{f,w,x;i,j+\frac{1}{2}}\right]$$

$$U_y^{'-} = -\left\{\frac{\Delta t}{\Delta V \rho^0 \alpha_{Ff}}\right\}_{i,j-\frac{1}{2}}\left[\left\{p'\alpha_{Ff}\Delta A_y\right\}_{i,j} - \left\{p'\alpha_{Ff}\Delta A_y\right\}_{i,j-1} + \frac{p'_{i,j-1}+p'_{i,j}}{2}A_{w_{i,j-\frac{1}{2}}}n_{f,w,x;i,j-\frac{1}{2}}\right]$$

These two equations define our Poisson equation for the pressure. Once pressure is solved for we can compute the final velocities, using equation (3.8).

We see that pressure points with $\alpha_{Ff} = 0$, and at the same time $A_w n_{f,w,x} = 0$, will be cut out from the equation system.

The nice feature of the present equations is that they offer a complete machinery for computing cut-cell coefficient without doing any special treatment of cut cells. However, we may expect that some special treatment to compute α_{Ff} may be necessary.

The handling of in/out-flow boundary conditions should be quite standard, and is not discussed here.

3.2 The single phase solution procedure

The solution procedure (fixed geometry, isothermal) is:

1) Compute fluid fractions (porosities), based on actual geometry.
2) Initialize flow and pressures.
3) Update fluid properties.
4) Solve starred momentum equations (5.5), using appropriate wall boundary conditions
5) Compute coefficients for the velocity pressure coupling, equation (3.3)
6) Assemble and solve pressure correction equation (3.7)
7) Update pressures and velocities, latter according to equation

3.3 To be done in next steps

1) The suggested cut cell method should be refined and tested
2) The method is to be extended to multifield flows, including moving walls. For steady walls the previously suggested method should be possible to apply with a minimum of adjustments
3) The complete multiphase method, including moving walls should be given.
4) Finally; include the semi-Lagrangian methods for time and advection into the solution strategy for the complete system.

4 Multiphase flow equations

Now we work with fields and phases. We use notation $\alpha^{k;l}$, telling that the volume fraction $\alpha^{k;l}$ is the volume fraction of a field *k* which is submerged in a phase *l*. The continuous phase *l* is then denoted $\alpha^{l;l}$. The field velocity is $U^{k;l}$, and where the continuous phase velocity is $U^{l;l}$.
In order to support which fields are active or not we may apply a field indicator $\Upsilon^{k;l}$, where,

$$\Upsilon^{k;l} = \begin{cases} 1\,; \text{ Field exists} \\ 0; \text{ Field non-existing} \end{cases} \tag{4.1}$$

, and which is linked to character tables k="phase name", and l="phase name". The l-table may be (1,2,3,4,5)=(gas,oil,water,sand, wall_1), with an identical table for k. In this notation we select that for k=l this represents the case where the field is the continuous phase. All water is represented by $\alpha^{k;3}$, and where continuous water is $\alpha^{3;3}$, gas bubbles in water is $\alpha^{1;3}$ and sand particles in water is $\alpha^{4;3}$. If sand is considered as a continuous phase we will have that $\Upsilon^{4;4}=1$. Still fields like $\alpha^{i\neq 4;4}$ may normally be irrelevant and would not exist. We note that $\alpha^{1;4}$ is dispersed gas inside the continuous sand phase. There may be situations where bubbles in a granular fluid may be a useful concept. Here we have only one wall type, represented by wall fraction $\alpha^{5;5}$, and where $\Upsilon^{5;5}=1$ and $\Upsilon^{i<5;5}=0$.

4.1 Special interface notation

For interfaces we will use a special notation which handle the precise situation. We use the notation, exemplified by the interfacial area:

$$\mathbf{A}_{k;m\uparrow m;m} \tag{4.2}$$

Here the area vector is representing the interface of field k, submerged into m (k;m), and the continuous field (m;m). For dispersed fields we have that $\mathbf{A}_{k;m\uparrow m;m} \equiv \mathbf{A}_{k;m}$. However, for continuous fields, having an interface between (k;k) and (m;m) we have to apply $\mathbf{A}_{k;k\uparrow m;m}$, as $\mathbf{A}_{k;k\uparrow m;m} \neq \mathbf{A}_{k;m}$.

4.2 Multiphase mass equations

To arrive at the formal transport equation for mass we use the formalism provided in ([2], [3] and [4]). Now the transport equation for the mass of a field k, submerged in continuous phase m, is:

$$\frac{\partial}{\partial t}\int_{V^{k;m}} \rho^{k;m} dV = -\int_{S_{k;m}} \rho^{k;m}\mathbf{u}^{k;m}\cdot\mathbf{n}^{k;m} dS$$
$$\underbrace{-(1-\delta_{km})\int_{A_{k;m\uparrow m;m}} \rho^{k;m}\left(\mathbf{u}^{k;m}-\mathbf{u}_{I,k;m\uparrow m;m}\right)\cdot\mathbf{n}_{k;m\uparrow m;m} dS}_{\text{k is dispersed in m}} \qquad (4.3)$$
$$\underbrace{-\delta_{km}\sum_{j=1}^{L}\int_{A_{m;m\uparrow j;m}} \rho^{m;m}\left(\mathbf{u}^{m;m}-\mathbf{u}_{I,m;m\uparrow j;m}\right)\cdot\mathbf{n}_{m;m\uparrow j;m} dS}_{\text{j is dispersed in m}}$$

Here the summation over j includes all dispersed fields present in the control volume. The area $A_{m;m\uparrow j;m}$ express the interfacial area between fields $m;m$ and $j;m$. In general, all walls are treated as a phase or field which is stationary or moving. In this way there is no difference in the treatment of fluid-fluid and fluid-solid, or solid-solid interfaces. This will at a later stage allow for any dynamics of the "solids". Areas, volumes and vectors are handled as discussed in the single phase section and explained in Figure 6. In Figure 6 the field denoted wall, could be any continuous field, denoted by a volume fraction $\alpha^{k;k}$ and a velocity $\mathbf{u}^{k;k}$. The dispersed field denoted m could be a collection of different fields. When we now integrate over the fluid volume $V^{k;m}$ we find the intrinsic average of the density. Using $\alpha^{k;m}$ as field fraction of the control volume the field mass per volume in the complete control volume is $\hat{\rho}^{k;m} = \alpha^{k;m}\rho^{k;m}$. Here $\rho^{k;m}(p,T)$ is the intrinsic density of the field phase, or rather the phase labelled k (note that fields are subsets of a phase, where the thermodynamic properties, such as density, belongs to the phase.

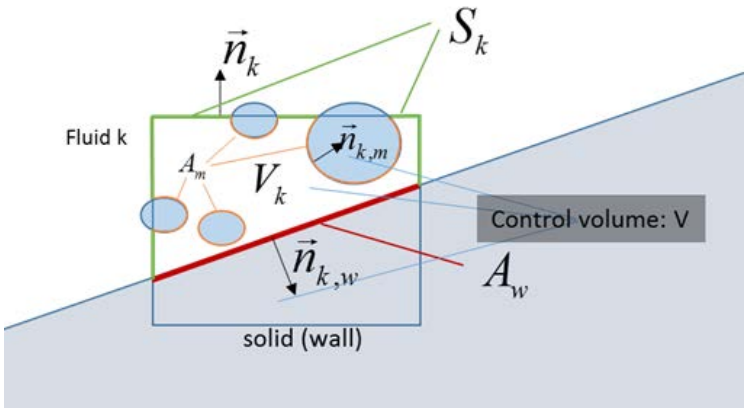

Figure 6 Control volume V, containing field k, cut by solid (or fluid-fluid interface), and by dispersed fields m.

The mass equation for a field *k* in the control volume V is then:

$$\frac{\partial}{\partial t}\left(\hat{\rho}^{k;l}\right) + \nabla\left(\hat{\rho}^{k;l}\mathbf{u}^{k;l}\right) = S^{k;l} \qquad (4.4)$$

Here the effective (extensive) density $\hat{\rho}^{k;l}$ is represented by:

$$\hat{\rho}^{k;l} = \alpha^{k;l}\rho^{k}(p, T^{k;l}) \tag{4.5}$$

, and where $\rho^{k}(p, T^{k;l})$ is the intrinsic density of the phase denoted as k. However, temperature and chemical composition of fields of a given phase may not be identical inside the same control volume provided that the temperature and compositions are not identical.

The volume constraint has to be fulfilled, stating that:

$$\sum_{l=1}^{L}\sum_{k=1}^{L}\alpha^{k;l} = 1.0 \tag{4.6}$$

At this stage we note that we in equation (4.6) have totally L different phases and types of walls. Each of these may have different appearances, named field.
The fields belonging to a zone (zone zk is represented by all fields which are contained inside the continuous fluid phase k. The volume fraction of the zone zk is then:

$$\alpha_{zm} = \sum_{k=1}^{L}\alpha^{k;m} \tag{4.7}$$

We further wants to keep track of special fields which are attached to a large scale (LSI) interface between continuous fields, such as $m;m$ and $j;j$. This is done by introduction of $\beta^{m;j;l}$. If we have a tiny oil film at the air-water interface, the volume of oil per interface area is represented by:

$$\beta^{oil;water;gas} \equiv \beta^{oil;gas;water} \Leftrightarrow \beta^{2;3;1} \equiv \beta^{2;1;3} \tag{4.8}$$

Similarly, a condensed film on water on wall_1 would be denoted $\beta^{water;wall\_1,gas} \equiv \beta^{water;gas,wall\_1}$, while a adsorbed gas on the oil-wall_2 interface would be represented by: $\beta^{gas;wall\_2,oil} \equiv \beta^{gas;oil,wall\_2}$
To keep track of the physics inside the oil film the most natural choice would be to represent the film by a Lagrangian representation. Then all necessary transport equations for the film, and the coupling with the Eulerian mesh, will have to be solved using the Lagrangian methods. Alternatively, we may formulate Eulerian transport equations for the surface mass β and properties, also handling these as an Eulerian fields. We leave this for now, but realize that handling transport of surface concentrations may be very useful for multiple applications.
We will assume that the interface fields will not displace resolved fluids (film thin compared to grid size), and can therefore be handled at a later stage and in a simplified manner.

4.3 Multiphase momentum equations

4.3.1 Dispersed fields

The momentum balance for the momentum of a dispersed field marked k in phase l, can for a computational cell can be written as:

$$\begin{aligned}&\frac{\partial}{\partial t}\int_{V^{k;l}}\rho^{k;l}\mathbf{u}^{k;l}dV=\int_{V^{k;l}}\rho^{k;l}\mathbf{g}dV\\&+\int_{S^{k;l}}\left(-p^{l;l}\mathbf{I}+\boldsymbol{\tau}^{l;l}\right)\cdot\mathbf{n}^{k;l}dS+\int_{A_{k;l\uparrow l;l}}\left(-p^{l;l}\mathbf{I}+\boldsymbol{\tau}^{l;l}\right)\cdot\mathbf{n}_{k;l\uparrow l;l}dS\\&-\int_{S^{k;l}}\rho^{k;l}\mathbf{u}^{k;l}\mathbf{u}^{k;l}\cdot\mathbf{n}^{k;l}dS-\int_{A_{k;l\uparrow l;l}}\rho^{k;l}\mathbf{u}^{k;l}\left(\mathbf{u}^{k;l}-\mathbf{u}_{I,k;l\uparrow l;l}\right)\cdot\mathbf{n}_{k;l\uparrow l;l}dS\end{aligned}\tag{4.9}$$

The volume integrals are first evaluated, $\frac{\partial}{\partial t}\int_{V^{k;l}}\rho^{k;l}\mathbf{u}^{k;l}dV=\Delta V\frac{\partial}{\partial t}\hat{\rho}^{k;l}\mathbf{u}^{k;l}$, and $\int_{V^{k;l}}\rho^{k;l}\mathbf{g}dV=\Delta V\hat{\rho}^{k;l}\mathbf{g}$.

