Equation Summary of a Filtered Two-Fluid Model Implemented in OpenFOAM®

Federico Municchi, Stefan Radl

January 5, 2018 - v1.0

Chapter 1

Governing equations for filtered TFM

The following equations have been extracted from Cloete [1], and are presented here in a slightly modified version.

1.1 Filtered mass conservation equations

$$\frac{\partial}{\partial t}\left(\rho_\mathrm{s}\overline{\phi}_\mathrm{s}\right) + \boldsymbol{\nabla}\cdot\left(\rho_\mathrm{s}\overline{\phi}_\mathrm{s}\widetilde{\boldsymbol{u}}_\mathrm{s}\right) = 0 \tag{1.1}$$

$$\frac{\partial}{\partial t}\left(\rho_\mathrm{g}\overline{\phi}_\mathrm{g}\right) + \boldsymbol{\nabla}\cdot\left(\rho_\mathrm{g}\overline{\phi}_\mathrm{g}\widetilde{\boldsymbol{u}}_\mathrm{g}\right) = 0 \tag{1.2}$$

1.2 Filtered momentum conservation equations

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\rho_\mathrm{s}\overline{\phi}_\mathrm{s}\widetilde{\boldsymbol{u}}_\mathrm{s}\right) + \boldsymbol{\nabla}\cdot\left(\rho_\mathrm{s}\overline{\phi}_\mathrm{s}\widetilde{\boldsymbol{u}}_\mathrm{s}\widetilde{\boldsymbol{u}}_\mathrm{s}\right) = -\overline{\phi}_\mathrm{s}\boldsymbol{\nabla}\overline{p} - \boldsymbol{\nabla}\cdot\left(\overline{\boldsymbol{\Sigma}_\mathrm{s}^\mathrm{meso}} + \overline{\boldsymbol{\Sigma}_\mathrm{s}^\mathrm{fric}} + \overline{\boldsymbol{\Sigma}_\mathrm{s}^\mathrm{micro}}\right)\\ &+ \widetilde{\boldsymbol{f}_{gs}} - \overline{\phi_\mathrm{s}'\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}_\mathrm{g}'} + \rho_\mathrm{s}\overline{\phi}_\mathrm{s}\mathbf{g}\end{aligned} \tag{1.3}$$

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\rho_\mathrm{g}\overline{\phi}_\mathrm{g}\widetilde{\boldsymbol{u}}_\mathrm{g}\right) + \boldsymbol{\nabla}\cdot\left(\rho_\mathrm{g}\overline{\phi}_\mathrm{g}\widetilde{\boldsymbol{u}}_\mathrm{g}\widetilde{\boldsymbol{u}}_\mathrm{g}\right) = -\overline{\phi}_\mathrm{g}\boldsymbol{\nabla}\overline{p} - \boldsymbol{\nabla}\cdot\left(\overline{\boldsymbol{\Sigma}_\mathrm{g}^\mathrm{meso}} + \overline{\boldsymbol{\Sigma}_\mathrm{g}^\mathrm{micro}}\right)\\ &- \widetilde{\boldsymbol{f}_{gs}} + \overline{\phi_\mathrm{s}'\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}_\mathrm{g}'} + \rho_\mathrm{g}\overline{\phi}_\mathrm{g}\mathbf{g}\end{aligned} \tag{1.4}$$

1.3 Summary of Unclosed Terms

- Filtered gas-solid drag force $\widetilde{\boldsymbol{f}_{gs}}$. Note, this force does not include the (filtered) buoyancy force, since it is already considered in the $\boldsymbol{\nabla}\overline{p}$ term.
- The mesoscale interphase force $\overline{\phi_\mathrm{s}'\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}_\mathrm{g}'}$. This force is often neglected, and hence not discussed any further in what follows.

- The filtered stress tensors. They are often modelled by adopting a Boussinesq approach, i.e., the stress is split into a pressure and viscosity-based term, as well as (if necessary) a bulk viscosity-based term. More details are provided in Chapter 3.

Chapter 2

Drag force models for filtered TFM

2.1 Structure of drag closures

2.1.1 Classical approach relying on a heterogeneity index

In classical models, the mesoscale interphase forces are lumped into the drag force. Also, one assumes that the difference between the filtered and the microscale drag coefficient can be expressed with a heterogeneity index $\boldsymbol{H_D}$ (i.e., essentially a correction function):

$$\widetilde{\boldsymbol{f}_{\mathrm{gs}}} - \overline{\phi_{\mathrm{s}}' \boldsymbol{\nabla} \cdot \boldsymbol{\sigma}_{\mathrm{g}}'} = \boldsymbol{H_D} \; \widetilde{\beta} \; (\widetilde{\boldsymbol{u}}_{\mathrm{g}} - \widetilde{\boldsymbol{u}}_{\mathrm{s}}) \tag{2.1}$$

Notice that $\widetilde{\beta}$ has the functional form of the microscopic drag, but it is calculated using filtered quantities. Also, $\boldsymbol{H_D}$ is typically modeled as $H_D \; \boldsymbol{I}$, i.e., an isotropic correction factor is employed. In the present description $\boldsymbol{H_D}$ is retained as a (symmetric) tensorial quantity to ensure generality. In most situations, however, it will be sufficient to consider off-diagonal elements of this tensor to be zero [1].

The following properties of $\boldsymbol{H_D}$ must hold;

- $\boldsymbol{H_D} \to \mathbf{1}$ for sufficiently small filter sizes (i.e., ”well-resolved” simulations).
- $\boldsymbol{H_D} \to \mathbf{1}$ in the dilute (i.e., a single particle sedimenting at its terminal speed) and dense limit (i.e., a closely-packed, hence homogeneous, particle suspension sedimenting at steady state).

The heterogeneity index can be expressed as a function of multiple markers. Popular choices for these markers are:

- filter size Δ_f
- filtered solid volume fraction $\overline{\phi}_{\mathrm{s}}$
- filtered slip velocity $\widetilde{u}_{gs,i} = \widetilde{u}_i - \widetilde{v}_i$. This velocity can be scaled in order to have a dimensionless marker, which is preferable.

2.1.2 Advanced approach relying on a correction factor and slip velocity

This approach has been proposed by Cloete [1], and closures relying on this approach will be documented after publication. Cloete [1] also introduces a new class of markers to improve the predictive quality of the closures.

