EFECTS OF SOFT-SPHERE MODEL PARAMETERS IN THE SIMULATION OF SLAGGING GASIFIERS

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Abstract

The correct prediction of the interaction of char and ash particles with confining walls in an entrained-flow slagging gasifier calls for a proper assessment of the parameters governing the dynamics of impacts between particles consisting of partially or fully converted coal and a surface partially covered by a viscous layer of molten ash. The limiting conditions of these interactions are: unconverted rigid and non-sticky coal particles versus fully converted plastic and sticky ash particles, on one side, and rigid bare non-sticky walls versus sticky walls covered by a flowing layer of molten ashes, on the other. A DEM simulation model has been used to explore how the presence of multiple particles in the near-wall region of the gasifier affects the effective deposition rates of char and ash onto the confining walls, hence the rate of rebound. The formation of a dense layer of particles in proximity of the walls' surface is critically affected by particle–wall interaction. This study is focused on the effects of selected simulation parameters on the dynamical patterns of particle impact under the four limiting regimes, and on the choice of parameters that more closely represent particle–wall interaction under realistic process conditions.

Introduction

The use of coal as primary energy source, to be socially accepted, requires a deep transformation of the related technology. Integrated coal gasification (such as IGCC) is among the most promising technologies from the efficiency and environmental point of view. This study focuses on gasifier chambers operated under slagging entrained-flow conditions. The onset of a slag layer (molten ash) flowing down the gasifier's walls, the interaction by impact between char/ash particles and slag layer, the constitution of a dense-dispersed phase close to slag layer where char particles that cannot be accommodated on the slag layer's surface accumulate, are all aspects able to profoundly affect the gasifier's performance and therefore deserve investigation. In the recent past, this research group has studied the topic from both experimental [1,2] and simulation modelling [3,4] point of view. This work extends the latter aspect. Two simplified configurations are introduced, that focus on the region of interface between the gasifier's walls (possibly covered by the slag) and the particle-laden flow in the surroundings. At this scale, order of centimeters, particles can be singled out and the interactions predicted by adopting highly accurate computational methods as the Discrete Element Method (DEM), with particle interaction described with a soft-sphere approach (details in [4]). The presence of a bare wall or of a wall covered by slag, as well as the impingement of unreacted char or ash particles, can be represented by changing some of the properties that govern the interaction during the impacts, one of the most important being the stickiness behavior [5]. Several empirical models available in the literature adopt a criterion based on the particles viscosity as a rule to determine the deposition rates of impinging particles onto the slag layer [6]. In our model, as reported in Fig. 1, the possible role of particle–particle interaction is accounted for as well, starting from the observation that a segregated dense-dispersed particle phase can form in the proximity of the slag layer [7]. This as a consequence of a very high flux of particles per surface unit, with the rebounding particles shielding the wall to the approaching ones, or due to the deposition of particles over the interface that in this way is transformed into a complex solid–liquid system constituting the effective interface of interaction between impinging particles and walls (along the non-sticky portion of slag reported in the lowest part of Fig. 1).

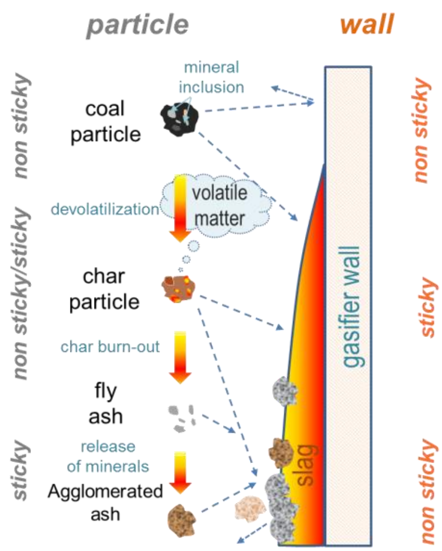

Figure 1. Possible interactions between coal particles at different levels of conversion and confining interfaces.

In this preliminary study, two limiting stickiness levels are assumed: a fully sticky behaviour, typical of ash particles or molten slag surface, and a fully non-sticky behaviour, typical of unconverted char particles or refractory rigid walls. Being in the DEM approach both particles and walls modelled with the same set of properties, a single parameter can be adopted to mark these behaviour: the coefficient of restitution ε. It determines the energy returned to the particle after the impact. Then an impact is considered sticky when almost all the energy is dissipated, while non-sticky when the particle rebounds retaining almost all the kinetic energy possessed before the impact.