Here the extensive density is $\hat{\rho}^{k;l}=\alpha^{k;l}\rho^{k;l}$ and $\mathbf{u}^{k;l}$ is the volume and mass averaged velocity inside the fluid volume.

The pressure and viscous stresses, acting on the part of the surface of the total control volume V (see Figure 6) which is cut by field k, is given by:

$$\int_{S^{k;l}}\left(-p^{l;l}\mathbf{I}+\boldsymbol{\tau}^{l;l}\right)\cdot\mathbf{n}^{k;l}dS\tag{4.10}$$

The field k;l is the local dispersed phase, where the pressure and stress is exerted by the continuous phase l. However, if the field fulfils k=l it is a continuous field, and $(p^{l;l},\boldsymbol{\tau}^{l;l})$ is the pressure and viscous stress of the phase itself.
The surface integral can be converted into a divergence of volume averaged quantities, using well known theorems ([2], [3] and [4]), stating that:

$$\int_{S^{k;l}}\boldsymbol{\psi}^{k;l}\cdot\mathbf{n}^{k;l}dS=\nabla\cdot\int_{V^{k;l}}\boldsymbol{\psi}^{k;l}dV=V\nabla\cdot\left\langle\boldsymbol{\psi}^{k;l}\right\rangle^{e}\tag{4.11}$$

Here the brackets denotes that $\left\langle\boldsymbol{\psi}^{k;l}\right\rangle^{e}$ is an extensive volume average. The area $s^{k;l}$ is the part of the surface of the control volume which is occupied by the field (k;l) (see Figure 6).

Applying equation (4.11) to equation (4.10) we obtain:

$$\int_{S^{k;l}}\left(-p^{l;l}\mathbf{I}+\boldsymbol{\tau}^{l;l}\right)\cdot\mathbf{n}^{k;l}dS=V\nabla\cdot\left\langle-p^{l;l}\mathbf{I}+\boldsymbol{\tau}^{l;l}\right\rangle^{e}=V\nabla\cdot\left(-\alpha^{k;l}\left\langle p^{l;l}\right\rangle^{i}\mathbf{I}+\alpha^{k;l}\left\langle\boldsymbol{\tau}^{l;l}\right\rangle^{i}\right)\tag{4.12}$$

Above the brackets denote volume averages and superscripts e and i denotes extensive and intensive averages, respectively.

The extensive volume average of a property φ is represented by:

$$\left\langle \varphi^{k;l} \right\rangle^{e} = \frac{1}{V} \int_{V^{k;l}} \varphi dV \tag{4.13}$$

Similarly, the intensive average is given by,

$$\left\langle \varphi^{k;l} \right\rangle^{i} = \frac{1}{V^{k;l}} \int_{V^{k;l}} \varphi dV \tag{4.14}$$

and the two are related by:

$$\left\langle \varphi^{k;l} \right\rangle^{e} = \frac{V^{k;l}}{V} \left\langle \varphi^{k;l} \right\rangle^{i} = \alpha^{k;l} \left\langle \varphi^{k;l} \right\rangle^{i} \tag{4.15}$$

Using our preferred notation we write:

$$\int_{S^{k;l}} \left(-p^{l;l}\mathbf{I} + \boldsymbol{\tau}^{l;l} \right) \cdot \mathbf{n}^{k;l} dS = V \nabla \cdot \left(-\alpha^{k;l} p^{l;l}\mathbf{I} + \alpha^{k;l} \boldsymbol{\tau}^{l;l} \right) \tag{4.16}$$

Using the same treatment for the convection terms, we obtain:

$$\begin{aligned} &\int_{S^{k;l}} \rho^{k;l} \mathbf{u}^{k;l} \mathbf{u}^{k;l} \cdot \mathbf{n}^{k;l} dS = V \nabla \cdot \left\langle \rho^{k;l} \mathbf{u}^{k;l} \mathbf{u}^{k;l} \right\rangle^{e} \equiv V \nabla \cdot \left(\alpha^{k;l} \rho^{k;l} \left\langle \mathbf{u}^{k;l} \mathbf{u}^{k;l} \right\rangle^{i} \right) \\ &= V \nabla \cdot \left(\alpha^{k;l} \rho^{k;l} \left(\left\langle \delta \mathbf{u}^{k;l} \delta \mathbf{u}^{k;l} \right\rangle^{i} + \left\langle \mathbf{u}^{k;l} \right\rangle^{i} \left\langle \mathbf{u}^{k;l} \right\rangle^{i} \right) \right) \end{aligned} \tag{4.17}$$

Here $\left\langle \mathbf{u}^{k;l} \right\rangle^{i}$ is the field internal, mass and volume averaged velocity. $\delta \mathbf{u}^{k;l}$ is the cell internal variation of deviation between averaged velocity and actual field velocity. As we will assume that the volume averaged quantities expressed on the numerical grid is smoothly varying in space, the deviatoric velocity $\delta \mathbf{u}^{k;l}$ and stress $\left\langle \delta \mathbf{u}^{k;l} \delta \mathbf{u}^{k;l} \right\rangle^{i}$ is a result of the deviation between the smooth volume averaged field and the true local value. As the system may have many possible realization the quantities we work with express ensembles of multiple realizations. The equations presented next will all be volume and ensemble averaged. The ensemble averaged velocities are mass weighed (Favre averaged). Details about the averaging procedure are found in the **Appendix**. In applications which involve turbulent flow we add turbulence by one more layer of ensemble averaging. This process will include one more deviatoric velocity $\mathbf{u}''^{k;l}$. The impact of turbulence is modification of the closure coefficient, and the physics can be incorporated in the presented physical and numerical framework. We may note that velocitied with a tilde, $\tilde{\mathbf{u}}$, represent a Favre averaged velocity. The convection terms may now be written as:

$$\int_{S^{k;l}} \rho^{k;l} \mathbf{u}^{k;l} \mathbf{u}^{k;l} \cdot \mathbf{n}^{k;l} dS = V \nabla \cdot \left(\alpha^{k;l} \rho^{k;l} \left(\overline{\delta \mathbf{u}^{k;l} \delta \mathbf{u}^{k;l}} + \mathbf{u}^{k;l} \mathbf{u}^{k;l} \right) \right) \tag{4.18}$$

The overbar in $\overline{\delta \mathbf{u}^{k;l} \delta \mathbf{u}^{k;l}}$ represents ensemble average. The forces acting on field k, inside the volume V, are represented by:

$$\int_{A_{k;l \uparrow l;l}} \left(-p^{l;l}\mathbf{I} + \boldsymbol{\tau}^{l;l} \right) \cdot \mathbf{n}_{k;l \uparrow l;l} dS \tag{4.19}$$

Equation (4.19) express the fluid forces acting on the boundaries $k;l \uparrow l;l$, with common interface area $A_{k;l\uparrow l;l}$. In order to handle equation (4.19) we split the pressure and viscous stress tensor into two parts:

$$\begin{aligned} p^{l;l} &= \left\langle p^{l;l} \right\rangle^i + p^{l;l}{}' \\ \boldsymbol{\tau}^{l;l} &= \left\langle \boldsymbol{\tau}^{l;l} \right\rangle^i + \boldsymbol{\tau}^{l;l}{}' \end{aligned} \tag{4.20}$$

Here the brackets denotes the smooth and volume averaged pressure and stress fields, while $p^{l;l}{}'$ and $\boldsymbol{\tau}^{l;l}{}'$ are the deviations caused by the local hydrodynamics. These deviatoric fields are responsible for all local hydrodynamics forces such as drag, lift and virtual mass.

The surface integral in equation (4.19), expressing hydrodynamic forces inside the volume V, can be rewritten as:

$$\begin{aligned} &\int_{A_{k;l\uparrow l;l}} \left(-p^{l;l}\mathbf{I} + \boldsymbol{\tau}^{l;l}\right)\cdot \mathbf{n}_{k;l\uparrow l;l} dS = \int_{A_{k;l\uparrow l;l}} \left(-p^{l;l}\mathbf{I} + \boldsymbol{\tau}^{l;l}\right)\cdot \mathbf{n}_{k;l\uparrow l;l} dS + \int_{S^{k;l}} \left(-p^{l;l}\mathbf{I} + \boldsymbol{\tau}^{l;l}\right)\cdot \mathbf{n}^{k;l} dS - \int_{S^{k;l}} \left(-p^{l;l}\mathbf{I} + \boldsymbol{\tau}^{l;l}\right)\cdot \mathbf{n}^{k;l} dS \\ &\approx \cancel{\left(-\left\langle p^{l;l}\right\rangle^i \mathbf{I} + \left\langle \boldsymbol{\tau}^{l;l}\right\rangle^i\right) \int_{S_k + A_{k;l\uparrow l;l}} 1\cdot \mathbf{n}_k dS} + \int_{A_{k;l\uparrow l;l}} \left(-p^{l;l}{}'\mathbf{I} + \boldsymbol{\tau}^{l;l}{}'\right)\cdot \mathbf{n}_{k;l\uparrow l;l} dS + \int_{S^{k;l}} \left(-p^{l;l}{}'\mathbf{I} + \boldsymbol{\tau}^{l;l}{}'\right)\cdot \mathbf{n}^{k;l} dS - \int_{S^{k;l}} \left(-p^{l;l}\mathbf{I} + \boldsymbol{\tau}^{l;l}\right)\cdot \mathbf{n}^{k;l} dS \\ &= \int_{A_{k;l\uparrow l;l}} \left(-p^{l;l}{}'\mathbf{I} + \boldsymbol{\tau}^{l;l}{}'\right)\cdot \mathbf{n}_{k;l\uparrow l;l} dS - \left(-\left\langle p^{l;l}\right\rangle^i \mathbf{I} + \left\langle \boldsymbol{\tau}^{l;l}\right\rangle^i\right)\cdot \int_{S^{k;l}} \mathbf{n}^{k;l} dS \\ &= \int_{A_{k;l\uparrow l;l}} \left(-p^{l;l}{}'\mathbf{I} + \boldsymbol{\tau}^{l;l}{}'\right)\cdot \mathbf{n}_{k;l\uparrow l;l} dS - V\cdot\left(-\left\langle p\right\rangle^i \mathbf{I} + \left\langle \boldsymbol{\tau}\right\rangle^i\right)\cdot \nabla \alpha_k \end{aligned} \tag{4.21}$$

We may now combine equations (4.12) and (4.21) to obtain:

$$\begin{aligned} &\int_{S^{k;l}} \left(-p^{l;l}\mathbf{I} + \boldsymbol{\tau}^{l;l}\right)\cdot \mathbf{n}^{k;l} dS + \int_{A_{k;l\uparrow l;l}} \left(-p^{l;l}\mathbf{I} + \boldsymbol{\tau}^{l;l}\right)\cdot \mathbf{n}_{k;l\uparrow l;l} dS \\ &= \nabla\cdot\left(-\alpha^{k;l}\left\langle p^{l;l}\right\rangle^i \mathbf{I} + \alpha^{k;l}\left\langle \boldsymbol{\tau}^{l;l}\right\rangle^i\right) + \int_{A_{k;l\uparrow l;l}} \left(-p^{l;l}{}'\mathbf{I} + \boldsymbol{\tau}^{l;l}{}'\right)\cdot \mathbf{n}_{k;l\uparrow l;l} dS - V\cdot\left(-\left\langle p^{l;l}\right\rangle^i \mathbf{I} + \left\langle \boldsymbol{\tau}^{l;l}\right\rangle^i\right)\cdot \nabla \alpha^{k;l} \\ &= \alpha^{k;l}\nabla\cdot\left(-\left\langle p^{l;l}\right\rangle^i \mathbf{I} + \left\langle \boldsymbol{\tau}^{l;l}\right\rangle^i\right) + \int_{A_{k;l\uparrow l;l}} \left(-p^{l;l}{}'\mathbf{I} + \boldsymbol{\tau}^{l;l}{}'\right)\cdot \mathbf{n}_{k;l\uparrow l;l} dS \end{aligned} \tag{4.22}$$

In equation (4.22) the smooth (volume averaged) pressure and stress field are handled by the first term. The sub-scale stresses, representing the dispersed fields, are represented by the integral of deviations in stress and pressure, must be limited to dispersed fields only. For the hydrodynamic interaction term in equation (4.22),

$$\int_{A_{k;l\uparrow l;l}} \left(-p^{l;l}{}'\mathbf{I} + \boldsymbol{\tau}^{l;l}{}'\right)\cdot \mathbf{n}_{k;l\uparrow l;l} dS\,, \tag{4.23}$$

we have that this term only involves dispersed phases. As we will see later, the LSI and solid wall stresses will be handled by the similar term, but now when we are dealing with the momentum equations for the continuous fields.