2.2 Closures for the heterogeneity index

2.2.1 Igci & Sundaresan 2011

This isotropic closure is documented in Igci & Sundaresan [2]. This publication details on 2D and 3D results. While the former are applicable to large domains, the latter are applicable to comparably small cell sizes (i.e., small filter sizes have been used in the development of this closure). In what follows, only the 2D results are summarized (see Table 2 in Igci & Sundaresan [2]).

$$H_D = 1 - h_\phi(\overline{\phi}_\mathrm{s}) h_{Fr}(\Delta_f) \tag{2.2}$$

Here the filter-size-based Froude number is defined as $Fr_{filter} = v_t^2/(g\Delta_f)$. The individual terms are closed as follows

$$h_\phi = \begin{cases} 2.7\overline{\phi}_\mathrm{s}^{-0.234} & \overline{\phi}_\mathrm{s} < 0.0012 \\ -0.019\overline{\phi}_\mathrm{s}^{-0.455} + 0.963 & 0.0012 \leq \overline{\phi}_\mathrm{s} < 0.014 \\ 0.868\,\exp(0.38\overline{\phi}_\mathrm{s}) - 0.176\,\exp(-119.2\overline{\phi}_\mathrm{s}) & 0.014 \leq \overline{\phi}_\mathrm{s} < 0.25 \\ -4.59 \cdot 10^{-5}\,\exp(19.75\overline{\phi}_\mathrm{s}) + 0.852\,\exp(-0.268\overline{\phi}_\mathrm{s}) & 0.25 \leq \overline{\phi}_\mathrm{s} < 0.455 \\ (\overline{\phi}_\mathrm{s} - 0.59)(-1501\overline{\phi}_\mathrm{s}^3 + 2203\overline{\phi}_\mathrm{s}^2 - 1054\overline{\phi}_\mathrm{s} + 162) & 0.455 \leq \overline{\phi}_\mathrm{s} < 0.59 \\ 0 & 0.59 \leq \overline{\phi}_\mathrm{s} \end{cases} \tag{2.3}$$

$$h_{Fr} = \frac{Fr_{filter}^{-1.3}}{Fr_{filter}^{-1.3} + 1.5} \tag{2.4}$$

2.2.2 Milioli et al. 2013

This isotropic closure is documented in Milioli et al. 2013 [3], and based on large 2D resolved simulations. The authors define a dimensionless filter size as $\Delta_f^* = g\Delta_f/v_t^2$, and a dimensionless slip velocity as $\widetilde{u}_{gs}^* = \widetilde{u}_{gs}/v_t$. Note, that the magnitude of the filtered slip velocity is used. The following assumptions apply inherently to this closure:

- There are two versions of this closure: (i) a two marker version that relies on $\overline{\phi}_\mathrm{s}$ and $\widetilde{u}_{gs}^*$. The filter (and hence grid) size is NOT used as a marker. (ii) a three-marker version in which the function f_{lin} (see below) also depends on the dimensionless filter size. In what follows only version (i) is discussed (for version ii see the appendix of Milioli et al. 2013 [3]).

- The two-marker version of the closure is valid for $\Delta_f^* >\sim 25$ only.
- For smaller Δ_f^* coefficients are changing, reaching a constant value at large Δ_f^*. Thus, one might use the three-marker version for small grid sizes.
- Two possible functions (envelopes) named $h_{env,1}$ and $h_{env,2}$ can be considered. The latter function is simpler and should not deteriorate the results significantly.

The correlation is expressed as

$$H_D = 1 - \min\left(h_{env,1}(\overline{\phi}_s) \text{ or } h_{env,2}(\overline{\phi}_s), h_{lin}(\widetilde{u}^*_{gs})\right) \tag{2.5}$$

With parameters:

$$\begin{aligned}
h_{env,1} &= \begin{cases} \dfrac{0.5643(1+\overline{\phi}_s)\overline{\phi}_s^{0.15}}{0.5766\overline{\phi}_s^{0.3}+0.1997}, & 0 < \overline{\phi}_s \leq 0.10 \\ 0.8428 + 0.6393\overline{\phi}_s - 0.6743\overline{\phi}_s^{2}, & 0.1 < \overline{\phi}_s \leq 0.54 \\ \dfrac{0.4099(0.65-\overline{\phi}_s)^{0.25}}{\overline{\phi}_s^{-0.25} - 0.9281}, & 0.54 < \overline{\phi}_s \leq 0.65 \\ 0, & \overline{\phi}_s < 0.65 \end{cases} \\
h_{env,2} &= 0.8428 + 0.6393\overline{\phi}_s - 0.6743\overline{\phi}_s^{2}, \qquad 0 > \overline{\phi}_s \leq 0.65 \\
h_{lin} &= \begin{cases} f_\infty h_1, & h_1 > 0 \\ 0, & h_1 < 0 \end{cases} \\
f_\infty &= 0.882\left(2.145 - \frac{7.8\widetilde{u}^{*1.8}_{gs}}{7.746\widetilde{u}^{*1.8}_{gs} + 0.5586}\right) \\
h_1 &= \frac{1.6\widetilde{u}^*_{gs}+4}{7.9\widetilde{u}^*_{gs}+0.08}\overline{\phi}_s + 0.9394 - \frac{0.22}{0.6\widetilde{u}^*_{gs}+0.01}
\end{aligned} \tag{2.6}$$

2.2.3 Schneiderbauer & Pirker 2014

This isotropic closure is documented in Schneiderbauer & Pirker [4], and applicable to comparably small cell sizes (i.e., small filter sizes have been used in the development of this closure). This is a three marker-based closure that relies on $\overline{\phi}_s$, $\widetilde{u}^*_{gs}$ (i.e., the filtered slip velocity scaled with the terminal settling speed of an isolated particle), and a dimensionless filter size $\Delta_f^+ = \Delta_f / L_{char}$ with $L_{char} = v_t^2/g\ Fr^{-2/3}$. Note, that the magnitude of the filtered slip velocity is used.

The proposed correlation is:

$$H_D = \left[1 - h_\phi(\overline{\phi}_s)h_\Delta(\Delta_f^+)\right] H_u(\overline{\phi}_s, \Delta_f^+, \widetilde{u}^*_{gs}) \tag{2.7}$$

The individual terms are closed as follows

$$\begin{aligned}
H_u(\overline{\phi}_\mathrm{s}, \Delta_f, \widetilde{u}^*_{gs}) &= \left(\widetilde{u}^*_{gs}\right)^{-C f_u^\Delta(\Delta_f^+) f_u^\phi(\overline{\phi}_\mathrm{s})} \\
C &\approx 9 \\
f_u^\phi(\overline{\phi}_\mathrm{s}) &= \overline{\phi}_\mathrm{s}\left(\phi^{\max} - \overline{\phi}_\mathrm{s}\right) \\
f_u^\Delta(\Delta_f^+) &= \frac{\Delta_f^{+5}}{\Delta_f^{+5} + 1024}
\end{aligned} \tag{2.8}$$

$$h_\phi(\overline{\phi}_\mathrm{s}) = \frac{-6.743\overline{\phi^*}^2 + 6.728\overline{\phi^*}}{\overline{\phi^*}^3 - 7.247\overline{\phi^*}^2 + 6.289\overline{\phi^*} + 0.384}, \quad \overline{\phi^*} = \frac{\overline{\phi}_\mathrm{s}}{\phi^{\max}} \tag{2.9}$$

$$h_\Delta(\Delta_f^+) = \frac{\Delta_f^{+2.664}}{\Delta_f^{+2.664} + 25.89} \tag{2.10}$$

2.2.4 Sarkar et al. 2016

This isotropic closure is documented in the study of Sarkar et al. 2016 [5], and based on 3D resolved simulations. The authors define a dimensionless filter size as $\Delta_f^* = g\Delta_f/v_t^2$, and a dimensionless slip velocity as $\widetilde{u}^*_{gs} = \widetilde{u}_{gs}/v_t$. Note, that the magnitude of the filtered slip velocity is used. The following assumptions apply inherently to this closure:

- The closure reported below is valid for $\Delta_f^* > 1.3495$ only.
- The closure does not respect the limit of zero correction for large volume fractions. Thus, it cannot be used for very dense flows.

