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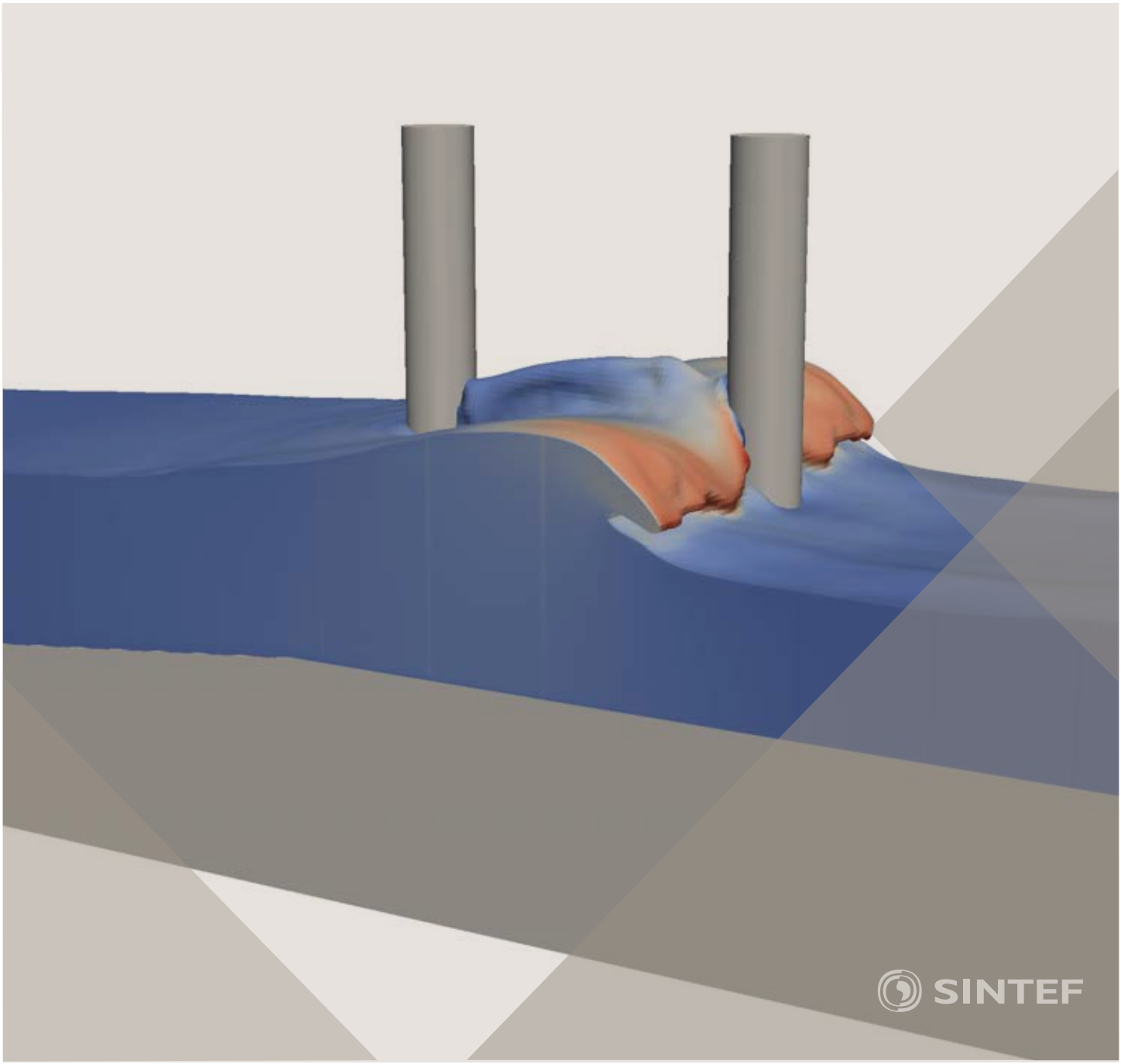

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Editors:
Jan Erik Olsen and Stein Tore Johansen

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PREFACE

This book contains all manuscripts approved by the reviewers and the organizing committee of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in May/June 2017 and is also known as CFD2017 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focuses on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. In addition pragmatic modelling concepts and bio-mechanical applications have become an important part of the conference. The papers in this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are included in the proceedings. 108 contributions were presented at the conference together with six keynote presentations. A majority of these contributions are presented by their manuscript in this collection (a few were granted to present without an accompanying manuscript).