If we for a start only include hydrodynamic drag in equation (4.23), we have that :

$$\int_{A_{k;l\uparrow l;l}} \left(-p'^{l;l}\mathbf{I}+\boldsymbol{\tau}'^{l;l}\right)\cdot\mathbf{n}_{k;l\uparrow l;l}dS = \overline{\frac{\alpha^{k;l}\rho^{k;l}}{\left(\frac{\rho^{k;l}\cdot\left(d^{k;l}\right)^2}{18\mu^{l;l}}\right)}\left(\frac{C_D\,\mathrm{Re}_p^{\,k;l}}{24}\right)\left(\mathbf{u}^{l;l}-\mathbf{u}^{k;l}\right)}$$

$$=\frac{\alpha^{k;l}\rho^{k;l}}{\left(\frac{\rho^{k;l}\cdot\left(d^{k;l}\right)^2}{18\mu^{l;l}}\right)}\left(\frac{C_D\,\mathrm{Re}_p^{\,k;l}}{24}\right)\left(\mathbf{u}^{l;l}-\mathbf{u}^{k;l}\right)+\mathbf{f}'_{\mathbf{H},k;l\uparrow l;l} \tag{4.24}$$

The overbar on the drag term implies ensemble averaging of the entire term. In the final expressions $\mathbf{u}^{k;l}$ denotes a volume and ensemble averaged velocity.

Similarly, if we have k=l, the field is continuous and the drag force is the sum of forces exerted by all the fields suspended in field (k;l):

$$\sum_{j=1}^{L}\int_{A_{k;l\uparrow j;l}} \left(-p^{l;l}\mathbf{I}+\boldsymbol{\tau}^{l;l}\right)\cdot\mathbf{n}_{k;l\uparrow j;l}dS = \overline{\sum_{j=1}^{L}\frac{\alpha^{j;l}\rho^{j;l}}{\left(\frac{\rho^{j;l}\cdot\left(d^{j;l}\right)^2}{18\mu^{l;l}}\right)}\left(\frac{C_D\,\mathrm{Re}_p^{\,j;l}}{24}\right)\left(\mathbf{u}^{j;l}-\mathbf{u}^{k;l}\right)}$$

$$=\sum_{j=1}^{L}\frac{\alpha^{j;l}\rho^{j;l}}{\left(\frac{\rho^{j;l}\cdot\left(d^{j;l}\right)^2}{18\mu^{l;l}}\right)}\left(\frac{C_D\,\mathrm{Re}_p^{\,j;l}}{24}\right)\left(\mathbf{u}^{j;l}-\mathbf{u}^{k;l}\right)+\sum_{j=1}^{L}\mathbf{f}'_{k;l\uparrow j;l} \tag{4.25}$$

Note that we will start with assuming that we have only one particle diameter in each computational volume. Extending to poly dispersed systems is rather trivial, but the consequence is huge amounts of data and extremely slow computations. However, significant physics may be represented by using transported particulate diameters (by separate transport equation)[5].

In equations (4.24) and (4.25) $\mathbf{f}'_{\mathbf{H}}$ represents the remaining hydro-dynamical forces, not accounted for

If we now just look at the transient term and the drag term we have, using equation (4.25):

$$\frac{\partial}{\partial t}\left(\alpha^{k;l}\rho^{k;l}\mathbf{u}^{k;l}\right)\sim \overline{\sum_{j=1}^{L}\frac{\alpha^{j;l}\rho^{j;l}}{\left(\frac{\rho^{j;l}\cdot\left(d^{j;l}\right)^2}{18\mu^{l;l}}\right)}\left(\frac{C_D\,\mathrm{Re}_p^{\,j;l}}{24}\right)\left(\mathbf{u}^{j;l}-\mathbf{u}^{k;l}\right)}$$

$$=\sum_{j=1}^{L}K^{j;l}\left(\mathbf{u}^{j;l}-\mathbf{u}^{k;l}\right)+\sum_{j=1}^{L}\mathbf{f}'_{k;l\uparrow j;l} \tag{4.26}$$

This far we have not considered properly the issues of which field is continuous or dispersed. We next generalize (4.24) - (4.26) to become:

$$\frac{\partial}{\partial t}\left(\alpha^{k;l}\rho^{k;l}\mathbf{u}^{k;l}\right)\sim$$

$$\underbrace{\left(1-\delta_{kl}\right)\left(K^{k;l}\left(\mathbf{u}^{l;l}-\mathbf{u}^{k;l}\right)+\mathbf{f}'_{\mathbf{H},k;l\uparrow l;l}\right)}_{\text{k is dispersed in l}}+\underbrace{\delta_{kl}\left(\sum_{j=1}^{L}K^{j;l}\left(\mathbf{u}^{j;l}-\mathbf{u}^{k;l}\right)+\sum_{j=1}^{L}\mathbf{f}'_{k;l\uparrow j;l}\right)}_{\text{j is dispersed in l}} \tag{4.27}$$

The friction coefficient in equation (4.27) is given by:

$$K^{k;l} = \frac{\alpha^{k;l}\rho^{k;l}}{\left(\frac{\rho^{k;l}\cdot\left(d^{k;l}\right)^2}{18\mu^{l;l}}\right)}\left(\frac{C_D\,\mathrm{Re}_p^{\,k;l}}{24}\right) \tag{4.28}$$

Here we introduced the Kronecker delta δ_{kl} , which will pick out values when k=l ($\delta_{kk}=1$, $\delta_{kl}=0$ for k $\neq l$). As a consequence, the first RHS term in equation (4.27) picks out the drag force when field (k;l) is a dispersed field ($k \neq l$). In this case the second term with $\delta_{kl}=0$, will disappear. In case the field (k;l) is a continuous field ($k = l$), the first term disappears and the second term includes the drag force exerted by all field submerged into continuous phase k.

We note that in equation (4.27) we have an ensemble average $\overline{K^{k;l}\left(\mathbf{u}^{l;l}-\mathbf{u}^{k;l}\right)}$ of the drag force. In the case of Stoke law drag (linear, $\frac{C_D\,\mathrm{Re}_p^{\,k;l}}{24}=1$), we have that

k disp i l : $\overline{K^{k;l}\left(\mathbf{u}^{l;l}-\mathbf{u}^{k;l}\right)}=\left(\frac{K^{k;l}}{\alpha^{k;l}}\right)\overline{\left(\alpha^{k;l}\mathbf{u}^{l;l}-\alpha^{k;l}\mathbf{u}^{k;l}\right)}$

$$=\left(\frac{K^{k;l}}{\alpha^{k;l}}\right)\overline{\left(\alpha^{k;l}\left(\widetilde{\mathbf{u}^{l;l}}+\mathbf{u}^{"l;l}\right)-\alpha^{k;l}\widetilde{\mathbf{u}^{k;l}}\right)}=\left(\frac{K^{k;l}}{\alpha^{k;l}}\right)\overline{\alpha^{k;l}\mathbf{u}^{"l;l}}+\left(\frac{K^{k;l}}{\alpha^{k;l}}\right)\left(\overline{\alpha^{k;l}}\widetilde{\mathbf{u}^{l;l}}-\overline{\alpha^{k;l}}\widetilde{\mathbf{u}^{k;l}}\right) \tag{4.29}$$

$$\rightarrow\left(\frac{K^{k;l}}{\alpha^{k;l}}\right)\overline{\alpha^{k;l}\mathbf{u}^{"l;l}}+\left(\frac{K^{k;l}}{\alpha^{k;l}}\right)\left(\alpha^{k;l}\mathbf{u}^{l;l}-\alpha^{k;l}\mathbf{u}^{k;l}\right)$$

The arrow above denote that the velocities and volume fractions are true ensemble averages, but we drop the overbars for convenience.

We may further note that in the case of Stokes law $\left(\frac{K^{k;l}}{\alpha^{k;l}}\right)$ is constant, not depending on the volume fraction, as long as we do not consider hindered settling effects.

Based on the above consideration we may write the complete momentum equation as:

$$\frac{\partial}{\partial t}\left(\alpha^{k;l}\rho^{k;l}\mathbf{u}^{k;l}\right)+\nabla\cdot\left(\alpha^{k;l}\rho^{k;l}\left(\overline{\delta\mathbf{u}^{k;l}\delta\mathbf{u}^{k;l}}+\mathbf{u}^{k;l}\mathbf{u}^{k;l}\right)\right)=\alpha^{k;l}\rho^{k;l}\mathbf{g}$$
$$+\alpha^{k;l}\nabla\cdot\left(-\left\langle p^{l;l}\right\rangle^{i}\mathbf{I}+\left\langle\boldsymbol{\tau}^{l;l}\right\rangle^{i}\right)$$
$$+\underbrace{\left(1-\delta_{kl}\right)K^{k;l}\left\{\left(\mathbf{u}^{l;l}-\mathbf{u}^{k;l}\right)+\frac{\overline{\alpha^{k;l}\mathbf{u}^{"l;l}}}{\alpha^{k;l}}\right\}}_{\text{k is dispersed in l}}+\underbrace{\delta_{kl}\sum_{j=1}^{L}K^{j;l}\left\{\left(\mathbf{u}^{j;l}-\mathbf{u}^{l;l}\right)-\frac{\overline{\alpha^{j;l}\mathbf{u}^{"l;l}}}{\alpha^{j;l}}\right\}}_{\text{j is dispersed in l}}$$
$$\underbrace{-\left(1-\delta_{kl}\right)\int\limits_{A_{k;l\uparrow l;l}}\rho^{k;l}\mathbf{u}^{k;l}\left(\mathbf{u}^{k;l}-\mathbf{u}_{I,k;l\uparrow l;l}\right)\cdot\mathbf{n}_{k;l\uparrow l;l}dS}_{\text{k is dispersed in l}}$$
$$\underbrace{-\delta_{kl}\sum_{j=1}^{L}\int\limits_{A_{l;l\uparrow j;l}}\rho^{l;l}\mathbf{u}^{l;l}\left(\mathbf{u}^{l;l}-\mathbf{u}_{I,l;l\uparrow j;l}\right)\cdot\mathbf{n}_{l;l\uparrow j;l}dS}_{\text{j is dispersed in l}} \tag{4.30}$$