The proposed correlation is:

$$H_D = 1 - \min\left[\left(a + \frac{b}{\widetilde{u}^*_\mathrm{gs}}\right)\overline{\phi}_\mathrm{s}^{\,c\left(\frac{1}{\Delta_f} - 1\right) + \frac{d}{\widetilde{u}^*_\mathrm{gs}}}, c_\mathrm{max}\right] \tag{2.11}$$

With coefficients: $a = 0.9506$, $b = 0.1708$, $c = 0.049$, $d = 0.3358$ and $c_\mathrm{max} = 0.97$.

2.2.5 Cloete 2017

This isotropic closure is documented in the PhD thesis [1]. The author defines a scaled dimensionless filter size as $\Delta_f^* = g\Delta_f/v_t^2 - \Delta^*_\mathrm{fine}$, and a dimensionless slip velocity as $\widetilde{u}^+_{gs} = \widetilde{u}_{gs}/v_{hom}$. Here v_{hom} is the steady state sedimentation velocity of a homogeneous suspension at the filtered volume fraction. Note, that the magnitude of the filtered slip velocity is used. Δ^*_fine is the dimensionless fine grid resolution, which was 0.1285. Scaling of the dimensionless filter size ensures that the correct vanishes in case the grid resolution approaches that of the fine grid simulation.

The proposed correlation is:

$$
\begin{aligned}
-\log_{10}(H_D) = \operatorname{atan}(x_1\Delta_f^*\overline{\phi}_\mathrm{s}) \\
\operatorname{atan}(x_2\Delta_f^* max(\overline{\phi}_\mathrm{max} - \overline{\phi}_\mathrm{s}, 0)) \\
\operatorname{atan}(x_3\Delta_f^*)\left(\frac{2}{\pi}\right)^3 \\
\left(x_4\log_{10}(\widetilde{u}_{gs}^+) + x_5\Delta_f^{*x_6} + x_7\left(\log_{10}(\widetilde{u}_{gs}^+)\right)^2\left[1 - \frac{\operatorname{atan}(x_8\Delta_f^*)}{\pi/2}\right]\right) \\
if - \log_{10}(H_D) < 0 :\ H_D = 1
\end{aligned}
\tag{2.12}
$$

The following choice of constants is proposed:

$$
\begin{aligned}
x_1 = 36.6, x_2 = 22.6, x_3 = 1.68, x_4 = 0.835, x_5 = 0.140, \\
x_6 = 0.188, x_7 = 1.33, x_8 = 3.28, \overline{\phi}_\mathrm{max} = 0.551
\end{aligned}
\tag{2.13}
$$

2.3 Microscale drag closures

These are well established in literature, and are availalbe in standard simulation tools. The current implementation is based on the models available in the OpenFOAM 4.x github repository.

Chapter 3

Stress models for filtered TFM

3.1 Preliminary remarks related to stress closures

- $\nabla \cdot \boldsymbol{\sigma}'_{\mathrm{g}}$ can be approximated with $\boldsymbol{\nabla} p'$ since gas-phase deviatoric stress components are typically negligible.
- Often, the Boussinesq approach is chosen to close the stresses. However, often this is inadequate for the mesoscale stress component [1]. To fix this, one might (i) add an anisotropic components of the stress tensor $\overline{\boldsymbol{\sigma}}^{i}_{q,a}$, or (ii) simply provide closures for all components of the stress tensor. The item (ii) can be realized with item (i) by simply setting the Boussinesq terms zero. Thus, item (i) has been implemented in the current library, following - in principle - the spirit of Sarkar et al. [5].

The following general expression for stress description is used (i.e., an 'extended' Boussinesq description) to close the stress for each phenomenon i:

$$
\begin{aligned}
\overline{\boldsymbol{\Sigma}^{\mathrm{i}}_{\mathrm{q}}} = \left[p^{\mathrm{i}}_{\mathrm{q}} - \lambda^{\mathrm{i}}_{\mathrm{q}} \mathrm{tr}\left(\mathbf{D}_{\mathrm{q}}\right)\right] \mathbf{I} - 2\mu^{\mathrm{i}}_{\mathrm{q}} \mathbf{S}_{\mathrm{q}} + \overline{\boldsymbol{\sigma}}^{i}_{q,a}, \\
\mathrm{q} = \mathrm{s}, \mathrm{g} \quad \mathrm{i} = \mathrm{meso}, \mathrm{fric}, \mathrm{micro}
\end{aligned}
\tag{3.1}
$$

The following additional relations are used (see, for example, Milioli et al. [3]):

$$
\begin{aligned}
\mathbf{D}_{\mathrm{q}} &= \frac{1}{2}\left[\boldsymbol{\nabla}\widetilde{\boldsymbol{u}}_{\mathrm{q}} + \left(\boldsymbol{\nabla}\widetilde{\boldsymbol{u}}_{\mathrm{q}}\right)^{T}\right], \\
\mathbf{S}_{\mathrm{q}} &= \mathbf{D}_{\mathrm{q}} - \frac{1}{3}\mathrm{tr}\left(\mathbf{D}_{\mathrm{q}}\right)\mathbf{I}, \\
\mathrm{S}_{\mathrm{q}} &= \sqrt{2\mathbf{S}_{\mathrm{q}} : \mathbf{S}_{\mathrm{q}}}
\end{aligned}
\tag{3.2}
$$

The term $\lambda^{\mathrm{i}}_{\mathrm{q}}$ is the bulk viscosity. A classical expression therefore would be $\lambda^{\mathrm{i}}_{\mathrm{q}} = -\frac{2}{3}\mu^{\mathrm{i}}_{\mathrm{q}}$. If not otherwise specified, the bulk viscosity is set to zero.