The organizing committee would like to thank everyone who has helped with review of manuscripts, all those who helped to promote the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: ANSYS, SFI Metal Production and NanoSim.

Stein Tore Johansen & Jan Erik Olsen

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IMPLEMENTING THE KINETIC THEORY OF GRANULAR FLOWS INTO THE LAGRANGIAN DENSE DISCRETE PHASE MODEL

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ABSTRACT

The dense discrete phase model (DDPM) is a promising method for detailed simulation of fluidized bed reactors. It can resolve particle clusters on much coarser grids than the conventional two fluid model (TFM) and allows for a more natural inclusion of particle size distributions. However, the discrete nature of the DDPM presents challenges when implementing the kinetic theory of granular flows (KTGF), which is required for adequate predictions of fluidized bed behaviour. This paper outlines several methods for accomplishing this task. A good match with experimental and TFM data was achieved with different methods for implementing the KTGF, thus building confidence in the DDPM as a method for fluidized bed reactor modelling. It was also shown that the model completely fails in dilute riser flows when the KTGF is only partially implemented or neglected completely.

Keywords: Kinetic theory of granular flows, dense discrete phase model, granular temperature, fluidized bed.

NOMENCLATURE

Greek Symbols

α Volume fraction
Δt Time step size [s]
ϕ_{gs} Interphase energy exchange rate [W/m^3]
γ_Θ Energy dissipation rate [W/m^3]
Θ Granular temperature [m^2/s^2]
ρ Density [kg/m^3]
$\bar{\bar{\tau}}$ Stress tensor [kg/m.s^2]
τ_c Collisional relaxation time [s]
$\vec{v}$ Velocity vector [m/s]
$\vec{v}'$ Uncorrelated velocity vector [m/s]
ω_Θ Granular temperature generation [m^2/s^3]

Latin Symbols

d Diameter [m]
e_{ss} Particle-particle restitution coefficient
$\vec{F}$ Specific force vector [N/kg]
F_D Drag force coefficient [1/s]
$\vec{g}$ Gravitational acceleration [m/s^2]
g_0 Radial distribution function
k_Θ Granular temperature diffusion coefficient [kg/m.s]
K_{sg} Interphase momentum exchange coefficient [kg/m^{3}s]
n_p Number of particle parcels in a cell
p Pressure [Pa]
t Time [s]

Sub/superscripts

g Gas
p Particle
pc Particle parcel
s Solids

Acronyms

CFD Computational fluid dynamics
DDPM Dense discrete phase model
fTFM Filtered two fluid model
GT Granular temperature
KTGF Kinetic theory of granular flows
ODE Ordinary differential equation
PDE Partial differential equation
RHS Right hand side
TFM Two fluid model
ToGT Transport of granular temperature

INTRODUCTION

Fluidized bed reactors are used across a wide range of process industries. The complex flow patterns, tightly coupled with mass and heat transfer phenomena, present challenges related to the design and operation of these reactors. These challenges have motivated several decades of research into accurate modelling of fluidized beds, both in terms of 1D phenomenological models and more fundamental CFD approaches.

The most established CFD approach is the two fluid model (TFM) closed by the kinetic theory of granular flows (KTGF) (Jenkins and Savage 1983, Gidaspow,

Bezburuah et al. 1992). In this method, particles in the fluidized bed are modelled as a fluid and closure laws are derived to model the dispersive effects of particle collisions and random translations as stresses experienced by this granular fluid. Closure laws derived from the KTGF are based on the likeness of granular motions to the motions of gas molecules, leading to a modelled pressure and viscosity.