The momentum equation above is valid for all flowing fields in the system, but is for now limited to laminar flows. We note two terms here, where the first one is the momentum dispersion:

$$\left[\overline{\delta\mathbf{u}^{k;l}\delta\mathbf{u}^{k;l}}\right]_{i,j}=\overline{\delta u_i^{\,k;l}\delta u_j^{\,k;l}}=\Gamma_{b,sub}\nabla\mathbf{u}^{k;l}\delta_{ij}-\Gamma_{sub}\left(\frac{\partial u_i^{\,k;l}}{\partial x_j}+\frac{\partial u_j^{\,k;l}}{\partial x_i}\right) \tag{4.31}$$

The coefficients $\Gamma_{b,sub}$ and Γ_{sub} express for now bulk and shear viscosities for sub-cell agitation, such as granular stresses. Later we will add turbulent stresses into the model. It can be shown that when we work with volume, mass and ensemble weighed velocities the only terms that will be modified are the effective viscosity in equation (4.31) and the hydrodynamic exchange terms. In the current formulation we will have to add turbulent dispersion into $\mathbf{f}'_{\mathbf{H},k;l\uparrow l;l}$. The sub cell drag dispersion force is typically modelled as:

$$\mathbf{f}'_{\mathbf{H},k;l\uparrow l;l}=\left(\frac{K^{k;l}}{\alpha^{k;l}}\right)\overline{\alpha^{k;l}\mathbf{u}^{"l;l}}\approx-K^{k;l}\lambda_{sub}^{\;k;l}\nabla\alpha^{k;l} \tag{4.32}$$

The sub cell drag dispersion can be modelled due to Brownian motions or granular dispersion. If the flow is turbulent we have to add a turbulent dispersion coefficient, typically slaved to the turbulent momentum dispersion coefficient (turbulent kinematic viscosity), such as $\lambda_{sub}^{\;k;l}\Rightarrow\lambda_{sub}^{\;k;l}+\frac{\nu_t}{Sc_t}$, where ν_t is a turbulent diffusivity for the continuous phase and Sc_t is a turbulent Schmidt number for the turbulent dispersion of the dispersed field.

Now, in the cases where dispersed fields are created or annihilated at the LSI between continuous domains, significant mechanical mass transfer will take place. In such cases the mass transfer terms in equations (4.4) and (4.30) have to be extended to handle mechanical mass transfer.

4.3.2 Continuous fields

Based on the generic averaging theorems ([2], [3] and [4]), the momentum equation for a continuous field is written as

$$\begin{aligned}
&\frac{\partial}{\partial t}\int_{V^{l;l}} \rho^{l;l}\mathbf{u}^{l;l}dV = \int_{V^{l;l}} \rho^{l;l}\mathbf{g}dV \\
&+\int_{S^{l;l}} \left(-p^{l;l}\mathbf{I}+\boldsymbol{\tau}^{l;l}\right)\cdot\mathbf{n}^{l;l}dS - \sum_{\substack{\text{All dispersed}\\ \text{fields k;l in l;l}}} \int_{A_{k;l\uparrow l;l}} \left(-p^{l;l}\mathbf{I}+\boldsymbol{\tau}^{l;l}\right)\cdot\mathbf{n}_{k;l\uparrow l;l}dS \\
&\underbrace{-\sum_{\substack{\text{All continuous fields m;m,}\\ \text{interacting with l;l}}} \int_{A_{m;m\uparrow l;l}} \left(-p^{l;l}\mathbf{I}+\boldsymbol{\tau}^{l;l}\right)\cdot\mathbf{n}_{m;m\uparrow l;l}dS}_{LSI_wall} \\
&-\int_{S^{l;l}} \rho^{l;l}\mathbf{u}^{l;l}\mathbf{u}^{l;l}\cdot\mathbf{n}^{l;l}dS - \sum_{\substack{\text{All other fields k}\\ \text{inside volume}}} \int_{A_{k;l\uparrow l;l}} \rho^{l;l}\mathbf{u}^{l;l}\left(\mathbf{u}^{l;l}-\mathbf{u}_{I,k;l\uparrow l;l}\right)\cdot\mathbf{n}_{l;l\uparrow k;l}dS
\end{aligned} \tag{4.33}$$

All terms in equation (4.33) except one has been developed and discussed above. The new term is marked with *LSI_wall*. Shear and normal stresses at solids walls or LSIs are handled by this term, as these are stresses and pressures resolved on the scale of the control volume V.

$$\sum_{\substack{\text{All continuous fields m;m,}\\ \text{interacting with l;l}}} \int_{A_{m;m\uparrow l;l}} \left(-p^{l;l}\mathbf{I}+\boldsymbol{\tau}^{l;l}\right)\cdot\mathbf{n}_{m;m\uparrow l;l}dS \tag{4.34}$$

For now disregarding the interfacial pressure difference due to curvature, we may drop the pressure contributions and assume that all phases share the same pressure. This simplification may lead to problems in certain cases and will be analysed at a later stage. At the LSI as well as solid walls the jump condition for mass flow normal to the interface must always be fulfilled.

By application of the method discussed in Chapter 2.3.1, we may write the tangential LSI exchange force as

$$\int_{A_{m;m\uparrow l;l}} \boldsymbol{\tau}^{l;l}\cdot\mathbf{n}_{m;m\uparrow l;l}dS_{m;m\uparrow l;l} \simeq \left(\boldsymbol{\tau}^{l;l}\right)_{m;m\uparrow l;l}\cdot\mathbf{n}_{m;m\uparrow l;l}\Delta S_{m;m\uparrow l;l} \tag{4.35}$$

This may further; take example for the x-velocity component (refers to equation (2.26)), being expressed as

$$F_{w,x} = -\tau_{Aw}n_{t,x} - \chi_w n_{t,x}\left(u_x - U_{LSI,x}\right), \tag{4.36}$$

which we generalize to

$$\left(\boldsymbol{\tau}^{l;l}\right)_{m;m\uparrow l;l}\cdot\mathbf{n}_{m;m\uparrow l;l}\Delta S_{m;m\uparrow l;l} = \boldsymbol{\Theta}_{m;m\uparrow l;l} + \Phi_{m;m\uparrow l;l}\left(\mathbf{u}_{m;m\uparrow l;l} - \mathbf{u}^{l;l}\right) \tag{4.37}$$

The coefficients $\boldsymbol{\Theta}_{m;m\uparrow l;l}$ and $\Phi_{m;m\uparrow l;l}$ are defined by equations (2.20) - (2.26). We may further note that for a solid wall (4.37) will use $\mathbf{u}^{m;m}$ as the wall velocity. If the interface is moving we must consider Newton's 3rd law. For each interface, now neglecting interface mass transfer, we have the relation:

$$\begin{aligned}
&\left(\boldsymbol{\tau}^{l;l}\right)_{m;m\uparrow l;l}\cdot\mathbf{n}_{m;m\uparrow l;l}\Delta S_{m;m\uparrow l;l}=\left(\boldsymbol{\tau}^{m;m}\right)_{l;l\uparrow m;m}\cdot\mathbf{n}_{l;l\uparrow m;m}\Delta S_{l;l\uparrow m;m}\\
&\qquad\qquad\Updownarrow\\
&\boldsymbol{\Theta}_{m;m\uparrow l;l}+\Phi_{m;m\uparrow l;l}\left(\mathbf{u}_{m;m\uparrow l;l}-\mathbf{u}^{l;l}\right)=\boldsymbol{\Theta}_{l;l\uparrow m;m}+\Phi_{l;l\uparrow m;m}\left(\mathbf{u}_{m;m\uparrow l;l}-\mathbf{u}^{m;m}\right)
\end{aligned}\tag{4.38}$$

As a result of (4.38) we obtain the interface velocity:

$$\mathbf{u}_{m;m\uparrow l;l}=\frac{\Theta_{m;m\uparrow l;l}-\Theta_{l;l\uparrow m;m}+\left(\mathbf{u}^{m;m}\Phi_{l;l\uparrow m;m}-\mathbf{u}^{l;l}\Phi_{m;m\uparrow l;l}\right)}{\left(\Phi_{l;l\uparrow m;m}-\Phi_{m;m\uparrow l;l}\right)}\ ,\tag{4.39}$$

and finally for the exchange force:

$$\begin{aligned}
&\left(\boldsymbol{\tau}^{l;l}\right)_{m;m\uparrow l;l}\cdot\mathbf{n}_{m;m\uparrow l;l}\Delta S_{m;m\uparrow l;l}\\
&=\left(\frac{\Phi_{l;l\uparrow m;m}\boldsymbol{\Theta}_{m;m\uparrow l;l}-\Phi_{m;m\uparrow l;l}\boldsymbol{\Theta}_{l;l\uparrow m;m}}{\Phi_{l;l\uparrow m;m}-\Phi_{m;m\uparrow l;l}}\right)+\left(\frac{\Phi_{m;m\uparrow l;l}\Phi_{l;l\uparrow m;m}}{\Phi_{l;l\uparrow m;m}-\Phi_{m;m\uparrow l;l}}\right)\left(\mathbf{u}^{m;m}-\mathbf{u}^{l;l}\right)
\end{aligned}\tag{4.40}$$

The suggested method is ready for application of wall functions. The quantities entering into equation (4.36) (or (2.26)) , like $n_{t,x},\tau_{Aw}$ and χ_w are readily computed from wall functions.

As a result, the LSI forces acting on the field *k;l* is given by;

$$\delta_{kl}\sum_{\substack{\text{All continuous fields m;m,}\\ \text{interacting with l;l}}}\left(\boldsymbol{\psi}_{l;l\uparrow m;m}+\vartheta_{l;l\uparrow m;m}\left(\mathbf{u}^{m;m}-\mathbf{u}^{l;l}\right)\right)\ ,\tag{4.41}$$

and where the coefficients are given by:

$$\begin{aligned}
\boldsymbol{\psi}_{l;l\uparrow m;m}&=\boldsymbol{\psi}_{m;m\uparrow l;l}=\left(\frac{\Phi_{l;l\uparrow m;m}\boldsymbol{\Theta}_{m;m\uparrow l;l}-\Phi_{m;m\uparrow l;l}\boldsymbol{\Theta}_{l;l\uparrow m;m}}{\Phi_{l;l\uparrow m;m}-\Phi_{m;m\uparrow l;l}}\right)\\
\vartheta_{l;l\uparrow m;m}&=\vartheta_{m;m\uparrow l;l}=\left(\frac{\Phi_{m;m\uparrow l;l}\Phi_{l;l\uparrow m;m}}{\Phi_{l;l\uparrow m;m}-\Phi_{m;m\uparrow l;l}}\right)
\end{aligned}\tag{4.42}$$

4.4 Simplified model equations

Here we neglect molecular and mechanical mass transfer. Then the mass conservation equation in (4.4) becomes:

$$\frac{\partial}{\partial t}\left(\hat{\rho}^{k;l}\right)+\nabla\left(\hat{\rho}^{k;l}\mathbf{u}^{k;l}\right)=0 \tag{4.43}$$

We note that due the mass weighted ensemble averaging we have that for the fluctuation velocity component $\left\langle \hat{\rho}^{k;l}\mathbf{u}''^{k;l}\right\rangle \equiv 0$, resulting in equation (4.43). Similarly, the momentum equation in (4.30) is written