3.2 Closures for mesoscale stresses

3.2.1 Milioli et al. 2013 with Schneiderbauer and Pirker 2014 modification

This simple Boussinesq-based model is based on the work of Milioli et al. [3] with a modification proposed by Schneiderbauer and Pirker [4]. The dimensional filtered viscosities are closed using the dimensional filter size and shear rate, as well as the phase density:

$$\mu_{\mathrm{s}}^{\mathrm{meso}} = C_{\mu,\mathrm{s}}^{\mathrm{meso}} \rho_s \Delta_f^2 \mathrm{S}_{\mathrm{s}}, \quad \mu_{\mathrm{g}}^{\mathrm{meso}} = C_{\mu,\mathrm{g}}^{\mathrm{meso}} \rho_g \Delta_f^2 \mathrm{S}_{\mathrm{g}} \tag{3.3}$$

We note in passing that in the literature [3] expressions for normalized stresses and viscosities are provided, and that Schneiderbauer and Pirker [4] use a dimensionless filter sizes that is scaled differently from that in [3]. Pressures are calculated similarly, but using a different exponent on the filter size. Based on dimensional quantities one arrives at:

$$p_{\mathrm{s}}^{\mathrm{meso}} = C_{p,\mathrm{s}}^{\mathrm{meso}} \rho_s \left(\frac{v_t^2}{g}\right)^{\frac{-2}{7}} \Delta_f^{\frac{16}{7}} \mathrm{S}_{\mathrm{s}}^2, \;\; p_{\mathrm{g}}^{\mathrm{meso}} = C_{p,\mathrm{g}}^{\mathrm{meso}} \rho_g \left(\frac{v_t^2}{g}\right)^{\frac{-2}{7}} \Delta_f^{\frac{16}{7}} \mathrm{S}_{\mathrm{g}}^2 \tag{3.4}$$

The closure constants provided by Milioli et al. [3] in the slightly modified form [4] read for the solid phase:

$$C_{\mu,\mathrm{s}}^{\mathrm{meso}} = 0.105\overline{\phi}_{\mathrm{s}} + \frac{0.001\overline{\phi}_{\mathrm{s}}}{\phi_{\mathrm{s}}^{\max}\left(\phi_{\mathrm{s}}^{\max} - \overline{\phi}_{\mathrm{s}}\right)} \tag{3.5}$$

$$C_{p,\mathrm{g}}^{\mathrm{meso}} = 0.17\overline{\phi}_{\mathrm{s}} + \frac{0.02325\overline{\phi}_{\mathrm{s}}}{\phi_{\mathrm{s}}^{\max}\left(\phi_{\mathrm{s}}^{\max} - \overline{\phi}_{\mathrm{s}}\right)^{\frac{3}{4}}} \tag{3.6}$$

For the gas phase, the corresponding expressions are

$$C_{\mu,\mathrm{g}}^{\mathrm{meso}} = 0.17 - 0.275\overline{\phi}_{\mathrm{s}}. \tag{3.7}$$

$$C_{p,\mathrm{g}}^{\mathrm{meso}} = 0.275 - 0.44\overline{\phi}_{\mathrm{s}}. \tag{3.8}$$

3.2.2 Sarkar et al. 2016

This extended Boussinesq-based model is based on the work of Sarkar et al. [5]. It features an anisotropic correction, specifically, normal stress differences are accounted for via the $\overline{\boldsymbol{\sigma}}_{s,a}$ term. The dimensional filtered viscosities are closed using the dimensional filter size and shear rate, as well as the phase density:

$$\mu_{\mathrm{s}}^{\mathrm{meso}} = C_{\mu,\mathrm{s}}^{\mathrm{meso}} \rho_s \left(\frac{v_t^2}{\mathrm{g}}\right)^{2/7} \Delta_f^{12/7} \mathrm{S}_{\mathrm{s}}, \qquad \mu_{\mathrm{g}}^{\mathrm{meso}} = C_{\mu,\mathrm{g}}^{\mathrm{meso}} \rho_g \Delta_f^2 \mathrm{S}_{\mathrm{g}} \tag{3.9}$$

Pressures are calculated similarly, and based on dimensional quantities one arrives at:

$$p_{\mathrm{s}}^{\mathrm{meso}} = C_{p,\mathrm{s}}^{\mathrm{meso}} \rho_s \left(\frac{v_t^2}{g}\right)^{-3/7} \Delta_f^{17/7} \mathrm{S}_{\mathrm{s}}^2, \;\; p_{\mathrm{g}}^{\mathrm{meso}} = C_{p,\mathrm{g}}^{\mathrm{meso}} \rho_g \left(\frac{v_t^2}{g}\right)^{-5/7} \Delta_f^{19/7} \mathrm{S}_{\mathrm{g}}^2 \tag{3.10}$$

The closure constants provided by Sarkar et al. [5] read for the solid phase:

$$C_{\mu,\mathrm{s}}^{\mathrm{meso}} = \frac{0.02518 \overline{\phi}_{\mathrm{s}}^{\,1.123}}{\phi_{\mathrm{s}}^{\mathrm{max}} - \overline{\phi}_{\mathrm{s}}} \tag{3.11}$$

$$C_{p,\mathrm{s}}^{\mathrm{meso}} = \frac{0.0236 \overline{\phi}_{\mathrm{s}}^{\,1.115}}{\phi_{\mathrm{s}}^{\mathrm{max}} - \overline{\phi}_{\mathrm{s}}} \tag{3.12}$$

For the gas phase, the corresponding expressions are:

$$C_{\mu,\mathrm{g}}^{\mathrm{meso}} = 0.0330 + 0.218 \overline{\phi}_{\mathrm{s}} - 0.485 \overline{\phi}_{\mathrm{s}}^2 \tag{3.13}$$

$$C_{p,\mathrm{g}}^{\mathrm{meso}} = 0.0661 + 0.0164 \overline{\phi}_{\mathrm{s}} - 0.194 \overline{\phi}_{\mathrm{s}}^2 \tag{3.14}$$

The anisotropic solid phase stess tensor $\overline{\boldsymbol{\sigma}}_{s,a}$ is calculated via:

$$\overline{\boldsymbol{\sigma}}_{s,a}^{\mathrm{meso}} = \begin{bmatrix} -\frac{1}{3} N_{\mathrm{s}}^{meso} & 0 & 0 \\ 0 & \frac{2}{3} N_{\mathrm{s}}^{meso} & 0 \\ 0 & 0 & -\frac{1}{3} N_{\mathrm{s}}^{meso} \end{bmatrix} \tag{3.15}$$

$$N_{\mathrm{s}}^{meso} = 2.6 p_{\mathrm{s}}^{\mathrm{meso}} \left(1 - \frac{\overline{\phi}_{\mathrm{s}}}{\phi_{\mathrm{s}}^{\mathrm{max}}}\right)^{1.2} \tag{3.16}$$