The TFM-KTGF approach has been developed to a good level of maturity over the past three decades. It gives good representations of small scale fluidized beds (Cloete, Zaabout et al. 2013, Cloete, Johansen et al. 2015), but cannot be used for 3D simulations of fluidized beds larger than laboratory scale (Cloete, Johansen et al. 2015). The reason for this restriction is the tendency of particles to cluster together during fluidization. This clustering behaviour strongly impacts all transfer phenomena inside the reactor and must be resolved to achieve accurate results. Due to the dynamic nature of these clusters, TFM-KTGF simulations generally require very fine spatial and temporal resolution, leading to great computational expense.

To overcome this challenge, a promising approach called the filtered TFM (fTFM) (Igci, Andrews et al. 2008) is currently under development. This approach utilizes multiscale modelling principles to derive models capable of modelling the presence of particle clusters on grid sizes larger than the cell size used in the CFD simulation, thereby reducing computational costs by several orders of magnitude. However, this approach is still under development.

The dense discrete phase model (DDPM) approach (Popoff and Braun 2007), which is the subject of this paper, is another promising method for reducing computational costs relative to the TFM. This approach tracks parcels of particles through the domain in the Lagrangian sense, but also interpolates information such as volume fraction and velocity onto an Eulerian computation grid. In this way, the DDPM eliminates numerical diffusion, thereby allowing clusters to be resolved on much fewer cells than the TFM, thus resulting in 1-2 orders of magnitude speed-up. Since particle clusters still need to be resolved, the DDPM approach remains limited for large reactors fluidizing fine powders (Cloete, Cloete et al. 2016), but it can simulate much larger reactors than the TFM. In addition, the method allows a more natural inclusion of the wide particle size distribution typical of many fluidized bed applications.

An important challenge related to the DDPM approach is the implementation of the KTGF for correctly modelling the effects of unresolved particle collisions on the motion of particle parcels. Due to the discrete nature of the DDPM, the flow fields interpolated onto the Eulerian grid from the Lagrangian particle data are not continuous, thus creating problems when implementing the KTGF where many gradient operations are required. It is also challenging to convect the granular temperature (kinetic energy in the random particle motions) – a key variable in the KTGF. This paper will investigate ways to incorporate the KTGF into the DDPM framework and evaluate the performance of the resulting DDPM-KTGF model in 2D riser flows.

SIMULATIONS

Model description

The DDPM is a hybrid Lagrangian-Eulerian approach, tracking the particle phase using Newton's second law (Eq. (1)), while gas-phase motion is solved by the Navier-Stokes equations (momentum conservation as in Eq. (2)). Solids phase volume fraction and velocity are interpolated from the particle data in each computational cell. A more complete presentation of the equation system is given in (Cloete, Johansen et al. 2012).

$$\frac{d\vec{\upsilon}_p}{dt} = F_D\left(\vec{\upsilon} - \vec{\upsilon}_p\right) + \frac{\vec{g}\left(\rho_p - \rho\right)}{\rho_p} + \vec{F}_{KTGF} \quad \textbf{(1)}$$

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g \vec{\upsilon}_g\right) + \nabla \cdot \left(\alpha_g \rho_g \vec{\upsilon}_g \vec{\upsilon}_g\right) = -\alpha_g \nabla p + \nabla \cdot \overline{\overline{\tau}}_g + \alpha_g \rho_g \vec{g} + K_{sg}\left(\vec{\upsilon}_s - \vec{\upsilon}_g\right) \quad \textbf{(2)}$$

Five different possibilities for modelling particle collisions and random translations are investigated in this work:

1. **No KTGF:** No additional modelling
2. **No ToGT:** Algebraic granular temperature conservation and modelling of the solids pressure
3. **Full KTGF:** Transport of granular temperature on the particle parcels and modelling of the full solids phase stress tensor
4. **Parcel relax:** The full KTGF implementation including a relaxation of parcel velocity to the mean in each cell
5. **Parcel GT:** Modelling granular temperature generation through the particle parcel velocity distribution in each cell and modelling the solids pressure

In the **"No KTGF"** approach, the final term in Eq. (1) is simply ignored to illustrate the effect of completely excluding the KTGF.