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\alpha^{k;l}\rho^{k;l}\mathbf{u}^{k;l}\right)+\nabla\cdot\left(\alpha^{k;l}\rho^{k;l}\mathbf{u}^{k;l}\mathbf{u}^{k;l}\right)=\alpha^{k;l}\rho^{k;l}\mathbf{g}+\alpha^{k;l}\nabla\cdot\left(-p^{l;l}\mathbf{I}+\boldsymbol{\tau}^{l;li}\right)+\nabla\cdot\left(\alpha^{k;l}\rho^{k;l}\Gamma_{sub}{}^{k;l}\nabla\mathbf{u}^{k;l}\right)\\&\underbrace{+\left(1-\delta_{kl}\right)K^{k;l}\left\{\left(\mathbf{u}^{l;l}-\mathbf{u}^{k;l}\right)+\left(\frac{\nu_t{}^{l;l}}{Sc_t{}^{l;l}}\frac{\nabla\overline{\alpha^{l;l}}}{\overline{\alpha^{l;l}}}-\frac{\nu_t{}^{l;l}}{Sc_t{}^{k;l}}\frac{\nabla\overline{\alpha^{k;l}}}{\overline{\alpha^{k;l}}}\right)\right\}}_{\text{k is dispersed in l}}+\underbrace{\delta_{kl}\sum_{j=1}^{L}K^{j;l}\left\{\left(\mathbf{u}^{j;l}-\mathbf{u}^{l;l}\right)-\left(\frac{\nu_t{}^{l;l}}{Sc_t{}^{l;l}}\frac{\nabla\overline{\alpha^{l;l}}}{\overline{\alpha^{l;l}}}-\frac{\nu_t{}^{l;l}}{Sc_t{}^{j;l}}\frac{\nabla\overline{\alpha^{j;l}}}{\overline{\alpha^{j;l}}}\right)\right\}}_{\text{j is dispersed in l}}\\&+\delta_{kl}\sum_{\substack{\text{All continuous fields m;m,}\\ \text{interacting with l;l}}}\left(\psi_{l;l\uparrow m;m}+\vartheta_{l;l\uparrow m;m}\left(\mathbf{u}^{m;m}-\mathbf{u}^{l;l}\right)\right)\end{aligned} \tag{4.44}$$

In equation (4.44) all symbols represent ensemble averages, and the velocities are mass weighed ensemble averages. The dispersion terms of type $\frac{\nu_t{}^{l;l}}{Sc_t{}^{j;l}}\frac{\nabla\overline{\alpha^{j;l}}}{\overline{\alpha^{j;l}}}$ are a result of equations (4.29) and (4.32), as well as the generalization proposed by Burns [6]. The last term contains all the large scale interface (LSI) and fluid-solid wall stresses. This will work fine as long at the interface is located away from cell boundaries. If this happens (will not be very frequent) the LSI exchange force will have to be modified. In the normal case the exchange force in the Cartesian x-direction (u velocity) may look like:

$$\left(\psi_{l;l\uparrow m;m}+\vartheta_{l;l\uparrow m;m}\left(\mathbf{u}^{m;m}-\mathbf{u}^{l;l}\right)\right)\vec{\mathbf{e}}_x=A_L+B_L(u_L^{m;m}-u_L^{l;l}) \tag{4.45}$$

L is here the cell index. However, if the LSI is very close to the cell face L-LYM we will have to replace (4.45) with:

$$\left(\psi_{l;l\uparrow m;m}+\vartheta_{l;l\uparrow m;m}\left(\mathbf{u}^{m;m}-\mathbf{u}^{l;l}\right)\right)\vec{\mathbf{e}}_x=A_L+B_L(u_{LYM}^{m;m}-u_L^{l;l}) \tag{4.46}$$

In this case the computational stencil is slightly changed, as we have momentum between two different fluids in two neighbouring computational cells.

We note that here the mixing stress term $\nabla\cdot\left(\alpha^{k;l}\rho^{k;l}\Gamma_{sub}{}^{k;l}\nabla\mathbf{u}^{k;l}\right)$ is simplified for the discussion purpose.

4.4.1 Pressure and viscous stress boundary conditions

In equation (4.44) the pressure and viscous stress field belongs to each fluid: However, as long as the flow is free the different continuous fields will exchange force and, except a capillary pressure at the interface the pressures can be assumed to be approximately identical in a given point in space, giving

$$p=p^{l;l}\ ;\ l=1,\ N \tag{4.47}$$

At inflow and outflow boundaries appropriate boundary conditions for pressure has to be applied. This will be discussed later.

The viscous stress internally in each continuous fluid is given by the local stress $\boldsymbol{\tau}^{l;l}$, controlled by the local viscosity $\mu^{l;l}$. The total viscous force on a control volume is represented by:

$$\mathbf{f} = \oint_{CV} \left(\alpha^{k;l} \nabla \cdot \left\langle \boldsymbol{\tau}^{l;l} \right\rangle^{i} + \nabla \cdot \left(\alpha^{k;l} \rho^{k;l} \Gamma_{sub}{}^{k;l} \nabla \mathbf{u}^{k;l} \right) \right) dV \tag{4.48}$$

The first part of (4.48) represents the viscous force by the continuous phase alone, while the latter part represents the added stress due to the volume-internal interactions between fluid and dispersed field, as well as dispersed field internal interactions. The from literature preferred treatment of this term as $\mathbf{f} \approx \oint_{CV} \nabla \cdot \left(\alpha^{k;l} \rho^{k;l} \Gamma_{effective}{}^{k;l} \nabla \mathbf{u}^{k;l} \right) dV$ seems questionable but possible.

More critical is the handling of the stresses at walls and LSIs. At all these interfaces we will have to use the methods elaborated in Chapter 2.3.1. It is important that the interface (LSI) shear forces respect Newton's third law and that the continuous filed velocities inside a volume sharing two or more continuous filed are implicitly coupled. This will be elaborated at a later stage.

5 Numerical discretization of the multi-fluid equations

5.1 Momentum equations

The momentum equation, disregarding mass transfer, reads (eq. (4.44)):

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\hat{\rho}^{k;l} \mathbf{u}^{k;l} \right) + \nabla \cdot \left(\hat{\rho}^{k;l} \mathbf{u}^{k;l} \mathbf{u}^{k;l} \right) = \hat{\rho}^{k;l} \mathbf{g} \\
&+ \alpha^{k;l} \nabla \cdot \left(- \left\langle p^{l;l} \right\rangle^{i} \mathbf{I} + \left\langle \boldsymbol{\tau}^{l;l} \right\rangle^{i} \right) + \nabla \cdot \left(\hat{\rho}^{k;l} \Gamma_{sub}{}^{k;l} \nabla \mathbf{u}^{k;l} \right) \\
&+ \left(1 - \delta_{kl} \right) K^{k;l} \left(\mathbf{u}^{l;l} - \mathbf{u}^{k;l} \right) + \delta_{kl} \sum_{j=1}^{L} K^{j;l} \left(\mathbf{u}^{j;l} - \mathbf{u}^{l;l} \right) \\
&+ \delta_{kl} \sum_{\substack{\text{All continuous fields m;m,} \\ \text{interacting with l;l}}} \left(\psi_{l;l \uparrow m;m} + \vartheta_{l;l \uparrow m;m} \left(\mathbf{u}^{m;m} - \mathbf{u}^{l;l} \right) \right) + \mathbf{S}^{k;l}
\end{aligned} \tag{5.1}$$

, and where the source term, assumed to be treated fully explicit, is given by:

$$\mathbf{S}^{k;l} = \underbrace{\left(1-\delta_{kl}\right) K^{k;l}\left(\frac{\nu_t^{\,l;l}}{Sc_t^{\,l;l}}\frac{\nabla\overline{\alpha^{l;l}}}{\overline{\alpha^{l;l}}} - \frac{\nu_t^{\,l;l}}{Sc_t^{\,k;l}}\frac{\nabla\overline{\alpha^{k;l}}}{\overline{\alpha^{k;l}}}\right)}_{\text{k is dispersed in l}}$$
$$-\underbrace{\delta_{kl}\sum_{j=1}^{L} K^{j;l}\left(\frac{\nu_t^{\,l;l}}{Sc_t^{\,l;l}}\frac{\nabla\overline{\alpha^{l;l}}}{\overline{\alpha^{l;l}}} - \frac{\nu_t^{\,l;l}}{Sc_t^{\,j;l}}\frac{\nabla\overline{\alpha^{j;l}}}{\overline{\alpha^{j;l}}}\right)}_{\text{j is dispersed in l}} \tag{5.2}$$

The terms of type $K^{k;l}\left(\mathbf{u}^{l;l}-\mathbf{u}^{k;l}\right)$ and $K^{j;l}\left(\mathbf{u}^{j;l}-\mathbf{u}^{l;l}\right)$ denotes friction between fields, and where we in the latter case sum over all fields j, dispersed in k=l.
As long as we can provide sub-models for the large scale interface friction we may simulate any fluid-fluid , or fluid-solid system, allowing both direct simulations and more coarse grained simulation possibilities.

The semi discretized momentum equation for *k* in *l* now reads:

$$\begin{aligned}
&\hat{\rho}^{0,k;l}\frac{u_i^{\,k;l}-u_i^{\,0,k;l}}{\Delta t} + \frac{\partial}{\partial x_j}\left(\hat{\rho}^{0,k;l}u_j^{\,0,k;l}u_i^{\,0,k;l}\right) - u_i^{\,0,k;l}\frac{\partial}{\partial x_j}\left(\hat{\rho}^{0,k;l}u_j^{\,0,k;l}\right)\\
&= -\alpha^{0,k;l}\frac{\partial}{\partial x_i}p + \alpha^{0,k;l}\frac{\partial}{\partial x_j}\tau_{ji}^{k;l} + \hat{\rho}^{0;k;l}g_i\\
&+\frac{\partial}{\partial x_j}\left(\hat{\rho}^{k;l}\Gamma_{sub}^{\,k;l}\frac{\partial}{\partial x_j}u_i^{\,k;l}\right) + \sum_{m;n}\widehat{K}_{m;n}^{k;l}\left(u_i^{\,m;n}-u_i^{\,k;l}\right) + S_i^{\,0,k;l}
\end{aligned} \tag{5.3}$$

The drag force in (5.3) has been generalized by:

$$\begin{aligned}
&\sum_{m;n}\widehat{K}_{m;n}^{k;l}\left(\mathbf{u}^{m;n}-\mathbf{u}^{k;l}\right) \equiv \left(1-\delta_{kl}\right)K^{k;l}\left(\mathbf{u}^{l;l}-\mathbf{u}^{k;l}\right) + \delta_{kl}\sum_{j=1}^{L}K^{j;l}\left(\mathbf{u}^{j;l}-\mathbf{u}^{l;l}\right)\\
&+\delta_{kl}\sum_{\substack{\text{All continuous fields m;m,}\\ \text{interacting with l;l}}}\left(\boldsymbol{\psi}_{l;l\uparrow m;m} + \vartheta_{l;l\uparrow m;m}\left(\mathbf{u}^{m;m}-\mathbf{u}^{l;l}\right)\right)
\end{aligned} \tag{5.4}$$

