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RADIATION HEAT TRANSFER WITHIN THE DISCRETE ELEMENT METHOD
- RELEVANCE, IMPLEMENTATION AND EXAMPLES -

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Abstract. Current developments in the energy sector increasingly demand the consideration of fuels with much larger particle sizes, either from alternative sources or due to a reduced pre-processing effort. In numerical simulations of such systems the particles can no longer be considered as non-colliding material points. Municipal waste incineration on grates or wood pellet combustion in domestic boilers are such examples, where the Discrete Element Method (DEM) can be applied to extend the Lagrange tracking of moving particles to a mechanically and thermally fully interacting flow of reacting granular material. In some situations where sufficiently large time scale differences between the processes in the gas phase and in the solid phase exist, distinctive interfaces can be identified between domains, thus allowing a different modelling in these regions. The treatment of the radiative heat transfer between such domains poses particular difficulties at the interfaces. Based on the two exemplary applications mentioned, details of the modelling approach are discussed and corresponding results presented.

1 INTRODUCTION

The theoretical description of fuel conversion processes and the numerical simulation of the equipment employed has gained considerable industrial application throughout the last two decades. Starting from the Eulerian gaseous fuel conversion in homogeneous multi-species turbulent flows, the further development led to the Lagrangian description of droplets or pulverized solid fuel particles. By tracking the material points representing these small particles, the movement and conversion within the flow field and the associated mass and heat transfer could be assessed. In many technically relevant applications collisions or any other direct interactions within the particulate phase could either be neglected or statistically represented.

The increasing exploitation of alternative fuel sources, especially biomass and agricultural residues, results in a growing significance of systems where much larger particles are directly converted. This largely avoids the otherwise required fuel preparation through energy intensive processes like cutting, crushing or grinding and thus supports the overall efficiency. With respect to the numerical simulation of such systems, the individual particles or objects must be considered as thermally thick and also often require a spatial resolution of the temperature field within each object. In addition, their mechanical interaction may dominate the flow of the solid phase while the transport processes associated with the interstitial gas phase still control the mass and heat transfer. A straightforward combined CFD/DEM approach, fully resolving the evolution of all relevant processes over time, may be applied in these situations, but still requires extremely large computational resources if systems of technical scale are considered. The assumption of steady state conditions in a part of the domain considered allows to reduce this effort.

2 EXAMPLES OF TECHNICAL APPLICATIONS

The application of DEM combined with the simulation of heat transfer and/or chemical reaction is still in an early phase of development and the application to systems of industrial or technical scale is scarce. If carried out, these investigations are complicated with respect to physics and chemistry, computationally very expensive and time consuming [2, 5]. Early applications and explorative investigations were possible for situations where the specific conditions eased these requirements to some extent. A DEM code developed at the Department of Energy Plant Technology [1, 3, 4] describes the particle motion and thermochemical processes of the reacting granular phase. The commercial CFD software package ANSYS FLUENT (Version 14.5) is connected with this code and used to solve the governing equations of the continuous fluid phase surrounding the particles.

Two examples of largely different geometric scale, namely the conversion of bulky material on the grate of a municipal waste incinerator and the combustion of wood pellets in a domestic heater will be presented and compared with respect to the heat transfer models applied.

2.1 Municipal waste incinerator

Thermal treatment, gently circumscribing ultimate combustion, is an efficient, ecologically favorable and long established process for the energetic utilization of municipal waste. In these systems the untreated material is introduced through a waste feeder chute into the furnace (approx. 60 MW_{th}) forming a waste layer on a grate of about 10 m length and 60 cm initial height. Moving bars mechanically induce the transport of this layer through the furnace, while it is passed by primary air from below.

The gas mixture leaving the upper surface of the layer consists of partially oxidized pyrolysis products, carbon monoxide and air. This flow enters the combustion chamber atop of the grate, becomes mixed with additional secondary air injected from the roof and/or the sidewalls and finally is converted under turbulent conditions (fig. 1). The harsh conditions in these combustion chambers render reliable measurements of gas temperatures, species concentrations or radiative fluxes technically ambitious and costly; within the waste layer they are virtually impossible. Thus only numerical simulations are left for the purpose of “looking” into details of these systems for optimization.