The **"No ToGT"** approach calculates the local generation and dissipation of granular temperature in each cell, but ignores convection and diffusion of granular temperature. This simplifying assumption reduces the granular temperature equation from a PDE to an ODE, simplifying implementation. However, this assumption is generally not valid in dilute systems as was selected for this study. The resulting granular temperature is then used to calculate the solids pressure, which is used to model the effect of particle collisions and random translations on the motion of particle parcels via the final term in Eq. (1):

$$\vec{F}_{KTGF} = \frac{-1}{\alpha_p \rho_p} \nabla \overline{\overline{\tau}}_s \approx \frac{-1}{\alpha_p \rho_p} \nabla p_s \quad \textbf{(3)}$$

As indicated in Eq. (3), this is also a simplifying assumption, ignoring the shear stress components of the solids stress tensor.

The **"Full KTGF"** approach completes the modelling described above by including the transport of granular temperature and the full stress tensor. Granular temperature is naturally convected on the particle parcels as described in (Cloete, Johansen et al. 2012) through the ODE shown in Eq. (4).

$$\frac{3}{2}\alpha_s\rho_s\frac{d\Theta}{dt} = \overline{\overline{\tau}}_s : \nabla\vec{\upsilon}_s + \nabla\cdot\left(k_\Theta\nabla\Theta\right) - \gamma_\Theta + \phi_{gs} \quad \textbf{(4)}$$

The second order derivatives present in the full stress tensor (Eq. (3)) require some smoothing of the solids velocity field interpolated from the particle data as described in (Cloete, Johansen et al. 2012).

An additional modification is made in the **"Particle relax"** approach by removing the parcel-scale granular temperature (caused by the difference between the velocities of the tracked particle parcels) in each cell. This is done through the relaxation term in Eq (5):

$$\tau_c = \left(\frac{24\alpha_s}{\sqrt{\pi}d_p}g_0\sqrt{\Theta_{pc}}\right)^{-1} \quad \textbf{(5)}$$

Each particle parcel is then accelerated according to a modified Eq. (3) where an additional particle acceleration is implemented which is proportional to the deviation of the particle velocity from the mean velocity in the cell:

$$\vec{F}_{KTGF} = \frac{-1}{\alpha_p\rho_p}\nabla\overline{\overline{\tau}}_s - \frac{\vec{\upsilon}'}{\tau_c} \quad \textbf{(6)}$$

The reasoning behind this action is to remove the additional dispersion of momentum and granular temperature by uncorrelated motions of the particle parcels in each cell. If the full kinetic theory is implemented as in the "Full KTGF" approach, the modelled granular temperature should account for all the effects of uncorrelated particle motions, implying that additional dispersive effects are superfluous.

Finally, the **"Parcel GT"** approach models the generation of granular temperature from the uncorrelated motions of particle parcels in each cell. This is done by implementing Eqs. (5) and (6) to relax particle parcels towards the mean velocity in each cell, but conserving energy by adding a generation of granular temperature. In fact, Eqs. (5) and (6) conserve momentum, but assume completely inelastic collisions, thereby dissipating all the kinetic energy associated with the uncorrelated particle motions. Granular temperature generation in each cell was therefore approximated from the projected difference in kinetic energy in the particle parcels before and after the relaxation in each timestep:

$$\omega_\Theta = \left(\sum_1^{n_p}\vec{\upsilon}_p^2 - \sum_1^{n_p}\left(\vec{\upsilon}_p - \frac{\vec{\upsilon}'}{\tau_c}\Delta t\right)^2\right)e_{ss}^2 \Big/ n_p\Delta t \quad \textbf{(7)}$$

The product of Eq. (7) and the particle mass then replaced the first term on the RHS of Eq. (4) to increase the granular temperature stored on each particle parcel. In addition, the second term on the RHS of Eq. (4) was neglected on the assumption that the uncorrelated motions of the particle parcels, each carrying a certain amount of granular temperature, adequately describe the diffusion of granular temperature.