Simulation of a lab-scale configuration

The first configuration analysed was a lab-scale cold flow setup to reproduce the experimental one proposed in [8]. A sketch of the computational domain is reported in Fig. 2. The value of ε adopted is 0.9 for non-sticky and 0.1 for sticky material.

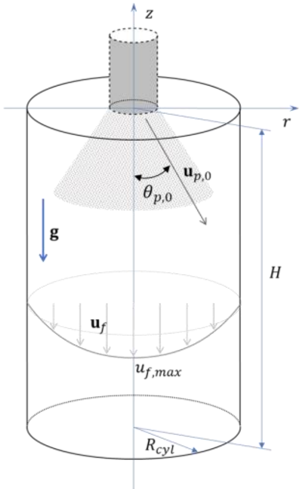

Figure 2. Setup of the simulation of the lab-scale experimental configuration.

A typical result of this investigation is reported in Fig. 3, where a snapshot of the particle distribution during fully-developed conditions is reported. Several interesting features can be detected. Stickiness of the wall mostly influences the reflection angle after the first impact. Sticky walls (SW) allow for an immediate formation of a layer of particles running adjacent to them. It is worth to note that the coupling with sticky particles (SP) leads to a layer that grows more rapidly than in the case of non-sticky particles (NSP). When non-sticky walls (NSW) are considered, a strong interaction of the reflecting particles converging to the axis of the cylindrical reactor leads to the formation, both for SP and NSP, of a dense layer of particles flowing in the bulk of the reactor. However, losing almost all their kinetic energy upon the first impact, NSP have a much lower velocity thus significantly increasing their residence time (i.e. burn-off in a real case) in the reactor.

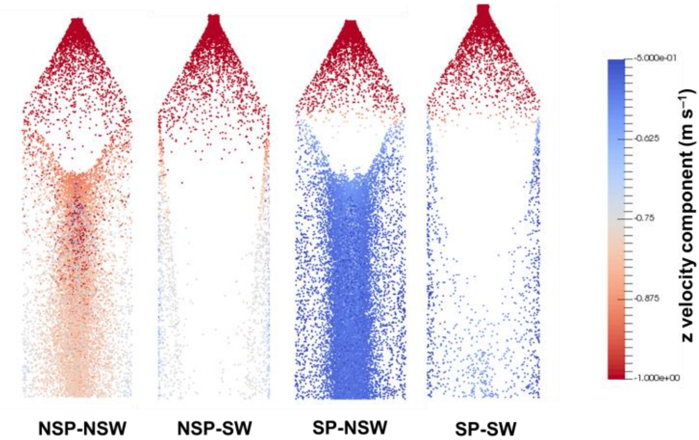

Figure 3. Particle distribution along the longitudinal section of the reactor in the four limiting regimes. Colors represent axial velocity magnitude.

Parametric investigation

Using the coefficient of restitution alone seems not adequate to reproduce all the changes in behaviour of particles used to mimic the impact of coal particles since their injection to the total conversion into ash. A second configuration was therefore considered to get a substantial reduction of the computational effort without losing most of the effects driving the interaction phenomena we want to observe. This new configuration has a very simple geometry, formed by a hexahedron as illustrated in Fig. 4. It aims at reproducing a small region adjacent to the interface close to the wall of a large-scale gasifier. Being in this case the dimension of the particles much smaller than the radius of curvature of the confining wall, it is reasonable (in extracting a small section of an annulus lying on the wall of the gasifier) to neglect the curvature of the section if the effects of the curvature, mostly the inertial centrifugal forces and the centripetal component of the dragging force acting on the particles, are substituted by a body force $\mathbf{F}_C$ equivalent to the resultant of the previous actions. Periodic conditions are assigned along the x and z directions. Along the y direction the front surface is an open surface that can be crossed by particles, while the back surface is the confining interface. Several parameters can be controlled in this configuration by changing the direction and intensity of $\mathbf{u}_f$ (velocity of the gas phase field) and the intensity of $\mathbf{F}_C$, whose combination determines angle and intensity of particles' impact, their acceleration after rebound, etc. Also the concentration of particles in proximity of the wall as well their total number can be varied in a large range of values due to the relatively low total number of particles required in this configuration to obtain a number of impacts per surface unit equivalent to that typically encountered in real gasifiers (about from 5000 to 50000).