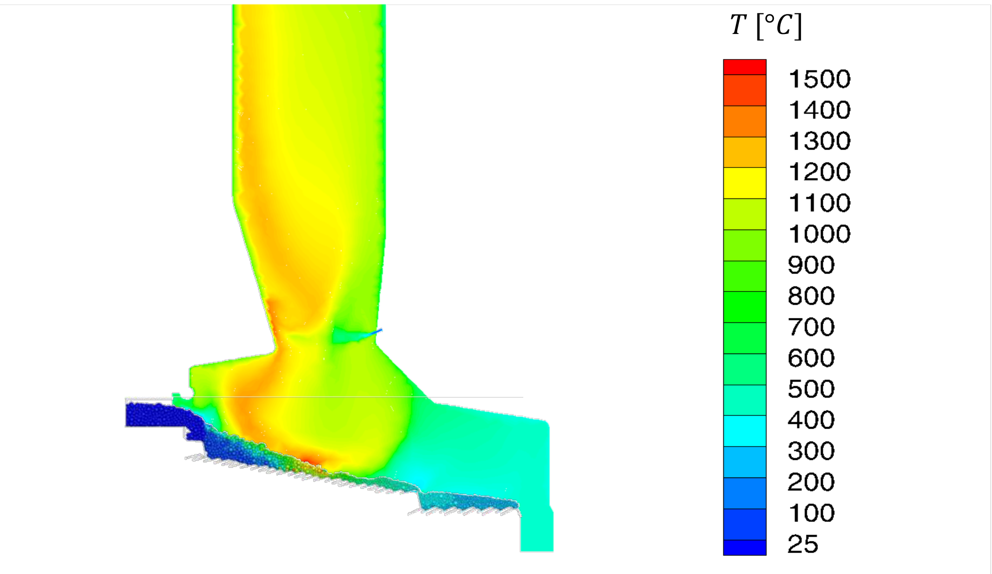

Figure 1: Temperature distribution in the boiler (gas phase) and in the bulk material (solid fuel) on the grate

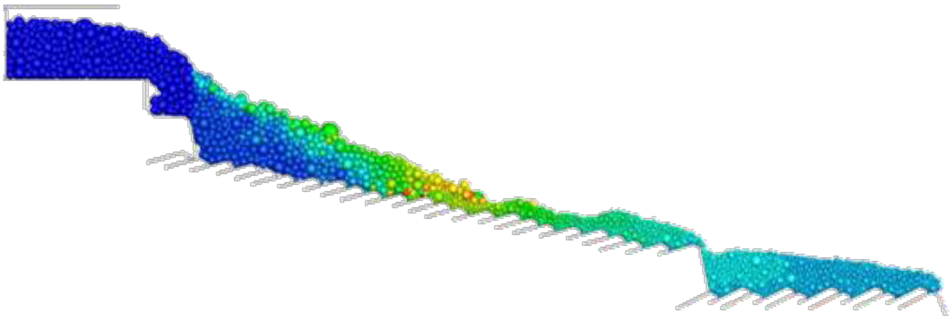

Figure 2: Close-up of the temperature distribution in the waste layer, scaled as in fig. 1.

As depicted in fig. 1 and fig. 2 the domain required for an overall simulation comprises of two distinctly different domains with respect to the prevailing physical and thermochemical conditions. While the fluid passes the combustion chamber in just a few seconds, the solid fuel (only a “strip”, 50 cm wide and containing approx.7500 particles is modeled) needs about 80 minutes to travel along the grate. Thus the overall time scales are wide apart, suggesting a separation at the boundary between fuel layer surface and combustion chamber.