To keep consistency with this parcel-scale approach to the KTGF implementation, the effect of granular temperature was implemented by simply displacing each parcel by the distance that would be covered by the uncorrelated motion in each timestep in a random direction:

$$\Delta x = \sqrt{\Theta}\Delta t \quad \textbf{(8)}$$

This simplified approach captures the essence of the KTGF by dispersing particles away from regions of high uncorrelated motions where many particle collisions and random translations would take place. This dispersion of particles carrying momentum and granular temperature then naturally leads to a dispersion of momentum and granular temperature without requiring additional modelling. Dispersion of a particle parcel into a cell with a very different mean velocity then leads to the generation of additional granular temperature since particle velocities in this parcel would be very different from that of the other particles in the cell.

Geometry, boundary conditions and material properties

A simple 2D planar geometry with periodic boundaries in the axial direction is utilized in this work (see Figure 1 and Figure 2 for visualization). This geometry has been used in detailed validation studies of the TFM approach in riser flows (Cloete, Amini et al. 2011). It will therefore be informative to observe whether the DDPM can achieve a similarly good match to experimental data as the TFM.

Similar to (Cloete, Amini et al. 2011), the geometry is 0.8 m in height and 0.076 m in width. The geometry was meshed with 8288 square cells – about 8 times fewer than was needed for the TFM study in (Cloete, Amini et al. 2011). The coarser mesh is due to the superior cluster resolution capability of the DDPM.

The side boundaries of the geometry were designated as walls with a no-slip boundary condition for the gas. For the solids, normal and tangential restitution coefficients of 0.9 and 0.2 were specified (FLUENT defaults). A more advanced formulation accounting for the granular temperature on each particle may be implemented in future works, but this simple implementation was deemed sufficient for this comparative study.

The top and bottom boundaries of the geometry were specified as periodic. A variable pressure gradient was specified across the geometry via a negative feedback mechanism to keep the average gas superficial velocity through the geometry close to 4.48 m/s (Cloete, Amini et al. 2011).

A total of 80000 particle parcels were included in the simulation so that the average solids volume fraction in the domain amounts to 0.0372. The particle size, density

and restitution coefficient were specified as 67 μm, 1500 kg/m^3 and 0.9 respectively. The gas was standard air at room temperature.

Solver settings

The commercial flow solver ANSYS Fluent 16 was used to complete the calculations. The phase coupled SIMPLE algorithm was used for pressure-velocity coupling, while all other variables were discretized using the QUICK scheme. First order temporal discretization was used since this was found to be adequate in (Cloete, Johansen et al. 2012).

