A NOVEL METHOD TO COUPLE DEM AND CFD TO SIMULATE TRANSPORT PHENOMENA IN SOLID BIOMASS FUEL BEDS

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Abstract
A new coupled DEM/CFD concept for the simulation of the transport processes in agitated fuel beds of thermally thick objects is presented. In contrast to other approaches, where a static interface between the fuel bed and the freeboard atop is predefined, the proposed method allows a continuous transition from the dense fuel bed, with a CFD mesh resolving the voids between the objects, to the freeboard, where much coarser meshes are sufficient. Momentum, heat and mass exchange at the interfaces to the fuel objects are calculated using wall functions, eliminating the requirement of shape specific correlations. Thermochemical source terms are determined by modeling conduction, drying and devolatilization within each fuel object in 3D. Local adaption of the effective viscosity accounts for different flow regimes; partial or full obstructions of the cell volumes are handled dynamically. First results show advantages of this concept especially for the simulation of agitated fuel beds.

Introduction and background
For fine fuel particles in the sub-mm range, the so called Euler-Lagrange description, where a representative number of material points associated with individual particle properties is numerically tracked through a reacting flow field, is the method of choice. This is valid since the actual particles are small with respect to the control volumes (CFD-cells) and only marginally influencing the flow field. Additionally, the individual particles are either far apart or collision can be described in a statistic manner, since particles collide only occasionally. Here, the interaction with the fluid phase can be safely modeled in a cell averaged fashion (many particles per CFD-cell) and particles do not displace a considerable amount of fluid. For larger fuel particles like solid biomass the situation is different, because the particles (further denoted as fuel objects), typically extend over the range of several CFD-cells. In these cases, the movement of the fuel objects is more or less controlled by the mechanical interaction among the fuel objects. Under these conditions the Discrete Element Method (DEM) provides an appropriate time resolved solution of the mechanical interaction and the resulting movement of the fuel objects. A challenging aspect evolves, if the interface between the fuel bed passed by combustion air and the freeboard atop is not stationary (as in [1]). This results in regions sparsely populated and
zones highly loaded with solids, both required to coexist and move across the same computational domain. One solution is the so called “porous media” DEM/CFD approach [2], where the DEM solution is tightly coupled with the CFD-solver and continuously updates the positions and velocities of the solid material. Semi-empirical models are used (for pressure loss, heat and mass transfer) but require averaging of the source terms across the CFD-cells. Although detailed information on the thermophysical/chemical processes inside the bulk of objects (sub-grid models, e.g. individual temperatures of objects) can be readily obtained, averaging across the CFD-cells filters the higher frequency part of this data. Unfortunately, these details strongly affect the conversion processes [6]. At this point the requirement of a finer mesh resolution (at least in the region populated by the solids) becomes obvious. In consequence, this results in CFD-cells fully covered by fuel objects where the porosity is zero, which cannot be handled by the current implementations of porous zone models. Immersed boundary methods [3] may be considered as an alternative to calculate details in the fuel bed, but reach their limits, especially when direct mechanical contact of fuel objects becomes relevant. Zambra et. al. [4] proposed a different approach, where the CFD-domain is modified “manually” at positions of solid objects to mimic their physical presence in the flow field. In the current work, this idea is coupled with the Discrete Element Method, which enables the dynamic calculation of the interaction (momentum, heat and mass transfer) of large numbers of arbitrarily moving objects, even of varying shape, within a flow field defined on a stationary mesh. This method is applied to a test case where movement of the solid fuel objects through stoking occurs during the conversion process, to demonstrate the capabilities of this approach.

**Solid object definition and transfer processes at the interfaces**

The fuel considered here is pelletized straw, which is approximated as a bulk of spherocylinders of constant size in the DEM simulation. This is a reasonable assumption, since the pellets contain up to 8 wt % ash and form a stable sintered matrix during conversion. The internal volume of the pellets is discretized with a tetrahedral finite volume mesh to allow simulation of the internal transport processes and to provide interface elements to the surrounding fluid phase. The CFD-domain defined in FLUENT consists of a three-dimensional finite volume mesh and requires (in areas where fuel objects may exist) a cell size smaller than the smallest object size. Since the CFD-cells and the details of their geometries are initially imported to the DEM code, the contact detection algorithm of the DEM continuously determines the CFD-cells fully contained in the object volume (blue) and the cells containing the interface of the two phases (green), as exemplified in fig 1a. A cross-sectional view of the straw pellet combustor targeted in this work is shown in fig 1b and 1c. The solid fuel objects (and the solid burner bowl components, blue), the fluid cells containing pellet surface elements (green) and the cells containing fluid only (red) are indicated. The fuel bed is considered either in a static state (fig 1b) or in a dynamic state when stoked (fig 1c) by vertical movement of the inner and outer cylinder.
Turbulent wall boundary conditions (which default to the laminar condition if the wall distance becomes small) are applied at each surface element of the respective DEM-object and collocated in the CFD-cell involved. Accordingly, $\bar{U}_{psf}$ the velocity of the cell center closest to the respective surface element is determined from equation 1:

$$\bar{U}_{psf} = \frac{\bar{U}_c \nu}{y_p C_{\mu}^{0.25} k^{0.5}} \cdot U^*$$  \hspace{1cm} (1)