With respect to the appropriate models, the combustion chamber may be represented as a conventional reactive multi-species turbulent steady state flow field, occasionally blown out small particles and their conversion may be readily described as transported and reacting material points using the commonly used particle tracking procedure.

The process on the grate with the waste-layer atop is dominated by the interaction of the mechanical transport and mixing of the bed, with the concurrent heat transfer, heterogeneous reaction in the bulk (drying, pyrolysis, char oxidation) and with the crossflowing primary air. Several grate designs based on different mechanical transport principles (forward acting, backward acting roller grates) coexist in the waste incineration technology. Depending on the specific grate design different combustion chamber layouts are favored (counter-current, co-current, center-flow firing). The example shown is a forward acting grate with counter-current firing [3].

Heating of the waste-layer, ignition of the combustible material contained therein and the resulting conversion rate, are to a large extent controlled by radiation from the combustion chamber above the layer. The intensity of the radiation incident on the layer surface tightly couples with the surface temperature of the particles in the top layer since radiation is transported “infinitely fast”. The height of the fuel layer is typically in the range of several decimeters, thus a considerable conversion of the gaseous components released within the bed appears to be a reasonable assumption; within the DEM model successive thermochemical equilibria are computed in the vertical direction. Since the major pressure loss occurs across the grate, an even distribution of the primary air passing through the fuel layer can be prescribed as the inlet boundary condition.

Typical municipal waste consists of a large variety of solid objects of widely varying size, shape, mechanical, physical and thermochemical properties. At this point any particle-based simulation method requires rigorous simplifications. This is not only due to the large number of objects involved but even more since the required data on the fuel, which (if known at all) is only available as long time averages. Combining detailed knowledge on the properties of individual fuel fractions (heat of reaction of different types of plastic material, wood, inert materials, water) and their respective content with known “typical” size distributions [7] allows to parametrize a “theoretical waste” which exhibits both, reasonable conversion behavior and transport properties resulting in realistic residence times on the grate. Therefore the actual geometric shape of the fuel objects may be reduced to cohesive spherical particles, interacting with each other and reducing size and cohesive forces during conversion. Since the large particles are thermally thick, their one-dimensional radial discretization allows to approximate their thermal inertance. Further details on the models and a comparison of results obtained with measurements in an actual incinerator may be found in [3].

The time scale associated with the final conversion of the products in the boiler is short if compared to the 80 minutes residence time. Therefore the movement, heating and reaction of the fuel objects need to be considered as unsteady processes, while the boiler atop always achieves steady state conditions within much shorter times. This provides the time scale difference required for a separation of the simulation into two distinct but coupled domains as described in chapter 2.4

2.2 Wood pellet furnace

The second example (fig. 3) discussed is a domestic heater (13 kW thermal) fired with wood pellets. This system differs in several aspects from the waste incinerator presented above. Obviously, the absolute scale of the system is much smaller, since the volume of the combustion chamber is only about 20 liter, installed atop a burner bowl of approximately 15 cm diameter which contains less than 1000 reacting particles during steady state and at nominal load. In contrast to the municipal waste, the wood pellets are geometrically and thermochemically well defined (cylindrical shape of 6 mm diameter and a length varying between 6 and 30 mm, known heating value, water content and measured temperature dependence of the gas release during pyrolysis). The initial geometry of the individual particles can be assumed to be preserved during drying (constant volume) and to be reduced in size during pyrolysis and char burnout (constant density), which roughly reflects the actual behavior during burnout. Since the primary air is introduced into the burner bowl from below and secondary air is injected radially through circular holes on the circumference at two different heights. The distribution of the air inflow through these ports is strongly controlled by the geometry of the air supply, thus the required boundary conditions can be determined in advance by a separate simulation of the distribution system.