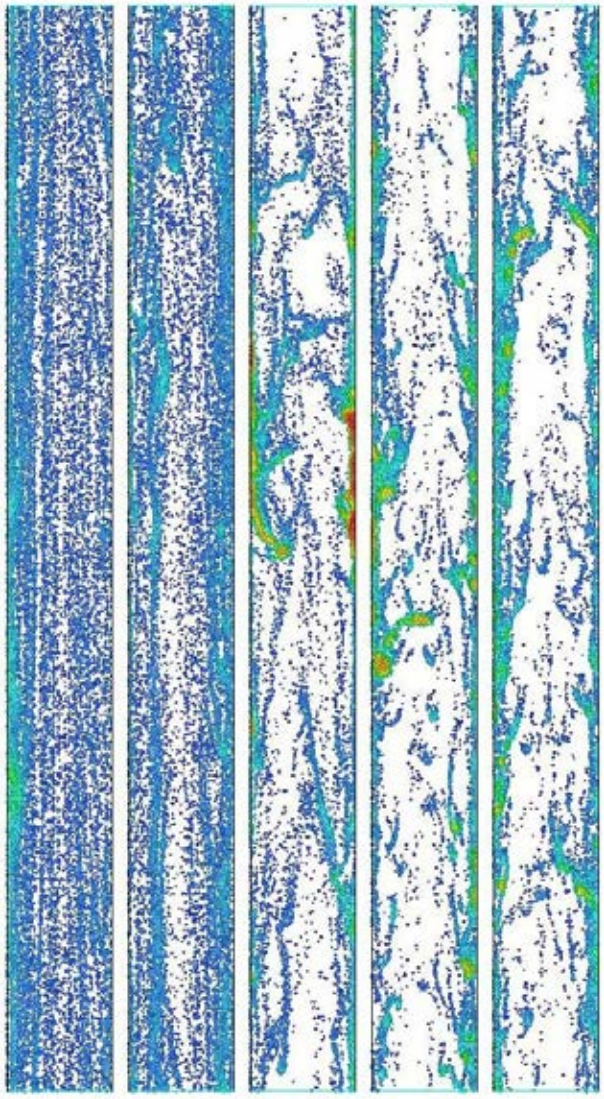

Figure 1: Instantaneous particle parcel positions for the five modelling approaches investigated in this study. Parcels are coloured according to local solids volume fraction where blue is zero and red is 0.6. From left to right: no KTGF implementation (No KTGF), no transport of granular temperature (No ToGT), complete KTGF implementation (Full KTGF), complete KTGF implementation with particle relaxation towards the mean velocity in each cell (Particle relax), and granular temperature generation from the uncorrelated motions between particle parcels (Parcel GT).

RESULTS

Qualitative analysis

Figure 1 shows instantaneous distributions of particle parcels in the geometry for the five different modelling approaches investigated in this study. It is clear that the first two approaches did not capture the expected clustering at the walls of the geometry, while the latter three approaches captured this phenomenon due to the more complete implementation of the kinetic theory of granular flows.

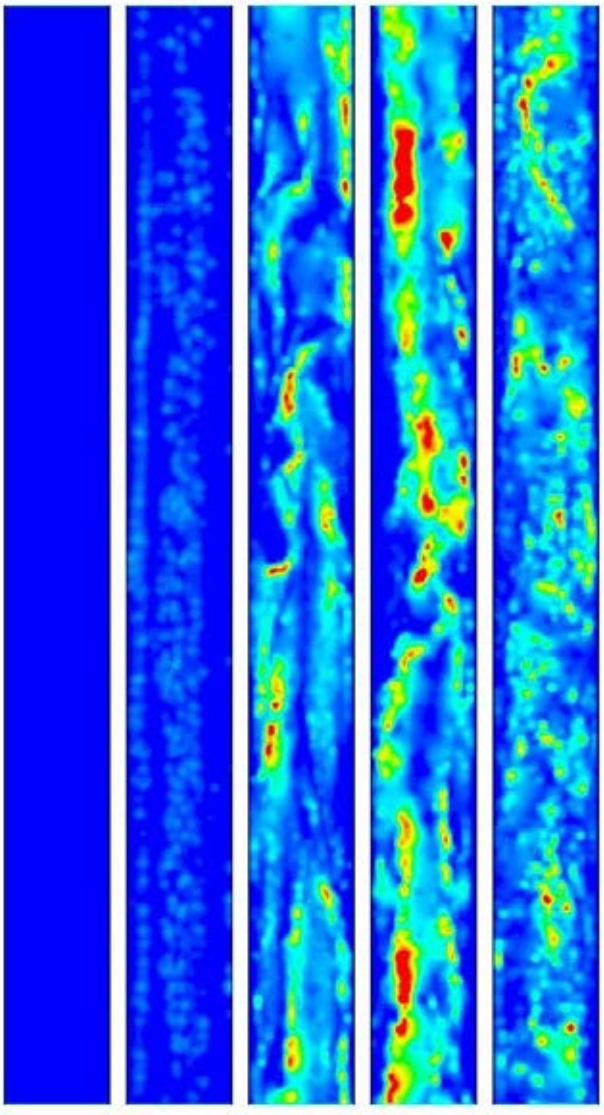

Figure 2: Instantaneous contours of granular temperature at the same instance as Figure 1. Blue represents zero and red 0.3 m^2/s^2.

Adequate representation of cluster formation at the walls of the geometry is primarily due to the formation of regions of high granular temperature in the dilute central regions of the geometry (Figure 2). These regions of high uncorrelated particle motion cause particles to migrate away from these regions towards the denser clusters at the walls. In these denser regions, granular temperature is rapidly dissipated due to inelastic collisions, thereby preserving the formed clusters until they are broken up by the rising gas flow (drag).