3.2.3 Cloete 2017

This Boussinesq-based model is based on the work of Cloete [1]. It models the solids stresses only (gas-phase stresses are neglected). The author defines a scaled dimensionless filter size as $\Delta_f^* = g\Delta_f / v_t^2 - \Delta_{\mathrm{fine}}^*$, and a dimensionless shear rate magnitude as $\mathrm{S}_{\mathrm{q}}^* = \mathrm{S}_{\mathrm{q}} / \left(\frac{g}{v_t}\right)$. The expression for the mesoscale solids pressure reads:

$$\frac{p_{\mathrm{s}}^{\mathrm{meso}}}{\rho_s v_t^2} = \frac{2}{\pi} x_1 \overline{\phi}_{\mathrm{s}}^{x_2} \operatorname{atan}\left(x_3 \Delta_f^{*x_4} \mathrm{S}_{\mathrm{s}}^{*x_5} \max(x_6 - \overline{\phi}_{\mathrm{s}}, 0)\right) \Delta_f^{*x_7} \mathrm{S}_{\mathrm{s}}^{*x_8 + x_9 \Delta_f^{*x_{10}}}$$
$$+ \frac{2}{\pi} x_{11} \overline{\phi}_{\mathrm{s}}^{x_{12}} \operatorname{atan}\left(x_{13} \max(x_{14} - \overline{\phi}_{\mathrm{s}}, 0)\right) \Delta_f^{*x_{15}}$$

$$(3.17)$$

with $x_1 = 0.774$, $x_2 = 1.72$, $x_3 = 0.403$, $x_4 = 0.610$, $x_5 = 1.19$, $x_6 = 0.684$, $x_7 = 1.57$, $x_8 = 1.00, x_9 = 0.331, x_{10} = -0.103, x_{11} = 0.123, x_{12} = 0.621, x_{13} = 2.89, x_{14} = 0.591, x_{15} = 1.05$.

The expression for the mesoscale solids viscosity reads (note the term S_s^* on the left hand side of the expression, i.e., a typical shear stress is modeled similar to the pressure):

$$\frac{\mu_\mathrm{s}^\mathrm{meso}}{\rho_s v_t^3/g}\mathrm{S}_\mathrm{s}^* = \frac{2}{\pi}x_1\overline{\phi}_\mathrm{s}^{x_2}\mathrm{atan}\left(x_3\Delta_f^{*x_4}\mathrm{S}_\mathrm{s}^{*x_5}\max(x_6-\overline{\phi}_\mathrm{s},0)\right)\Delta_f^{*x_7}\mathrm{S}_\mathrm{s}^{*x_8+x_9\Delta_f^{*x_{10}}} + \frac{2}{\pi}x_{11}\overline{\phi}_\mathrm{s}^{x_{12}}\mathrm{atan}\left(x_{13}\max(x_{14}-\overline{\phi}_\mathrm{s},0)\right)\Delta_f^{*x_{15}} \tag{3.18}$$

with $x_1 = 0.350$, $x_2 = 0.545$, $x_3 = 2.43$, $x_4 = 0.141$, $x_5 = 0.772$, $x_6 = 0.624$, $x_7 = 1.83$, $x_8 = 1.40, x_9 = 0.348, x_{10} = -0.0905, x_{11} = 0.130, x_{12} = -0.498, x_{13} = 3.58, x_{14} = 0.618, x_{15} = 0.968$.

3.2.4 Schneiderbauer's 2017 mixing length model

This model is based on the idea that the fluctuation energy k_q in each phase q can be predicted, e.g., based on an additional transport equation. Subsequently, it relies on a Boussinesq-based approach to close the stress tensor. Specifically, the equations provided by Schneiderbauer [6] read:

$$p_\mathrm{q}^\mathrm{meso} = \frac{2}{3}\overline{\phi}_\mathrm{q}\rho_q k_q, \qquad \mu_\mathrm{q}^\mathrm{meso} = \overline{\phi}_\mathrm{q}\mu_\mathrm{t,q} \tag{3.19}$$

$$\mu_\mathrm{t,q} = \rho_\mathrm{q}k_\mathrm{q}^{1/2}l_\mathrm{m,q} \tag{3.20}$$

$$l_\mathrm{m,q} = C_{\nu\mathrm{q}}\Delta_f \tag{3.21}$$

Where $C_{\nu\mathrm{s}} = 0.25$ and $C_{\nu\mathrm{g}} = 0.4$.

3.3 Closures for frictional stresses

Schneiderbauer and Pirker 2012

This model is based on the work of Schneiderbauer and Pirker [7], and relies on the so-called $\mu - I$ rheology. Thus, this model has not been specifically developed for filtered TFMs, but rather for well-resolved simulations based on a TFM.

The model relies in its core on the inertial number that is defined as follows:

$$I_s = \frac{2\mathrm{S}_\mathrm{s}d_\mathrm{s}}{\sqrt{p_\mathrm{s}^\mathrm{fr}/\rho_\mathrm{s}}} \tag{3.22}$$

The frictional pressure is closed as follows

$$p_{\mathrm{s}}^{\mathrm{fr}} = 4\rho_{\mathrm{s}} \left(\frac{b d_{\mathrm{s}} \mathrm{S}_{\mathrm{s}}}{\phi_{\mathrm{s}}^{\max} - \overline{\phi}_{\mathrm{s}}} \right)^2, \quad b = 0.2, \quad \phi_{\mathrm{s}}^{\max} = 0.6 \tag{3.23}$$

$$\mu_{\mathrm{s}}^{\mathrm{fr}} = \frac{\mu_i(I_s) p_{\mathrm{s}}^{\mathrm{fr}}}{2\mathrm{S}_{\mathrm{s}}} \tag{3.24}$$

$$\begin{aligned} &\mu_i(I_s) = \mu_i^{st} + \frac{\mu_i^c - \mu_i^{st}}{I_0/I_s + 1}, \\ &I_0 = 0.279, \quad \mu_i^{st} = \tan(20.9^\circ), \quad \mu_i^c = \tan(32.76^\circ) \end{aligned} \tag{3.25}$$

Warning: coefficients are given for mono-disperse glass particles! Also, regularization is necessary to elegantly handle the singularities for low shear rates and near the close packing limit.

Cloete 2017 model

This simple (pressure-based) model is based on the work of Cloete [1]. The author defines a scaled dimensionless filter size as $\Delta_f^* = g\Delta_f/v_t^2 - \Delta_{\mathrm{fine}}^*$, and a dimensionless shear rate magnitude as $\mathrm{S}_{\mathrm{q}}^* = \mathrm{S}_{\mathrm{q}}/\left(\frac{g}{v_t}\right)$. The expression for the frictional solids pressure reads:

$$\frac{p_{\mathrm{s}}^{\mathrm{meso}}}{\rho_s v_t^2} = \overline{\phi}_{\mathrm{s}}^{x_1} \Delta_f^{*x_2 + x_3 \Delta_f^{*x_4}} \left(x_5 \mathrm{S}_{\mathrm{s}}^{*x_6 + x_7 \Delta_f^{*x_8}} \Delta_f^{*x_9} + x_{10} \frac{e^{x_{11} \max(\overline{\phi}_{\mathrm{s}} - x_{12}, 0)}}{(\overline{\phi}_{\mathrm{s,max}} - \overline{\phi}_{\mathrm{s}})^{x_{13}}} \right) \tag{3.26}$$

with $x_1 = 2.78$, $x_2 = 1.00$, $x_3 = -0.0726$, $x_4 = 0.722$, $x_5 = 0.124$, $x_6 = 2.00$, $x_7 = -0.0689$, $x_8 = 0.684, x_9 = 0.807, x_{10} = 7.3810^{-6}, x_{11} = 36.0, x_{12} = 0.485, x_{13} = 3.64, \overline{\phi}_{\mathrm{s,max}} = 0.63$.