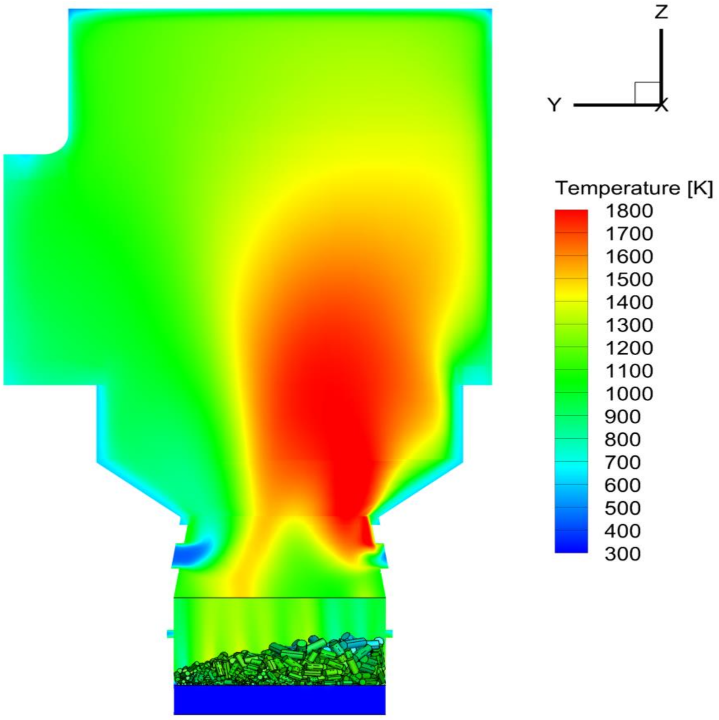

Figure 3: Temperature distribution in the fuel layer and the combustion chamber of a pellet fired domestic heater

As shown in fig. 4, the discrete fuel objects, the wood pellets, are discontinuously dropped onto the fuel layer through a chute. About 10 gram every 10 seconds are introduced to obtain an averaged fuel feed rate of 1.0 g/s. This results in an unsteady heating and conversion process within the burner bowl, every 10 seconds the onset of drying releases water vapor, subsequently volatiles and later on carbon monoxide (as the primary char conversion product) occur. Since the particles fall on a small area of the surface a distinctive movement of the particles in the bed is induced, being overlain by the particle size reduction resulting from char burnout. The average residence time of the pellets until full burnout is 375 seconds.

Similar as in the waste incinerator, the flow in the combustion chamber atop of the fuel bowl must be considered to be partially premixed, turbulent and three-dimensional, thus the reaction of the gaseous products is controlled by the spatially distributed release of the components from the reacting pellet bed and the mixing with the secondary air. Different descriptions (Eddy Dissipation/Eddy Dissipation Combustion) were compared, a detailed comparison may be found in [1].