For now we have not included the special cases for the LSI or wall perfectly aligned with the computational cell face, here represented by equation (4.46).
Similar to how we proceed for single phase flow, we do the first fractional step for the momentum equation:

$$\begin{aligned}
&\hat{\rho}^{0,k;l}\frac{u_i^{\,*,k;l}-u_i^{\,0,k;l}}{\Delta t} + \frac{\partial}{\partial x_j}\left(\hat{\rho}^{0,k;l}u_j^{\,0,k;l}u_i^{\,0,k;l}\right) - u_i^{\,0,k;l}\frac{\partial}{\partial x_j}\left(\hat{\rho}^{0,k;l}u_j^{\,0,k;l}\right)\\
&= -\alpha^{0,k;l}\frac{\partial}{\partial x_i}p^0 + \alpha^{0,k;l}\frac{\partial}{\partial x_j}\tau_{ji}^{k;l}(\mathbf{u}^*) + \hat{\rho}^{0;k;l}g_i\\
&+\frac{\partial}{\partial x_j}\left(\hat{\rho}^{k;l}\Gamma_{sub}^{\,k;l}\frac{\partial}{\partial x_j}u_i^{\,*,k;l}\right) + \sum_{m;n}\widehat{K}_{m;n}^{k;l}\left(u_i^{\,0,m;n}-u_i^{\,0,k;l}\right) + S_i^{\,0,k;l}
\end{aligned} \tag{5.5}$$

In this first step we solve implicitly for the viscous stresses (turbulent stresses to be included in this step later). As external forces, friction, stress and pressure gradient balance out by large, the explicit friction term is included.
By subtracting (5.5) from (5.3) we obtain:

$$\begin{aligned}
&\hat{\rho}^{0,k;l}\,\frac{u_i^{\,k;l}-u_i^{\,*,k;l}}{\Delta t}\\
&=-\alpha^{0,k;l}\,\frac{\partial}{\partial x_i}\left(p-p^0\right)+\cancel{\alpha^{0,k;l}\,\frac{\partial}{\partial x_j}\left(\tau_{ji}^{k;l}-\tau_{ji}^{k;l}(\mathbf{U}^*)\right)}\\
&+\cancel{\frac{\partial}{\partial x_j}\left(\hat{\rho}^{k;l}\Gamma_{sub}^{\,k;l}\,\frac{\partial}{\partial x_j}\left(u_i^{\,k;l}-u_i^{\,*,k;l}\right)\right)}\\
&+\sum_{m;n}\widehat{K}_{m;n}^{k;l}\left(u_i^{\,m;n}-u_i^{\,k;l}-u_i^{\,0,m;n}+u_i^{\,0,k;l}\right)
\end{aligned}\tag{5.6}$$

By neglecting the crossed out term in equation (5.6) we find that:

$$\begin{aligned}
&u_i^{\,k;l}-K_{m;n}^{k;l}\,\frac{\Delta t}{\hat{\rho}^{0,k;l}}\left(u_i^{\,m;n}-u_i^{\,k;l}\right)\\
&=u_i^{\,*,k;l}-K_{m;n}^{k;l}\,\frac{\Delta t}{\hat{\rho}^{0,k;l}}\left(u_i^{\,0,m;n}-u_i^{\,0,k;l}\right)-\alpha^{0,k;l}\,\frac{\Delta t}{\hat{\rho}^{0,k;l}}\,\frac{\partial}{\partial x_i}\,p'
\end{aligned}\tag{5.7}$$

Here we assume the summing convention for $K_{m;n}^{k;l}\,\frac{\Delta t}{\hat{\rho}^{0,k;l}}\left(u_i^{\,m;n}-u_i^{\,k;l}\right)$. We recognize that for (5.7) we may write

$$\mathbf{A}\mathbf{u}=\mathbf{b}-\Delta t\mathbf{a}\frac{\partial p'}{\partial x_i}\tag{5.8}$$

where

$$\mathbf{a}=\begin{bmatrix}\vdots\\ \alpha^{0,k;l}/\hat{\rho}^{0,k;l}\\ \vdots\end{bmatrix}\tag{5.9}$$

and

$$\mathbf{b}=\begin{bmatrix}\vdots\\ u_i^{\,*,k;l}-K_{m;n}^{k;l}\,\frac{\Delta t}{\hat{\rho}^{0,k;l}}\left(u^{0,m;n}-u^{0,k;l}\right)\\ \vdots\end{bmatrix}\tag{5.10}$$

So the solution for the velocities may be written as,

$$\mathbf{u}=\mathbf{A}^{-1}\mathbf{b}-\Delta t\mathbf{A}^{-1}\mathbf{a}\frac{\partial p'}{\partial x_i}\tag{5.11}$$

In a two phase flow with 4 fields **A** is a 4x4 matrix, in three phase flows we have a 9 x 9 matrix. For SIMCOFLOW we may limit ourselves (for now to) three phases, but allowing one extra field for oil at the air-water interface. We may note that the inversion of the local matrix **A** is crucial for a strong and implicit

momentum coupling between the dispersed and continuous fields. Accordingly, the operation in eq. (5.11) will affect all velocities if the system becomes sufficiently stiff. We are now ready to solve for the pressure field. The challenge here is that we have to fulfil the condition

$$\sum_{l=1}^{L}\sum_{k=1}^{L}\alpha^{k;l} = \sum_{l=1}^{L}\sum_{k=1}^{L}\frac{\hat{\rho}^{k;l}}{\rho_l} = 1.0 \tag{5.12}$$

In addition we have $N_{tot} = \sum_{l=1}^{L}\sum_{k=1}^{L}\Upsilon^{k;l}$ fields in our system, each with individual mass equations, and we have only one common pressure. However, we do not have to consider mass and momentum equations for fields which are rigid wall with zero velocity in the direction normal to the wall.

5.2 Obtaining a pressure equation

We start out with the mass equations for all "living" fields. We can now make a prediction of the field masses, using explicit interpolation.

$$\frac{\hat{\rho}^{*,k;l} - \hat{\rho}^{0,k;l}}{\Delta t} + \nabla\left(\hat{\rho}^{0,k;l}\mathbf{u}^{0,k;l}\right) = S^{*,k;l} \tag{5.13}$$

The final mass equation is:

$$\frac{\hat{\rho}^{k;l} - \hat{\rho}^{0,k;l}}{\Delta t} + \nabla\left(\hat{\rho}^{0,k;l}\mathbf{u}^{k;l}\right) = S^{k;l} \tag{5.14}$$

Subtraction the two equations above we obtain:

$$\frac{\hat{\rho}^{k;l} - \hat{\rho}^{*,k;l}}{\Delta t} + \nabla\left(\hat{\rho}^{0,k;l}\left(\mathbf{u}^{k;l} - \mathbf{u}^{0,k;l}\right)\right) = S^{k;l} - S^{*,k;l} \tag{5.15}$$

Note that eqs. (5.13) and (5.14) are both fully conserving mass, so no mass loss/gain is expected.

We can now insert eq. (5.15) into eq. (5.12), to obtain:

$$\sum_{l=1}^{L}\sum_{k=1}^{K(l)}\frac{\hat{\rho}^{*,k;l} - \Delta t\nabla\left(\hat{\rho}^{0,k;l}\left(\mathbf{u}^{k;l} - \mathbf{u}^{0,k;l}\right)\right) - \Delta t\left(S^{k;l} - S^{*,k;l}\right)}{\rho_l} = 1.0 \tag{5.16}$$

The equation above is re-organized as:

$$-\sum_{l=1}^{L}\sum_{k=1}^{K(l)}\frac{\Delta t\nabla\left(\hat{\rho}^{0,k;l}\left(\mathbf{u}^{k;l}-\mathbf{u}^{0,k;l}\right)\right)}{\rho_l}=1.0-\sum_{l=1}^{L}\sum_{k=1}^{K(l)}\frac{\hat{\rho}^{*,k;l}-\Delta t\left(S^{k;l}-S^{*,k;l}\right)}{\rho_l} \tag{5.17}$$

Equation (5.17) is now our pressure equation. We see that if the starred extensive densities, and possible mass source corrections, do not fulfil the volume sharing conditions, this will derive a pressure field variation, in order to restore correct volume sharing. Note that the new velocity is given by eq.(5.11), which can be written as:

$$\mathbf{u}=\mathbf{A}^{-1}\mathbf{B}-\mathbf{A}^{-1}\left(\alpha^{0,k;l}\frac{\Delta t}{\hat{\rho}^{0,k;l}}\right)\nabla p'\equiv\mathbf{u}^{**,k;l}-DU^{k;l}\nabla p' \tag{5.18}$$

The equation above defined following quantities:

$$\begin{aligned}&\left(\mathbf{A}^{-1}\mathbf{B}\right)^{k;l}=\mathbf{u}^{**,k;l}\\&DU^{k;l}=\left\{\mathbf{A}^{-1}\left(\alpha^{0,k;l}\frac{\Delta t}{\hat{\rho}^{0,k;l}}\right)\right\}^{k;l}\end{aligned} \tag{5.19}$$

The pressure correction equation (5.17) now reads:

$$\begin{aligned}&\sum_{l=1}^{L}\sum_{k=1}^{K(l)}\frac{\Delta t\nabla\left(\hat{\rho}^{0,k;l}DU^{k;l}\nabla p'\right)}{\rho_l}\\&-\sum_{l=1}^{L}\sum_{k=1}^{K(l)}\frac{\Delta t\nabla\left(\hat{\rho}^{0,k;l}\left(\mathbf{u}^{**,k;l}-\mathbf{u}^{0,k;l}\right)\right)}{\rho_l}\\&=1.0-\sum_{l=1}^{L}\sum_{k=1}^{K(l)}\frac{\hat{\rho}^{*,k;l}-\Delta t\left(S^{k;l}-S^{*,k;l}\right)}{\rho_l}\end{aligned} \tag{5.20}$$

In eq. (5.20) only pressure update p' and intrinsic phase densities $\hat{\rho}$ are not known. The temperature can be based on a first prediction. To improve convergence we may linearize the densities due to:

$$\frac{1}{\rho_l(p,T)}\approx\frac{1}{\rho_l(p^0,T^0)+\chi_l p'+\beta_l T'}\approx\frac{1-\chi_l p'/\rho_l^0-\beta_l T'/\rho_l^0}{\rho_l^0} \tag{5.21}$$

Using the linearization we obtain:

$$\Delta t\sum_{l=1}^{L}\sum_{k=1}^{K(l)}\frac{\cancel{1-\chi_l p'/\rho_l^0-\beta_l T'/\rho_l^0}}{\rho_l^0}\nabla\left(\hat{\rho}^{0,k;l}DU^{k;l}\nabla p'\right)$$
$$-\Delta t\sum_{l=1}^{L}\sum_{k=1}^{K(l)}\frac{1-\chi_l p'/\rho_l^0-\beta_l T'/\rho_l^0}{\rho_l^0}\left\{\nabla\left(\hat{\rho}^{0,k;l}\left(\mathbf{u}^{**,k;l}-\mathbf{u}^{0,k;l}\right)\right)+\left(S^{k;l}-S^{*,k;l}\right)\right\}$$
$$=1.0-\sum_{l=1}^{L}\sum_{k=1}^{K(l)}\left[\hat{\rho}^{*,k;l}-\Delta t\left(S^{k;l}-S^{*,k;l}\right)\right]\frac{1-\chi_l p'/\rho_l^0-\beta_l T'/\rho_l^0}{\rho_l^0}$$

(5.22)

5.3 The solution procedure is now:

1) Prediction of extensive densities, by equation (5.13)
2) A first prediction of the phase velocities, eq. (5.5). Here the stress terms are treated implicitly.
3) Establishing the momentum exchange matrix coefficients, equation (5.7) and (5.8), for the final momentum equation
4) Computing inverse of A matrix, equation (5.8).
5) Establishing the coefficients in the relation between final velocity and pressure update gradient, see equation (5.18)
6) By using the pressure correction (update) equation (5.22) , compute the pressure correction $p' = p - p^0$
7) Update pressure
8) Update all field velocities by equation (5.18)
9) Update extensive phase densities by equation (5.15)
10) Compute volume fractions, using $\alpha^{k;l} = \hat{\rho}^{k;l} / \rho_l(p,T)$. Checking $\sum_{l=1}^{L}\sum_{k=1}^{K(l)}\alpha^{k;l} - 1.0$.
11) Advance to next time step

Note that no iterations are planned here. However, it may be necessary to iterate the pressure equation (5.22). In this case, for the density in the denominator we use $\rho_l^0 \to \rho(p+p', T+T')$, or – we update the pressure and densities for each iteration.