3.4 Closures for microscale stresses

Sarkar et al. 2016

This is a simple model proposed by Sarkar et al. [5], and similar to their meso-scale model. The model is formulated in dimensional quantities.

$$\mu_s^{\mathrm{micro}} = C_{\mu,\mathrm{s}}^{\mathrm{micro}} \rho_s \left(\frac{v_t^2}{\mathrm{g}} \right)^{6/7} \Delta_f^{8/7} \mathrm{S}_{\mathrm{s}} \tag{3.27}$$

$$p_s^{\mathrm{micro}} = C_{p,\mathrm{s}}^{\mathrm{micro}} \rho_s \Delta_f^2 \mathrm{S}_{\mathrm{s}}^2 \tag{3.28}$$

The closure expressions for viscosity and pressure read as follows, respectively:

$$C_{\mu,\mathrm{s}}^{\mathrm{micro}} = \frac{0.00307\overline{\phi}_{\mathrm{s}}^{\,1.544}}{\phi_{\mathrm{s}}^{\max} - \overline{\phi}_{\mathrm{s}}} \tag{3.29}$$

$$C_{p,\mathrm{s}}^{\mathrm{micro}} = \frac{0.01797\overline{\phi}_{\mathrm{s}}^{\,1.645}}{\phi_{\mathrm{s}}^{\max} - \overline{\phi}_{\mathrm{s}}} \tag{3.30}$$

$\phi_{\mathrm{s}}^{\max} = 0.65$ needs to be used in this expression.

Chapter 4

Additional transport equations for filtered TFM

4.1 Mesoscale Kinetic energy transport equation

The following equations are based on Schneiderbauer [6].

4.1.1 Transport equation and closures

$$\begin{aligned}\frac{\partial\overline{\phi}_\mathrm{s}k_\mathrm{s}}{\partial t} + \boldsymbol{\nabla}\cdot\left(\overline{\phi}_\mathrm{s}k_\mathrm{s}\widetilde{\boldsymbol{u}}_\mathrm{s}\right) = &\underbrace{-\overline{\phi_\mathrm{s}\boldsymbol{u}_\mathrm{s}\boldsymbol{u}_\mathrm{s}}:\boldsymbol{\nabla}\widetilde{\boldsymbol{u}}_\mathrm{s}}_{\text{shear production}} + \underbrace{\frac{\widetilde{\beta}}{\rho_\mathrm{s}}\left(\overline{\phi_\mathrm{s}\boldsymbol{u}_\mathrm{s}\boldsymbol{u}_\mathrm{g}}:\overline{\phi_\mathrm{s}\boldsymbol{u}_\mathrm{s}\boldsymbol{u}_\mathrm{s}}\right)}_{\text{drag production}} \\ &-\underbrace{\overline{\phi}_\mathrm{s}\left(\epsilon-\frac{1}{\rho_\mathrm{s}}p_\mathrm{s}^\mathrm{micro}\overline{\boldsymbol{\nabla}\cdot\boldsymbol{u}_\mathrm{s}}\right)}_{\text{dissipation}} - \underbrace{\boldsymbol{\nabla}\cdot\left[\frac{1}{2}\overline{\phi_\mathrm{s}(\boldsymbol{u}_\mathrm{s}\cdot\boldsymbol{u}_\mathrm{s})\boldsymbol{u}_\mathrm{s}} + \frac{1}{\rho_\mathrm{s}}\overline{\boldsymbol{u}_\mathrm{s}\cdot(\boldsymbol{\Sigma}_\mathrm{s}^\mathrm{micro})'}\right]}_{\text{diffusion}} \\ &-\underbrace{\frac{1}{\rho_\mathrm{s}}\overline{\phi_\mathrm{s}\boldsymbol{u}_\mathrm{s}\boldsymbol{\nabla}p'}}_{\text{pressure work}}\end{aligned} \tag{4.1}$$

shear production:

$$\overline{\phi_\mathrm{s}\boldsymbol{u}_\mathrm{s}\boldsymbol{u}_\mathrm{s}}:\boldsymbol{\nabla}\widetilde{\boldsymbol{u}}_\mathrm{s} \approx 2\overline{\phi}_\mathrm{s}\nu_\mathrm{s}\mathbf{S}_\mathrm{s}:\mathbf{S}_\mathrm{s} \tag{4.2}$$

dissipation:

$$\overline{\phi}_\mathrm{s}\left(\epsilon-\frac{1}{\rho_\mathrm{s}}p_\mathrm{s}^\mathrm{micro}\overline{\boldsymbol{\nabla}\cdot\boldsymbol{u}_\mathrm{s}}\right) \approx C_{\epsilon\mathrm{s}}\overline{\phi}_\mathrm{s}\frac{k_\mathrm{s}^{3/2}}{l_\mathrm{m,s}}, \quad C_{\epsilon\mathrm{s}}\approx 1 \tag{4.3}$$

diffusion:

$$\boldsymbol{\nabla}\cdot\left[\frac{1}{2}\overline{\phi_\mathrm{s}(\boldsymbol{u}_\mathrm{s}\cdot\boldsymbol{u}_\mathrm{s})\boldsymbol{u}_\mathrm{s}} + \frac{1}{\rho_\mathrm{s}}\overline{\boldsymbol{u}_\mathrm{s}\cdot(\boldsymbol{\Sigma}_\mathrm{s}^\mathrm{micro})'}\right] \approx -\boldsymbol{\nabla}\cdot\left(\overline{\phi}_\mathrm{s}\frac{\nu_\mathrm{t,s}}{\mathrm{Sc}_\mathrm{s}}\boldsymbol{\nabla}k_\mathrm{s}\right), \quad \mathrm{Sc}_\mathrm{s}=\mathrm{const}$$

$$(4.4)$$

drag production:

$$\frac{\widetilde{\beta}}{\rho_\mathrm{s}}\left(\overline{\phi_\mathrm{s}\boldsymbol{u}_\mathrm{s}\boldsymbol{u}_\mathrm{g}} : \overline{\phi_\mathrm{s}\boldsymbol{u}_\mathrm{s}\boldsymbol{u}_\mathrm{s}}\right) \approx 2\overline{\phi}_\mathrm{s}\widetilde{\beta}\left(\xi_\mathrm{gs}\sqrt{k_\mathrm{g}k_\mathrm{s}} - k_\mathrm{s}\right) \tag{4.5}$$