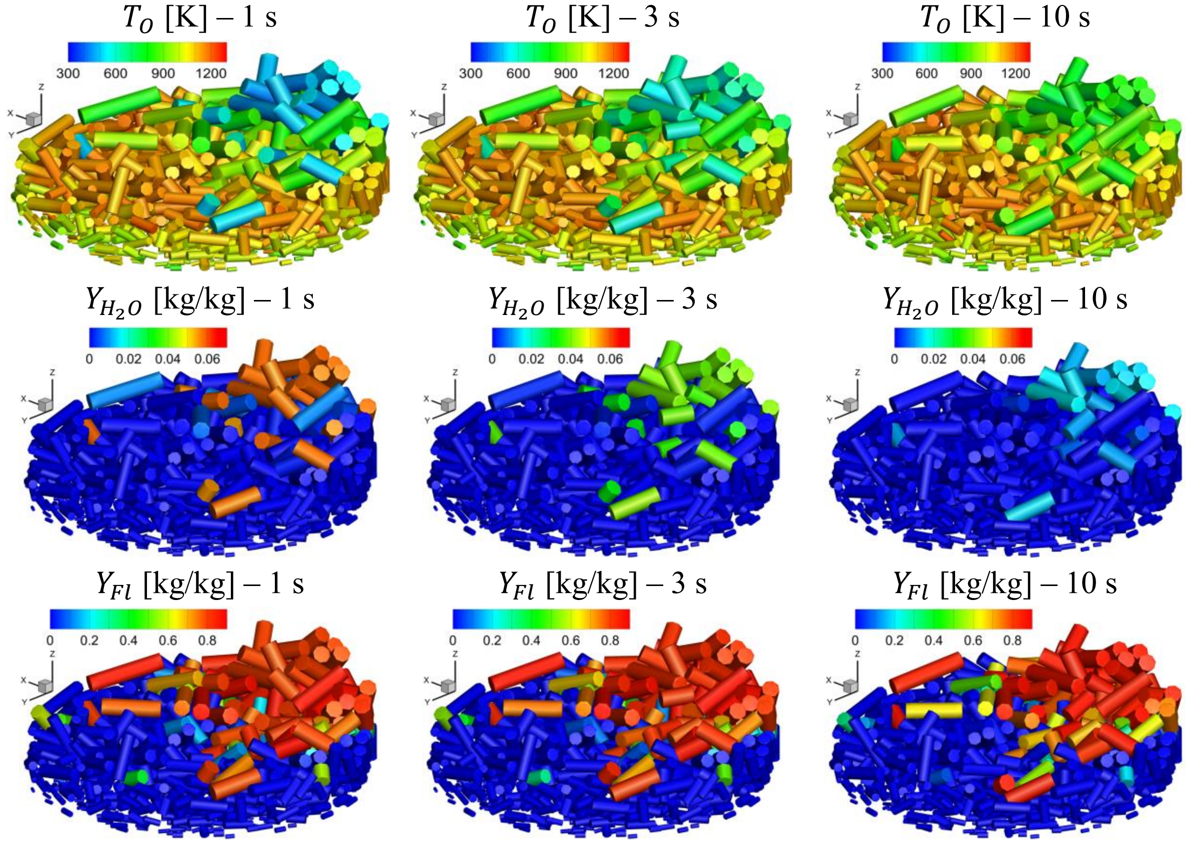

Figure 4: Surface temperature, water and volatile content of the pellets in the burner bowl

In contrast to the waste incineration, the pellet layer height is quite small and the residence time of the gaseous components released in the bed approaches the same magnitude as the time required for fuel conversion. Due to the essentially "laminar" conditions in the small gaps between the pellets and the constrained spatial mixing, a kinetic description (only one step global reaction of the hydrogen content) is required to allow for a partial conversion of pyrolysis products in the bed.

2.3 DEM-CFD coupling / radiative transfer

As previously shown, the surface of the waste layer and in the other case, the interface between the burner bowl and the combustion chamber atop, represent natural interfaces with a sufficient scale separation to allow for a separated but externally coupled (iteratively, via files and User Defined Functions) simulation of the overall system. Averaging the time resolved conversion on the grate or in the pellet bed over appropriate prescribed times (cycling time of the waste push rod and time between successive pellet additions) provides the inlet boundary conditions for a steady state simulation of the respective combustion chamber.