Quantitative analysis

Results presented in the previous section clearly showed that the inclusion of a proper KTGF implementation is essential for reasonable predictions in riser flows. The three complete KTGF implementations investigated in this work all performed well in a qualitative sense by predicting reasonable cluster formation and breakup behaviour at the walls (Figure 1). Quantitative results presented in this section will aim to better distinguish the differences between these three approaches.

Time averaged lateral profiles of solids volume fraction and axial velocity are shown in Figure 3 and Figure 4 for all five cases investigated in the study. It is clear that the incomplete KTGF implementations ("No KTGF" and "No ToGT") completely fail to predict the flow in the simulated riser section. This is especially evident in Figure 4 where very large upward velocities in the centre and downward velocities at the walls are shown. The reason for this great error is simply that the proper dispersion of momentum caused by the KTGF is not accounted for, thereby allowing very large velocity gradients to form. In addition, limited cross-stream particle parcel motion (due to the final term in Eq. (1) being very small or neglected) cause very few impacts with the wall to slow down falling particles. The result is a lateral velocity profile that is far too pronounced.

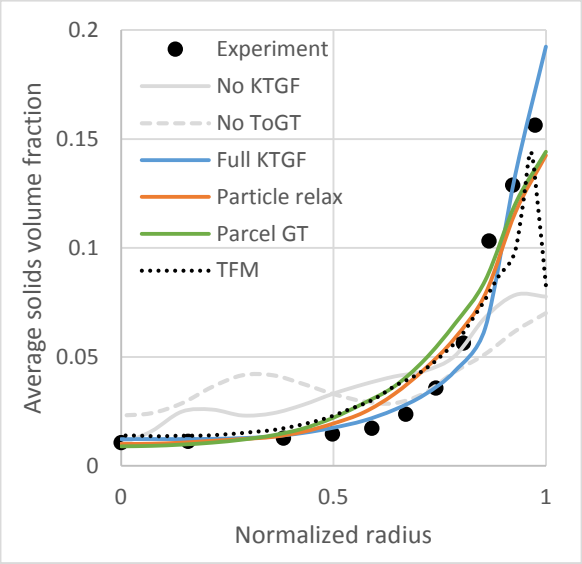

Figure 3: Time averaged lateral volume fraction profiles of the five cases compared to experiments (Yan and Zhu 2004) and TFM predictions (Cloete, Amini et al. 2011). Legend: No KTGF = no KTGF implementation, No ToGT = no transport of granular temperature, Full KTGF = Complete KTGF implementation, Particle relax = Complete KTGF implementation with particle relaxation towards the mean velocity in each cell, and Parcel GT = Granular temperature generation from the uncorrelated motions between particle parcels.

The three cases with more complete implementations of the KTGF perform much better. Figure 3 shows very similar profiles for the "Particle relax" and "Parcel GT" case, and a somewhat more pronounced lateral solids volume fraction profile for the "Full KTGF" case.

The similarity between the "Particle relax" and "Parcel GT" cases is the relaxation of particle parcels towards the mean cell velocity through Eqs. (5) and (6). This implementation has a large impact on particle parcel motion, but is strongly dependent on the granular temperature. Remarkably, the completely different methods used to represent the granular temperature in the "Particle relax" and "Parcel GT" cases returned similar granular temperature predictions (Figure 5). This is a positive result for the "Parcel GT" implementation, given its relative simplicity relative to the "Particle relax" and "Full KTGF" cases.

An important effect of the particle relaxation implementation in Eqs. (5) and (6) is that it slowed down falling particle clusters at the wall. This resulted from the effect of particle parcels hitting the wall and losing axial momentum (tangential restitution coefficient of 0.2) being transmitted to all parcels in the first cell next to the wall. Given that the cell size in this case was equivalent to 40 particle diameters, it is likely to be incorrect that parcels being slowed down on one side of the cell will exchange momentum with parcels on the opposite side of the cell. This implementation may therefore be grid dependent in regions of high solids velocity gradients (e.g. walls). Further work is needed on this topic.

It is clear from Figure 4 that the "Full KTGF" implementation resulted in more cluster slip at the walls because all particle parcels in the first cell next to the wall were not directly affected by momentum exchange with the wall as described in the previous paragraph.