4.1.2 Algebraic model

$$k_\mathrm{s} = \frac{1}{C_{\epsilon\mathrm{s}}^2}\left[-\frac{\widetilde{\beta}l_\mathrm{m,s}}{\rho_\mathrm{s}} + \sqrt{\left(\frac{\widetilde{\beta}l_\mathrm{m,s}}{\rho_\mathrm{s}}\right)^2 + 2\left(l_\mathrm{m,s}^2\ \mathbf{S}_\mathrm{s} : \mathbf{S}_\mathrm{s} + \frac{\xi_\mathrm{gs}\widetilde{\beta}l_\mathrm{m,s}k_\mathrm{g}^{1/2}}{\rho_\mathrm{s}}\right)}\right]^2 \tag{4.6}$$

$$l_\mathrm{m,s} = C_{\nu\mathrm{s}}\Delta_f \tag{4.7}$$

$$k_\mathrm{g} = \frac{1}{C_{\epsilon\mathrm{g}}^2}\left[-\frac{\overline{\phi}_\mathrm{s}\widetilde{\beta}l_\mathrm{m,s}}{\overline{\phi}_\mathrm{g}\rho_\mathrm{g}} + \sqrt{\left(\frac{\overline{\phi}_\mathrm{s}\widetilde{\beta}l_\mathrm{m,s}}{\overline{\phi}_\mathrm{g}\rho_\mathrm{g}}\right)^2 + 2\left(l_\mathrm{m,g}^2\ \mathbf{S}_\mathrm{g} : \mathbf{S}_\mathrm{g} + \frac{\xi_\mathrm{gs}\widetilde{\beta}\overline{\phi}_\mathrm{s}l_\mathrm{m,g}k_\mathrm{s}^{1/2}}{\overline{\phi}_\mathrm{g}\rho_\mathrm{g}}\right)}\right]^2 \tag{4.8}$$

$$l_\mathrm{m,g} = C_{\nu\mathrm{g}}\Delta_f \tag{4.9}$$

4.2 Volume fraction variance transport equation

4.2.1 Transport equation and closures

$$\begin{aligned}\frac{\partial\overline{\phi_\mathrm{s}^2}}{\partial t} + \boldsymbol{\nabla}\cdot\left(\overline{\phi_\mathrm{s}^2}\widetilde{\boldsymbol{u}}_\mathrm{s}\right) = &\underbrace{\overline{\phi_\mathrm{s}^2}\boldsymbol{\nabla}\cdot\widetilde{\boldsymbol{u}}_\mathrm{s}}_{\text{compression/dilation}} - \underbrace{2\overline{\phi_\mathrm{s}\boldsymbol{u}_\mathrm{s}}\boldsymbol{\nabla}\overline{\phi}_\mathrm{s}}_{\text{flow induced turbulence}} \\ &- \underbrace{2\overline{\overline{\phi}_\mathrm{s}\phi_\mathrm{s}\boldsymbol{\nabla}\cdot\boldsymbol{u}_\mathrm{s}} + \overline{\phi_\mathrm{s}^2\boldsymbol{\nabla}\cdot\boldsymbol{u}_\mathrm{s}}}_{\text{turbulent dissipation}} - \underbrace{\boldsymbol{\nabla}\cdot\left(\overline{\boldsymbol{u}_\mathrm{s}\phi_\mathrm{s}^2}\right)}_{\text{diffusion}}\end{aligned} \tag{4.10}$$

flow induced turbulence:

$$\overline{\phi_\mathrm{s}\boldsymbol{u}_\mathrm{s}} = \mathbf{e}\xi_{\phi\mathrm{s}}\sqrt{\frac{2}{3}\overline{\phi_\mathrm{s}^2}k_\mathrm{s}} \tag{4.11}$$

Where $\mathbf{e}$ is the unit vector (1,1,1), therefore the contribution is isotropic.

turbulent dissipation:

$$2\overline{\overline{\phi}_\mathrm{s}\phi_\mathrm{s}\boldsymbol{\nabla}\cdot\boldsymbol{u}_\mathrm{s}} + \overline{\phi_\mathrm{s}^2\boldsymbol{\nabla}\cdot\boldsymbol{u}_\mathrm{s}} = C_{\phi\mathrm{s}}\overline{\phi_\mathrm{s}^2}\frac{\epsilon_\mathrm{s}}{k_\mathrm{s}} \tag{4.12}$$

Where $C_{\phi\mathrm{s}} = 0.25$ is a model constant.
diffusion:

$$\boldsymbol{\nabla}\cdot\left(\overline{\boldsymbol{u}_\mathrm{s}\phi_\mathrm{s}^2}\right) = -\overline{\phi}_\mathrm{s}\nu_{\mathrm{t,s}}\boldsymbol{\nabla}\left(\frac{\overline{\phi_\mathrm{s}^2}}{\overline{\phi}_\mathrm{s}}\right) = -\overline{\phi}_\mathrm{s}\nu_{\mathrm{t,s}}\left(\frac{1}{\overline{\phi}_\mathrm{s}}\boldsymbol{\nabla}\overline{\phi_\mathrm{s}^2} - \frac{\overline{\phi_\mathrm{s}^2}}{\overline{\phi}_\mathrm{s}^2}\boldsymbol{\nabla}\overline{\phi}_\mathrm{s}\right) \tag{4.13}$$

4.2.2 Algebraic model

- turbulence is assumed to be produced and dissipated locally (i.e., transport is negligible)

$$\overline{\phi_\mathrm{s}^2} = \frac{8}{3}\frac{\xi_{\phi\mathrm{s}}^2 k_\mathrm{s}\left(\boldsymbol{\nabla}\overline{\phi}_\mathrm{s}\right)^2}{\left(\boldsymbol{\nabla}\cdot\widetilde{\boldsymbol{u}}_\mathrm{s} + C_{\phi\mathrm{s}}\dfrac{k_\mathrm{s}^{1/2}}{l_\mathrm{ms}}\right)^2}, \qquad \overline{\phi_\mathrm{g}^2} = \frac{8}{3}\frac{\xi_{\phi\mathrm{g}}^2 k_\mathrm{g}\left(\boldsymbol{\nabla}\overline{\phi}_\mathrm{g}\right)^2}{\left(\boldsymbol{\nabla}\cdot\widetilde{\boldsymbol{u}}_\mathrm{g} + C_{\phi\mathrm{g}}\dfrac{k_\mathrm{g}^{1/2}}{l_\mathrm{mg}}\right)^2}, \tag{4.14}$$

- volume fraction fluctuations are mostly determined by the volume fraction gradients
- fluctuations are high close to clusters
- denominators in the algebraic equations are always positive

realizability condition:

$$\boldsymbol{\nabla}\cdot\widetilde{\boldsymbol{u}}_\mathrm{s} + C_{\phi\mathrm{s}}C_{\epsilon\mathrm{s}}\frac{k_\mathrm{s}^{1/2}}{l_\mathrm{ms}} > 0, \qquad \boldsymbol{\nabla}\cdot\widetilde{\boldsymbol{u}}_\mathrm{g} + C_{\phi\mathrm{g}}C_{\epsilon\mathrm{g}}\frac{k_\mathrm{g}^{1/2}}{l_\mathrm{mg}} > 0, \tag{4.15}$$

Bibliography

[1] J. H. Cloete, Development of Anisotropic Filtered Two Fluid Model Closures, Phd thesis, Norwegian University of Science and Technology (2017).