6 Respecting the jump conditions

In the discussions above we have not considered some important jump conditions for the fluid-fluid interfaces.

The simplest version of the mass jump condition (no mass transfer) is that for the kl-interface we have:

$$\left[\left(\mathbf{u}^{k;k}-\mathbf{u}^{l;l}\right)\cdot\mathbf{n}_{k;k\uparrow l;l}\right]^{Interface}=0 \qquad (6.1)$$

Condition (6.1) assures that the velocities of the continues are identical, at the interface, and in the direction normal to the interface. If we use a VOF approach the phases have identical velocities in each computational volume. Then condition (6.1) is automatically assured. However, as we allow individual phase velocities in

interface cells the condition (6.1) must be explicitly impressed on the system. The only way this can be done is by allowing for phase specific pressures, i.e. all continuous fluid fields have their genuine field pressure.

6.1 Application of discretised mass jump condition

The mass jump condition is centred around point $\Psi_{i,j}$, as illustrated in Figure 7. For the interface referred to in eq. (6.1) the jump discrete jump condition is (constant grid spacings in all directions):

$$\begin{aligned}&\Psi_{i,j} = \\ &\frac{1}{2}\left(u^k_{i,j}+u^k_{i,j+1}-u^l_{i,j}+u^l_{i,j+1}\right)\cdot\frac{1}{2}\left(\alpha^k_{i+1,j}+\alpha^k_{i+1,j+1}-\alpha^k_{i,j}-\alpha^k_{i,j+1}\right)/\Delta x \\ &+\frac{1}{2}\left(v^k_{i,j}+v^k_{i+1,j}-v^l_{i,j}+v^l_{i+1,j}\right)\cdot\frac{1}{2}\left(\alpha^k_{i,j+1}+\alpha^k_{i+1,j+1}-\alpha^k_{i,j}-\alpha^k_{i+1,j}\right)/\Delta y \\ &=0\end{aligned} \tag{6.2}$$

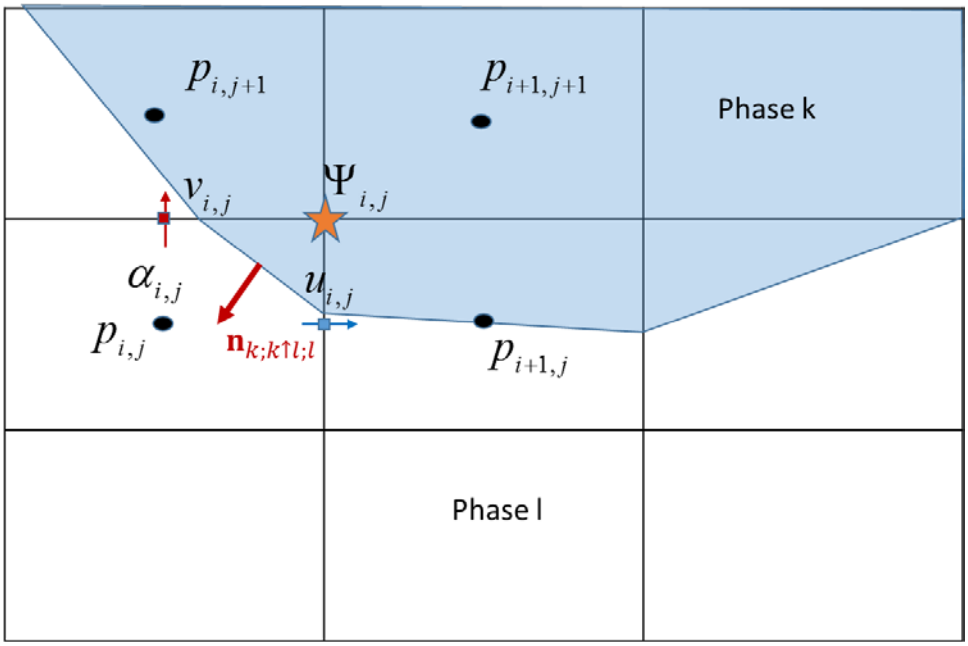

Figure 7 Stencil for mass jump condition is centred around point $\Psi_{i,j}$.

In equation (6.2) the interface normal is replaced by the volume fraction gradient. We may now take the extended to multiple pressures relation (5.18) and write as:

$$\mathbf{u}^k=\left(\mathbf{A}^{-1}\mathbf{B}\right)^k-\left(\mathbf{A}^{-1}\left(\alpha^{0,k;l}\frac{\Delta t}{\hat{\rho}^{0,k;l}}\right)\right)^k\nabla p^{k\,\prime}\equiv\mathbf{u}^{**,k;k}-DU^{k;k}\nabla p^{k\,\prime} \tag{6.3}$$

By combining equations (6.2) and (6.3) we obtain a relation that couples the gradients in phase (continuous field) pressures of the two fluid sharing the interface. The phase pressures must always adjust such that the condition (6.1) is fulfilled. Mass jump stencil in eq. (6.2) is compact as it involves pressures, volume fractions and velocities in only four cells for 2D (8 cells for 3D).

6.2 A better approach to handle the mass jump condition

First we may note that the mass equation has two forms. We simplify by neglecting dispersed fields and have incompressible fluids.

Standard form a): $$\frac{\partial}{\partial t}\alpha^{k;k} + \nabla\left(\alpha^{k;k}\mathbf{u}^{k;k}\right) = S^{k;k} \tag{6.4}$$

Alternative form b): $$\frac{1}{\Delta V}\sum_{m=1}^{N} A^{k;m}\mathbf{u}^{k;m}\cdot\mathbf{n}^{k;m} + \nabla\left(\alpha^{k;k}\mathbf{u}^{k;k}\right) = S^{k;k} \tag{6.5}$$

The first terms in (6.5) is an integral, but is represented by the semi-discrete form. Here $A^{k;m}$ is the interfacial area of and $\mathbf{n}^{k;m}$ is the interface normal vector, pointing out of fluid zone k, while $\mathbf{u}^{k;m}$ is the fluid velocity at the interface.
The two forms above, together, is identical to the statement :

$$\frac{\partial}{\partial t}\alpha^{k;k} = \frac{1}{\Delta V}\sum_{m=1}^{N} A^{k;m}\mathbf{u}^{k;m}\cdot\mathbf{n}^{k;m} \tag{6.6}$$

We may note that (6.6) tells that there is a direct link between the interface velocity and the time derivative of the volume fraction, *both taken at the very same moment.*

From the equations above we have that in a two-phase situation (gas (g) and liquid (l)) we have the jump condition:

$$\left[\left(\mathbf{u}^{g;l} - \mathbf{u}^{l;g}\right)\cdot\mathbf{n}_{l;l\uparrow g;g}\right]^{Interface} = 0, \tag{6.7}$$

and we wrote the two mass equations in the flux form:

$$\sum_{m=1}^{N} A^{l;g}\mathbf{u}^{l;l}\cdot\mathbf{n}_{l;l\uparrow g;g} + \nabla\left(\alpha^{l;l}\mathbf{u}^{l;l}\right) = S^{l;l} \tag{6.8}$$

$$\sum_{m=1}^{N} A^{g;l}\mathbf{u}^{g;g}\cdot\mathbf{n}_{g;g\uparrow l;l} + \nabla\left(\alpha^{g;g}\mathbf{u}^{g;g}\right) = S^{g;g} \tag{6.9}$$

As the interface areas are the same and the two normal vectors are of opposite sign, we can implement eq. (6.7) by adding eqs. (6.8) and (6.9):

$$\nabla\left(\alpha^{g;g}\mathbf{u}^{g;g}\right) + \nabla\left(\alpha^{l;l}\mathbf{u}^{l;l}\right) = S^{g;g} + S^{l;l} \tag{6.10}$$

Equation (6.10) is further consistent with

$$\alpha^{g} + \alpha^{l} = 1 \quad\Leftrightarrow\quad \frac{\partial}{\partial t}\left(\alpha^{g} + \alpha^{l}\right) = 0 \tag{6.11}$$

Note that above we used superscripts g and l to represent a simplified situation without dispersed fields.
The interesting part is that by assuring that the volume fractions sum to 1.0 we have taken case of the mass jump conditions, resulting in pressure equation that can be based on:

$$\sum_{m=1}^{N}\left(\frac{\alpha^{*,m,t^{n+1}} - \alpha^{m,t^{n}}}{\Delta t} + \nabla\left(\alpha^{m,t^{n}}\mathbf{u}^{m,t^{n+1}}\right) = S^{m,t^{n}}\right) \tag{6.12}$$

At this point we recognize that $\alpha^{*,m,t^{n+1}}$ is an explicit prediction of the continuous fluid fractions.

As we search a solution where $\sum_{m=1}^{N}\frac{\alpha^{m,t^{n+1}}}{\Delta t}=\frac{1}{\Delta t}$, we may write:

$$\sum_{m=1}^{N}\left(-\frac{\alpha^{m,t^{n}}}{\Delta t}+\nabla\left(\alpha^{m,t^{n}}\mathbf{u}^{m,t^{n+1}}\right)=S^{m,t^{n}}\right) \tag{6.13}$$

If the equations have been solved correctly at the previous time step we would have $\sum_{m=1}^{N}\frac{\alpha^{m,t^{n}}}{\Delta t}=\frac{1}{\Delta t}$.

However, this may not be perfectly true. Hence, the old time step contribution to the transient term is retained in eq. (6.13).

Furthermore, as $\sum_{m=1}^{N}\frac{\alpha^{*,m,t^{n}}}{\Delta t}\neq\frac{1}{\Delta t}$, we cannot expect the prediction to fulfil the mass jump conditions. Based on (5.18) we may write the velocity as:

$$\mathbf{u}^{m,t^{n+1}}=\mathbf{u}^{***,m}-DU^{m}\nabla p^{t^{n+1}} \tag{6.14}$$

Using eqs. (6.13) and (6.14) we obtain the pressure Poisson equation:

$$\frac{1}{\Delta t}+\sum_{m=1}^{N}\left(-\frac{\alpha^{m,t^{n}}}{\Delta t}+\nabla\left(\alpha^{m,t^{n}}\mathbf{u}^{***,m}\right)\right)=\sum_{m=1}^{N}\left(S^{m,t^{n}}+\nabla\left(\alpha^{m,t^{n}}DU^{m}\nabla p^{t^{n+1}}\right)\right) \tag{6.15}$$

By solving for the new pressure (eq. (6.15)) and updating the velocities (eq. (6.15), we can now find the final volume fraction. ***This must be done by redoing the calculation of the volume fractions, i.e. solving the equations (6.4) once more.*** *The solution method to compute* $\alpha^{m,t^{n+1}}$ *must be exactly the same as used when making the prediction* $\alpha^{*,m,t^{n}}$.

As the new velocities will fulfil equation (6.13), they will also fulfil $\sum_{m=1}^{N}\frac{\alpha^{m,t^{n+1}}}{\Delta t}\equiv 0$.