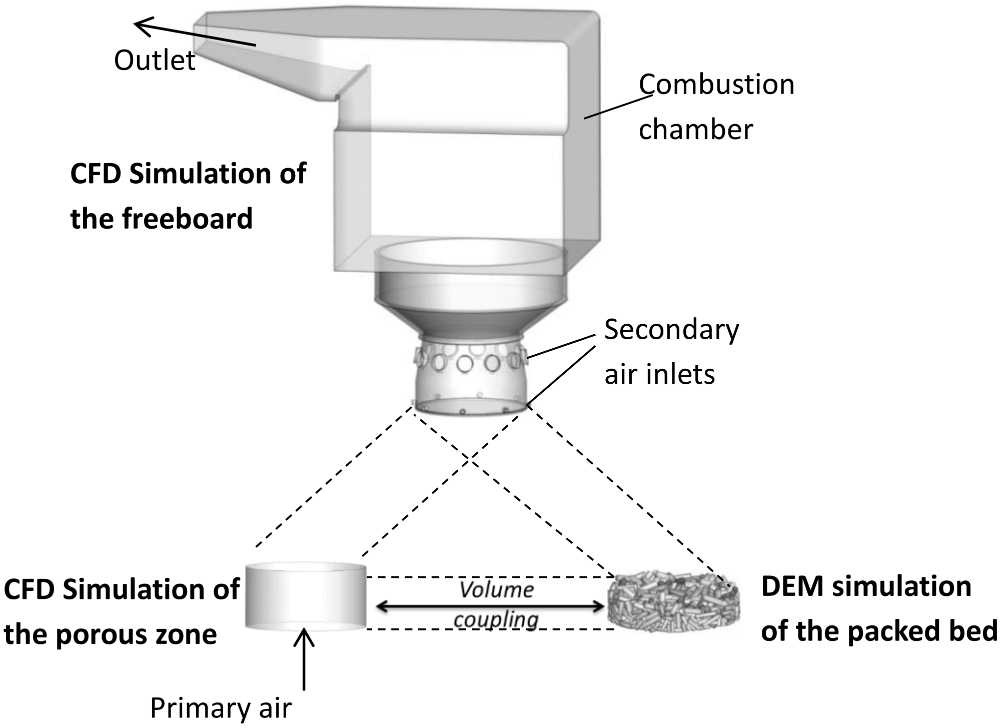

Figure 5: Data exchange concept for DEM/CFD coupling

Fig. 5 depicts this approach for the case of the pellet stove. While a two-dimensional, two-way interface is sufficient for the waste incinerator (steady state CFD in the combustion chamber and reacting, time resolved DEM on the grate), additional volume coupling is required for the process in the pellet burner bowl. Turbulent steady state simulation and time resolved "laminar" flow in the porous medium representing the pellet bed are not compatible enough to be treated in one single domain.

This results in three distinct computing tasks (CFD in the combustion chamber, CFD in fluid phase and reacting DEM for the solid particles in the burner bowl) which need to exchange data of mass and heat fluxes in tightly synchronized (and consistent) manner.

In this context the thermal radiation heat transfer requires specific attention since the overall system behavior and thus the rate of fuel conversion is distinctively influenced by the radiative fluxes. Any inconsistencies at this point add to the uncertainties already resulting from the many assumptions and simplifications contained in the other model components (e.g. fuel conversion, convective flow and diffusive mass transfer, thermochemical model).

From a general perspective the three-dimensional radiative transfer equation in an absorbing, emitting and scattering medium must be solved with respect to the boundary conditions imposed by multiple enclosing surfaces. The radiative intensity I in position $\vec{r}$ arriving from (or being emitted in) direction $\vec{s}$ can be obtained by integration of

$$\frac{dI(\vec{r},\ \vec{s})}{ds} + \kappa(s)\, I(\vec{r},\vec{s}) = a\, n^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_S}{4\pi} \int_0^{4\pi} I(\vec{r},\vec{s}\,)\, \phi(\vec{s}\cdot\vec{t}\,)\ d\Omega \qquad (1)$$

with the absorption coefficient **a**, the scattering coefficient $\boldsymbol{\varrho_S}$, the optical thickness $\kappa(s)$, the refractive index **n** of the gray medium passed, a scattering phase function $\boldsymbol{\phi}$ relating scattered to incident radiation and the Stefan-Boltzmann constant $\boldsymbol{\sigma}$. In the commonly used CFD tools several approximations to the solution of this equation do exist. A a comparison of the most popular models, the so called P-1, the Discrete Transfer Radiation Model (DTRM), the Discrete Ordinates Model (DO) and the Surface-to-Surface (S2S) model may be found in [6]. If the optical thickness of the participating medium is large, either due to a strong absorption or due to a "large" length scale, the P-1 model provides the most robust and efficient approach and is used in the waste incinerator simulations. In contrast, if the optical thickness is small and the radiative exchange is dominated by the direct exchange among the surfaces involved, like in the case of the pellet stove, the S2S model or the DO-model are reasonable choices.