[2] Y. Igci, S. Sundaresan, Constitutive Models for Filtered Two-Fluid Models of Fluidized Gas-Particle Flows, Industrial & Engineering Chemistry Research 50 (2011) 13190–13201.
URL dx.doi.org/10.1021/ie200190q

[3] C. C. Milioli, F. Milioli, W. S. Holloway, K. Agrawal, S. Sundaresan, Filtered Two-Fluid Models of Fluidized Gas-Particle Flows: New Constitutive Relations, AIChE Journal 59 (2013) 3265–3275. doi:10.1002/aic.14130.

[4] S. Schneiderbauer, S. Pirker, Filtered and heterogeneity-based subgrid modifications for gas–solid drag and solid stresses in bubbling fluidized beds, AIChE Journal 60 (3) (2014) 839–854.
URL http://onlinelibrary.wiley.com/doi/10.1002/aic.14321/abstract

[5] A. Sarkar, F. E. Milioli, S. Ozarkar, T. Li, X. Sun, Filtered sub-grid constitutive models for fluidized gas-particle flows constructed from 3-D simulations, Chemical EngineeringScience 152 (2016) 443–456. doi:10.1016/j.ces.2016.06.023.

[6] S. Schneiderbauer, A Spatially-Averaged Two-Fluid Model for Dense Large-Scale Gas-Solid Flows, AIChE Journal 63 (8) (2017) 3544–3562. arXiv:arXiv:1402.6991v1, doi:10.1002/aic.

[7] S. Schneiderbauer, A. Aigner, S. Pirker, A comprehensive frictional-kinetic model for gas–particle flows: Analysis of fluidized and moving bed regimes, Chemical Engineering Science 80 (2012) 279–292. doi:10.1016/j.ces.2012.06.041.
URL http://linkinghub.elsevier.com/retrieve/pii/S0009250912003971

Chapter 5

Appendix A - Schneiderbauer's theory

The following equations are based on Schneiderbauer [6], and are included here to illustrate how to close the mesoscale drag modification with a more theoretical ansatz.

- The filtered gas-solid drag is evaluated from a Taylor expansion of the microscopic drag coefficient

$$\begin{aligned}\beta = \beta\left(1-\overline{\phi}_{\mathrm{s}}, \widetilde{\mathbf{u}}, \widetilde{\mathbf{v}}\right) + \left.\frac{\partial \beta}{\partial v_j}\right|_{1-\overline{\phi}_{\mathrm{s}}, \widetilde{\mathbf{u}}, \widetilde{\mathbf{v}}} v_j^{''} \\ + \left.\frac{\partial \beta}{\partial u_j}\right|_{1-\overline{\phi}_{\mathrm{s}}, \widetilde{\mathbf{u}}, \widetilde{\mathbf{v}}} u_j^{''} - \left.\frac{\partial \beta}{\partial (1-\phi)}\right|_{1-\overline{\phi}_{\mathrm{s}}, \widetilde{\mathbf{u}}, \widetilde{\mathbf{v}}} \phi' + \mathrm{H.O.T.}\end{aligned} \tag{5.1}$$

Which is substituted into the filtered drag coefficient to yield the following equation:

$$\begin{aligned}\overline{\beta(v_i - u_i)} \approx \widetilde{\beta}\left[(\widetilde{v}_i - \widetilde{u}_i) + \sqrt{\frac{2}{3}\overline{\phi'^2}}\left(\frac{\xi_{\phi \mathrm{g}}\sqrt{k_{\mathrm{g}}}}{1-\overline{\phi}_{\mathrm{s}}} + \frac{\xi_{\phi s}\sqrt{k_{\mathrm{s}}}}{\overline{\phi}_{\mathrm{s}}}\right)\right] \\ + \left.\frac{\partial \beta}{\partial v_i}\right|_{1-\overline{\phi}_{\mathrm{s}}, \widetilde{\mathbf{u}}, \widetilde{\mathbf{v}}}\left[\frac{2}{3}\left(k_{\mathrm{g}} - \xi_{\mathrm{gs}}\sqrt{k_{\mathrm{g}}k_{\mathrm{s}}}\right) + \frac{\xi_{\phi \mathrm{g}}}{1-\overline{\phi}_{\mathrm{s}}}\sqrt{\frac{2}{3}k_{\mathrm{g}}\overline{\phi'^2}}(v_i - u_i)\right] \\ + \left.\frac{\partial \beta}{\partial u_i}\right|_{1-\overline{\phi}_{\mathrm{s}}, \widetilde{\mathbf{u}}, \widetilde{\mathbf{v}}}\left[\frac{2}{3}\left(\xi_{\mathrm{gs}}\sqrt{k_{\mathrm{g}}k_{\mathrm{s}}} - k_{\mathrm{s}}\right) + \frac{\xi_{\phi \mathrm{s}}}{\overline{\phi}_{\mathrm{s}}}\sqrt{\frac{2}{3}k_{\mathrm{s}}\overline{\phi'^2}}(v_i - u_i)\right] \\ - \left.\frac{\partial \beta}{\partial (1-\phi_{\mathrm{s}})}\right|_{1-\overline{\phi}_{\mathrm{s}}, \widetilde{\mathbf{u}}, \widetilde{\mathbf{v}}}\sqrt{\frac{2}{3}\overline{\phi'^2}}\left(\xi_{\phi g}\sqrt{k_{\mathrm{g}}} - \xi_{\phi \mathrm{s}}\sqrt{k_{\mathrm{s}}}\right)\end{aligned} \tag{5.2}$$

Therefore the filtered drag force requires closures for:

- the turbulent kinetic energies k_{g}, k_{s}

- and the bulk density fluctuations $\overline{\phi'^2}$

The additional linear correlation parameters ξ are:

$$\xi_{\mathrm{gs}} \approx 0.8, \quad \xi_{\phi\mathrm{s}} \approx 0.1, \quad \xi_{\phi\mathrm{g}} \approx -0.5\left(1-\overline{\phi}_{\mathrm{s}}\right) \tag{5.3}$$

The factor H_D is expressed as:

$$\boldsymbol{H_D} = \frac{\left.\frac{\partial\beta}{\partial(1-\phi_{\mathrm{s}})}\right|_{1-\overline{\phi}_{\mathrm{s}},\tilde{\mathbf{u}},\tilde{\mathbf{v}}} \sqrt{2\overline{\phi'^2}}\left(\xi_{\phi\mathrm{g}}\sqrt{k_{\mathrm{g}}} - \xi_{\phi\mathrm{s}}\sqrt{k_{\mathrm{s}}}\right)}{\widetilde{\beta}(\widetilde{\boldsymbol{u}}_{\mathrm{g}} - \widetilde{\boldsymbol{u}}_{\mathrm{s}})} \tag{5.4}$$

Thus, this theory only allows one to model isotropic correction to the drag at the moment.