With the friction velocity

$$U_\tau = \bar{U}_{fsf} - (\bar{U}_{fsf} \cdot \vec{F}_n) \cdot \vec{F}_n$$  \hspace{1cm} (2)

Here $\bar{U}_{fsf}$ is the velocity vector of the closest fluid cell and $\vec{F}_n$ is the normal vector of the particle surface element. $U^*$ and $C_{\mu}$ are defined as in [5]. $y_p$ is the distance from the particle surface to the CFD-cell center, $\nu$ is the dynamic viscosity and $k$ is the turbulent kinetic energy. Heat and mass transfer from the particle surface elements follows Reynolds analogy. For further explanations we refer to [6]. Sources for the turbulent kinetic energy and values for the turbulent dissipation rate are calculated accordingly. Finally, the CFD-cells fully covered by the fuel objects are modified such that they are no longer passed by the flow (setting the transported values and the transport coefficients accordingly). This results in an acceleration of the fluid around the solid objects and automatically creates a pressure drop satisfying momentum conservation.

**Treatment of the viscous terms**

In the test case considered (fig. 1b, c), the essentially laminar flow in the fuel bed and the turbulent flow field in the freeboard atop are required to be solved simultaneously and within the same domain. This requires an adaptive treatment of the viscous terms in the Navier-Stokes equations. As proposed in [7] the effective viscosity entering the equation is modified according to the local conditions (VLES), ranging from laminar in the void of the bulk to fully turbulent in the freeboard. As a first step
and in order to verify the applicability of the proposed approach, numerical results from a LES simulation of two side-by-side spheres [8] were compared to a corresponding simulation using the new approach on a coarser mesh. Figure 2 compares the time averaged velocity fields of the two methods, indicating a reasonable conformance.

![Figure 2. Comparison of the LES and VLES-DEM approach](image)

**Processes within the fuel objects**

As a prerequisite to describe drying and pyrolysis within the thermally thick fuel objects, the temporal development of the temperature is determined by solving Fourier’s Law within the particle (simultaneously for all objects involved). Drying of the particle is modeled with a latent heat and mass sink term for each particle cell with T>373.15 K and YH2O>0.0 as in equation 5 and 6:

\[
Q_{lt} = m_{Cell} c_p, cell (T_{Cell} - T_{vap})
\]  (5)

\[
dm_{H2O} = \frac{Q_{lt}}{h_{lt}}
\]  (6)

Devolatilization is modeled using a macro kinetic one-step Arrhenius behavior:

\[
dm_{vol} = k_{vol} e^{-\frac{E_1}{RT}} dt
\]  (7)

Coefficients( \(k_{vol} = 4.017e^{-7} [kg/s] \), \(E_1 = 23791[J/kgK]\)) for the devolatilization rate were obtained from experiments with straw pellets (D=7 mm, moist.=7.2 [wg %], vol.=71.5 [wg%], ash=7.7 [wg%] (raw)) as performed by [9]. Char combustion is accounted for a described in [2].
Results and Discussion
Figure 3 illustrates snapshots of the results obtained from the simulation. A horizontal cross sectional view through the top layer of the fuel bed is depicted. The first row shows results from a stationary fuel bed while the second row shows the respective results when stoking is applied.

Figure 3. Profiles of the fluid (T, left) and solid fuel objects (T, vol., moist., right)

The leftmost image presents the gas phase temperatures, whereas the next three images visualize pellet temperatures, the remaining volatile and the moisture content after 100 seconds of operation (still in an early conversion stage: char combustion already initiated due to radiative heat transfer by electrically heated walls (1000 K) above the fuel bed, but prior to gas flame ignition in the freeboard; passed by air of 300 K). The temperature distributions in the fixed bed show distinct local variations of the temperature level, both for the gas phase and the solid phase. If stoking is applied, temperatures are overall lower, indicating the effect of homogenization, resulting in a significant decreased conversion.

Conclusion
A new CFD/DEM approach for the simulation of stoked solid fuel beds, describing the flow through the fuel layer and the freeboard simultaneously and within one joint computational domain, has been presented. Local transfer processes within the fuel objects can be considered with the spatial resolution required, thus the approach is applicable to thermally thick and complex shaped fuel objects. Although a mesh fine enough to resolve the void space between the objects is required, the new procedure avoids tedious and error prone immersed boundary interpolations or continuous time consuming re-meshing. An approach adapting the effective viscosity to the local requirements is applied and shows promising results. The approach described can be combined with different gas phase reaction models, an aspect not discussed here.
**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$C_{\mu}$</td>
<td>Model constant [-]</td>
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<tr>
<td>$D$</td>
<td>Diameter [mm]</td>
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<tr>
<td>$\tilde{F}_n$</td>
<td>Surface normal</td>
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<tr>
<td>$h$</td>
<td>Enthalpy [J/kg]</td>
</tr>
<tr>
<td>$k$</td>
<td>Turb. kin. energy [m²/s²]</td>
</tr>
<tr>
<td>$m$</td>
<td>Mass [kg]</td>
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<tr>
<td>$Q$</td>
<td>Energy [J]</td>
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<tr>
<td>$R$</td>
<td>Gas constant [J/kmol K]</td>
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<tr>
<td>$U$</td>
<td>Velocity [m/s]</td>
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<tr>
<td>$Y$</td>
<td>Mass fraction</td>
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<tr>
<td>$\nu$</td>
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<td>$\tau$</td>
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**References**


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