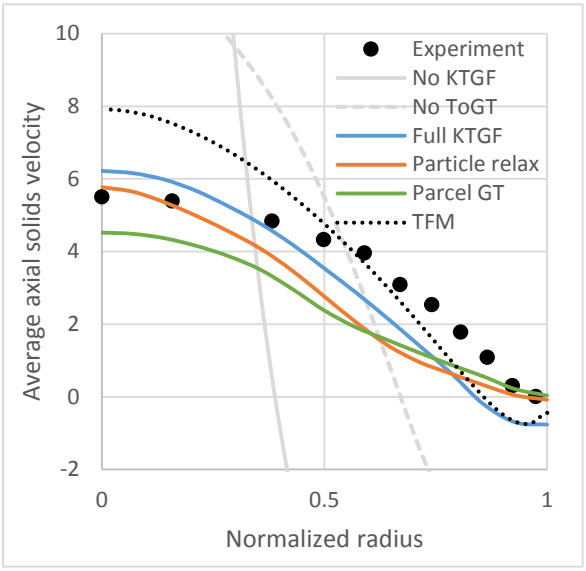

Figure 4: Time averaged lateral profiles of axial velocity compared to experiments (Yan and Zhu 2004) and TFM predictions (Cloete, Amini et al. 2011). Values were weighted by the solids volume fraction in the averaging process. See the caption of Figure 3 to interpret the legend.

The granular temperature profiles in Figure 5 show similar results for the three different cases with adequate KTGF implementations. The "Full KTGF" profile is shifted more towards the wall due to the formation of smaller, but more concentrated clusters at the wall (a higher solids concentration at the wall in Figure 3). As

mentioned earlier, the profile of the "Parcel GT" case is remarkably similar to the others even though a very different implementation of the KTGF was done in this case.

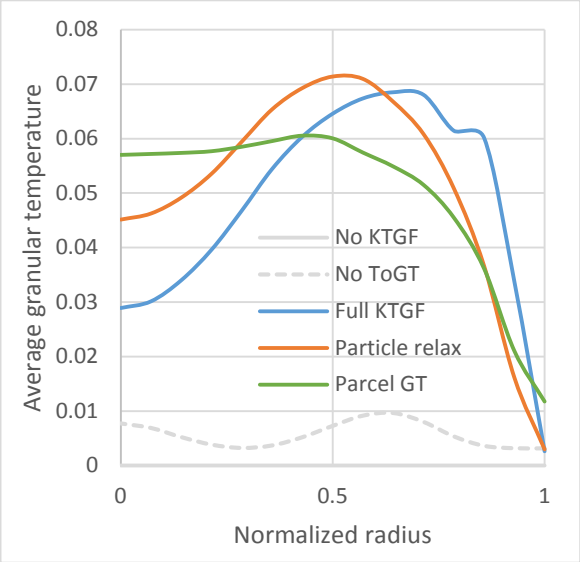

Figure 5: Time averaged lateral profiles of granular temperature. Values were weighted by the solids volume fraction in the averaging process. See the caption of Figure 3 to interpret the legend. Note that the "No KTGF" case has no granular temperature.

CONCLUSION

This paper presented five different methods for modelling dilute granular flows using the hybrid Lagrangian-Eulerian dense discrete phase model (DDPM). It was firmly established that proper implementation of the KTGF is essential for capturing the flow dynamics in riser flows. If this is not done, momentum dispersion is under-predicted and excessive velocity gradients can form.

Three different approaches to a more complete KTGF implementation all performed well when compared to experiments and predictions by the conventional Eulerian two fluid model (TFM). In all the approaches, transport of granular temperature is naturally completed by convecting a granular temperature property on each tracked particle parcel.

Results also showed that generation of granular temperature and the resulting momentum dispersion can be well approximated via data regarding the uncorrelated motions in the tracked particle parcels. This is a simpler approach relative to the conventional KTGF implementation where gradient operations are required, creating challenges due to the discrete nature of the DDPM.

In general, positive results from this study showed that different pathways exist towards a complete implementation of granular physics into the promising DDPM framework. Further evaluation of these methods in a broader range of cases is strongly recommended.

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