Here the major difficulty arises from the fact that the thermal radiation acts instantaneously between the surfaces and gas volumes involved. If a reacting fuel object changes its surface temperature over time, the resulting change in heat flux from the combustion chamber atop occurs immediately and thermal equilibration must be obtained before the next time step. This would require to solve (to converge) at least the radiation transport problem in the combustion chamber domain for every step of the DEM simulation, which currently is not possible with reasonable effort.

An “ad hoc” approach to resolve this conflict between steady state and time dependent solutions uses the domain interfaces such that a common, time averaged “radiative background temperature” T_{rad} is associated with the interfacing surface to compute on the particle side the time resolved heat exchange with the individual particles and on the other side the radiative exchange with the combustion chamber as a whole, iteratively balancing the integral heat flux. Figure 6 depicts, in order to show the sensitivity, the effect of a reduction of this radiative temperature on the conversion and particle temperature on the grate. As can be seen, 20 % difference in the value of T_{rad} decides between stable operation and full extinction of the reaction. Unfortunately the measurement of radiative fluxes in devices of technical scale is difficult and expensive, thus no direct comparison is currently available.

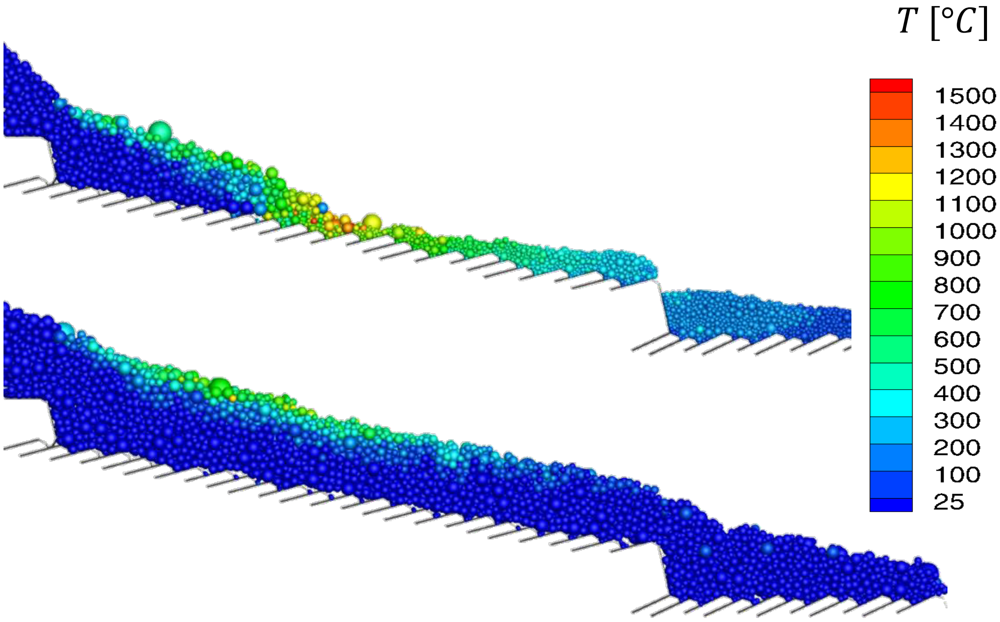

Figure 6: Particle temperatures and conversion on the grate of a municipal waste incinerator,
upper part: nominal operation,
lower part: radiation temperature at the interface reduced by 20%

3 CONCLUSIONS

Coupled CFD/DEM simulations are an emerging methodology for the numerical treatment of mechanically and thermally interacting and chemically reacting two phase flows with large reacting particles. Although, many details especially with respect to the generalisation of the modelling approaches require further investigation. First demonstrations and exemplary applications could be realized with quantitatively reasonable results. Thermal radiation in these systems requires special attention since it immediately transfers energy and therefore has a strong influence on the conversion rates, this complicates scale separation of the problem in time and space.

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