6.3 The momentum jump condition

The momentum jump condition between fluids 1 and 2 may be written as:

$$\dot{m}(\mathbf{u}_2-\mathbf{u}_1)+\left[\left(-p\mathbf{I}+\boldsymbol{\tau}\right)_2-\left(-p\mathbf{I}+\boldsymbol{\tau}\right)_1\right]\cdot\mathbf{n}+2\sigma H_s\mathbf{n}-\nabla_s\sigma=0 \tag{6.16}$$

Here $\dot{m}$ is the mass transfer rate across the interface, $\mathbf{n}$ is the normal vector pointing out of phase 2, H_s is the surface curvature, which may be positive or negative, σ is the surface tension and ∇_s is the surface gradient. In the case of no mass transfer and neglecting surface tension effects, we have for the normal stress:

$$p_1=p_2=p_{\text{interface}} \tag{6.17}$$

We consider the pressure force acting on a volume shared by continuous fluids k and l. The pressure force acting on the continuous fluids k can be written as:

$$\begin{aligned}\vec{f}^{\,k} &= -\nabla\left(\alpha_k p^k\right) + p^{I;k-l}\nabla\alpha_k \\ &\approx -\nabla\left(\alpha_k p^k\right) + \frac{1}{2}\left(p^l + p^k\right)\nabla\alpha_k \\ &= -\alpha_k \nabla p^k + \frac{1}{2}\left(p^l - p^k\right)\nabla\alpha_k\end{aligned} \tag{6.18}$$

Here we have approximated the interface pressure by:

$$p^{I;k-l} \approx \frac{1}{2}\left(p^l + p^k\right) \tag{6.19}$$

This approximation may be rough and may have to be improved at a later stage.
Similarly for the continuous fluids l, we have

$$\begin{aligned}\vec{f}^{\,l} &= -\nabla\left(\alpha_l p^l\right) + p^{I;k-l}\nabla\alpha_l \\ &\approx -\nabla\left(\alpha_l p^l\right) + \frac{1}{2}\left(p^l + p^k\right)\nabla\alpha_l \\ &= -\alpha_l \nabla p^l + \frac{1}{2}\left(p^k - p^l\right)\nabla\alpha_l\end{aligned} \tag{6.20}$$

The additional term $\frac{1}{2}\left(p^k - p^l\right)\nabla\alpha_l$ will contribute to accelerate the liquid into a region with gas if the liquid pressure is larger than the gas pressure.
We note that for a two fluid situation, adding the forces for the two phases (mixture assessment) we have:

$$\begin{aligned}\vec{f}^{\,k} + \vec{f}^{\,l} &= -\nabla\left(\alpha_k p^k\right) - \nabla\left(\alpha_l p^l\right) \\ &= -\nabla p; \quad p \equiv \frac{\alpha_k p^k + \alpha_l p^l}{\alpha_k + \alpha_l}\end{aligned} \tag{6.21}$$

The momentum jump condition assist the coupling of the two pressures sharing the interface.

As a consequence of equation (6.18) the expression for the new velocity (ref. eq. (6.3)) will now have the shape:

$$\mathbf{u}^k = \mathbf{u}^{**,k;k} + \left\{\mathbf{C}\otimes\mathbf{p}'\right\}^k \quad , \tag{6.22}$$

Where $\left\{\mathbf{C}\otimes\mathbf{p}'\right\}^k$ expresses that pressures of all phases may contribute to the new velocity of a given phase.

This means that for the liquid velocity (only x-component shown) we have :

$$u_x^l = u_x^{**,l} + A(p_{l;i,j}^l - p_{l;i+1,j}^l) + B(p_{l;i,j}^g - p_{l;i+1,j}^g) + C\left(p_{l;i,j}^l + p_{l;i+1,j}^l\right) + D(p_{l;i,j}^g + p_{l;i+1,j}^g), \tag{6.23}$$

Where A,B,C and D are known coefficients. We note that in regions where there is no large scale interface, i.e. $\left|\nabla\alpha_l\right| = \left|\nabla\alpha_g\right| = 0$, we have only one active pressure, and here the jump condition (6.1) is obsolete. We

need to assess both volume fraction gradients to address correctly solid walls. Close to a solid wall we have that only one of the two $|\nabla \alpha_k| = 0$.

We further note that in a vertex (ref Figure 7) where both $|\nabla \alpha_k| \neq 0$, sharing the interface, we have two active pressures. All cells included in the vertex have two active (different) phase pressures. The equation system is still well-posed and solvable as we have one more equation in the system, i.e. the mass jump condition.
We now assume that the mass jump condition is discretized according to (6.2). In all vertices where $\frac{\partial \alpha_l}{\partial x}, \frac{\partial \alpha_l}{\partial y} \neq 0$ we will have a mass jump equation. The vertices are only interior, not at the boundaries of the domain. Pressure cells which are contained in active vertices will connect to two active pressures, through some cell boundary, even if the cell itself has only one active pressure. Intuitively, the number of equations and unknown should match, but this has to checked in further details.

In a system with M continuous fluids we will need M different pressures to solve for.

7 Solution issues

Currently we have not discussed boundary conditions for inlets, outlets and possible free boundaries. This is left for now. However, we need to consider the overall solution strategy.

We have now basically split the universe into regions with one fluid being continuous (example is $\alpha^{l;l}$), and with several dispersed fields $\alpha^{k;l}$ existing only inside $\alpha^{l;l}$. For the local flow inside each continuous region, away from solid walls or fluid-fluid large scale interfaces, the model is expected to work fine without any surprises.

8 List of symbols

α	volume fraction
ρ	density (kg/m3)
ρ_l	intrinsic density of phase *l* (kg/m3)
$\hat{\rho}^{k;l}$	extensive phase density (kg/m3), $\hat{\rho}^{k;l} = \alpha^{k;l}\rho_l$
χ_l	variation of density with pressure at constant temperature: $\chi_l = \left.\frac{\partial \rho_l}{\partial p}\right\|_{T^0}$
β_l	thermal expansion coefficient: $\beta_l = \left.\frac{\partial \rho_l}{\partial T}\right\|_{p^0}$
τ	viscous stress term (Pa)
DU	defined by equation (5.19)
G	total external force (N/m^3)
$\widehat{K}^{k;l}_{m;n}$	Interface friction coefficient between velocity fields *m;n* and *k;l*
N_{tot}	total number of fields in the flow
p	pressure at end of time step (Pa)
S	source term
Δt	time step (s)

p' $p' = p - p^0$

T temperature at end of time step (K)

T' $T' = T - T^0$

$U^{k;l}$ field velocity of phase k, dispersed into phase *l*; (m/s)

U^{**} defined by equation (5.19)

Superskripts

0 previous time step

k;j field k, submerged into phase j

9 List of references

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10 Appendix

Some averaging rules, applicable to ensemble averaging of the drag force:

$$\begin{aligned} &\mathrm{K}\overline{\alpha_p\left(u-u_p\right)} = \mathrm{K}\left(\overline{\alpha_p\left(\tilde{u}+u''\right)} - \overline{\alpha_p\widetilde{u_p}}\right) \\ &= \mathrm{K}\left(\left(\overline{\alpha_p}\tilde{u}+\overline{\alpha_p u''}\right) - \overline{\alpha_p}\widetilde{u_p}\right) \\ &= \mathrm{K}\overline{\alpha_p}\left(\tilde{u}-\widetilde{u_p}\right) + K\overline{\alpha_p u''} \end{aligned} \qquad (10.1)$$

Velocity without index represents the fluid, and subscript p represents particles. Above the overbar is ensemble averaging. K is a coefficient which is assumed independent of velocity and α_p is the volume fraction of the dispersed phase. We have following relations, where the velocity is split into the direct

ensemble averaged velocity $\overline{u_p}$ and fluctuation $u_p^{'}$, or into the mass averaged velocity $\widetilde{u_p}$ and fluctuation $u_p^{"}$. A we assume that the density is constant we have that

$$\widetilde{u_p} \equiv \frac{\overline{\alpha_p \rho_p u_p}}{\overline{\alpha_p \rho_p}} = \frac{\overline{\alpha_p u_p}}{\overline{\alpha_p}} \quad , \tag{10.2}$$

and

$$\widetilde{u_p^{"}} \equiv \frac{\overline{\alpha_p \rho_p u_p^{"}}}{\overline{\alpha_p \rho_p}} = \frac{\overline{\alpha_p u_p^{"}}}{\overline{\alpha_p}} = 0 . \tag{10.3}$$

Useful relations are:

$$\text{A} : \quad \alpha u = \alpha\left(\overline{u} + u'\right) = \alpha\left(\tilde{u} + u"\right) \tag{10.4}$$

$$\text{B} : \quad \left(\overline{u} + u'\right) = \left(\tilde{u} + u"\right) \Rightarrow u" = \overline{u} - \tilde{u} + u' \tag{10.5}$$

$$\overline{u"} = \overline{u} - \tilde{u} \tag{10.6}$$

$$\left(\overline{\alpha u} + \overline{\alpha' u'}\right) = \overline{\alpha}\tilde{u} \Rightarrow = \overline{u"} = \overline{u} - \tilde{u} = -\frac{\overline{\alpha' u'}}{\overline{\alpha}} \tag{10.7}$$

If we extend to a generic N-phase multiphase flow, the correlation between a disperse field fraction α_i and fluid fluctuation velocity $u"$, becomes after using (10.5) and (10.7):

$$\begin{aligned} \overline{\alpha_i u"} &\overset{n-phase}{=} -\overline{\alpha_i}\frac{\overline{\alpha' u'}}{\overline{\alpha}} + \overline{\alpha_i' u'} \\ &= \frac{\overline{\alpha_i}}{\overline{\alpha}}\frac{\nu_{t,c}}{Sc_{t,c}}\nabla\overline{\alpha} - \frac{\nu_{t,i}}{Sc_{t,i}}\nabla\overline{\alpha_i} \\ &= \overline{\alpha_i}\left(\frac{\nu_{t,c}}{Sc_{t,c}}\frac{\nabla\overline{\alpha}}{\overline{\alpha}} - \frac{\nu_{t,i}}{Sc_{t,i}}\frac{\nabla\overline{\alpha_i}}{\overline{\alpha_i}}\right) \end{aligned} \tag{10.8}$$

Here and $\nu_{t,i}$ is a dispersion coefficient (kinematic viscosity) of dimension (m^2/s), and $Sc_{t,i}$ is a Schmidt number, expressing the relative strength of dispersion of dispersed fields and momentum dispersion of the continuous field.

Using our notation we may then write:

$$\overline{\alpha^{j;l}\mathbf{u}^{"l;l}} = \overline{\alpha^{j;l}}\left(\frac{\nu_t^{l;l}}{Sc_t^{l;l}}\frac{\nabla\overline{\alpha^{l;l}}}{\overline{\alpha^{l;l}}} - \frac{\nu_t^{l;l}}{Sc_t^{j;l}}\frac{\nabla\overline{\alpha^{j;l}}}{\overline{\alpha^{j;l}}}\right)$$
$$\overline{\alpha^{k;l}\mathbf{u}^{"l;l}} = \overline{\alpha^{k;l}}\left(\frac{\nu_t^{l;l}}{Sc_t^{l;l}}\frac{\nabla\overline{\alpha^{l;l}}}{\overline{\alpha^{l;l}}} - \frac{\nu_t^{l;l}}{Sc_t^{k;l}}\frac{\nabla\overline{\alpha^{k;l}}}{\overline{\alpha^{k;l}}}\right) \qquad (10.9)$$

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