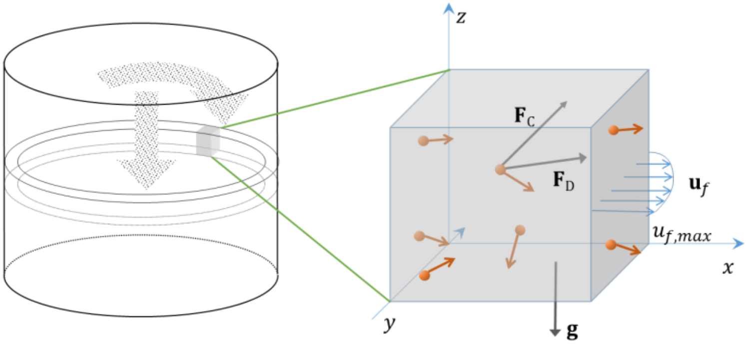

Figure 4. Setup of the simulation for the parametric investigation.

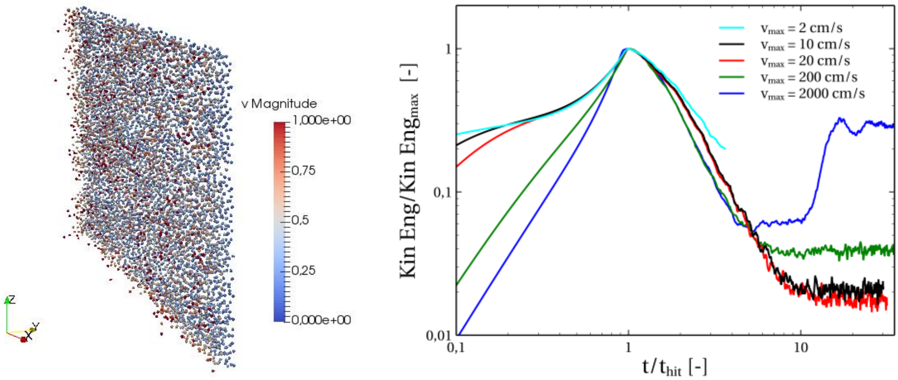

Figure 5. Left: snapshot of particle distribution on the surface, $u_{f,max}$=10 cm/s (velocity scale in m/s in the figure). Right: time evolution of normalized total kinetic energy at different values of $u_{f,max}$. SW–SP case.

The effect of the maximum velocity of the gas phase field $u_{f,max}$ is reported in Fig. 5 for the case of both SW and SP. The time has been normalized with respect to the time t_{hit} required by the injected particles to firstly hit the surface. The simulation for $u_{f,max}$=2 cm/s, despite the low number of particles adopted (4790), is very time-consuming because of the very small characteristic time (t_{hit}=1.1 s) with respect to the time step required for the stability of the soft-sphere contact model (10^{-7} s). All other simulations have evolved up to the establishment of fully-developed regimes. It results that, up to a velocity of 200 cm/s, an asymptotic behaviour is eventually recognized. However the dependence upon the velocity is not straightforward, with the minimum kinetic energy at regime conditions reached for $u_{f,max}$=20 cm/s. Further increasing the value of $u_{f,max}$ to 2000 cm/s, a new behaviour is observed with a temporary lowering of energy after first impact to an almost equilibrium phase. This is followed by a sudden increase of energy to be attributed to the detachment of most of the particles that are eventually dragged by the gas phase to reach a new, higher energy, equilibrium regime. In any case a full deposition of the bunch of injected particle arises.

Conclusions

The reported results clearly indicate the high complexity of the phenomenology under investigation. The proposed simplified configuration is being adopted to obtain a thorough parametric insight of the many parameters affecting this phenomenon, thus helping in determining the real regimes of particles interaction with the gasifiers' surfaces – an aspect that can strongly influence the residence time distribution (i.e., the overall burn-off degree) of reacting coal particles.

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References

[1] Troiano, M., Solimene, R., Salatino, P., Montagnaro, F., "Multiphase flow patterns in entrained-flow slagging gasifiers: physical modelling of particle-wall impact at near-ambient conditions", *Fuel Process. Technol.* 141: 106–116 (2016).

[2] Troiano, M., Santagata, T., Montagnaro, F., Salatino, P., Solimene, R., "Impact experiments of char and ash particles relevant to entrained-flow coal gasifiers", *Fuel* 202: 665–674 (2017).

[3] Ambrosino, F., Aprovitola, A., Brachi, P., Marra, F.S., Montagnaro, F., Salatino, P., "Entrained-flow gasification of coal under slagging conditions: relevance of fuel-wall interaction and char segregation to the properties of solid wastes", *Fuel* 114: 44–55 (2013).

[4] Marra, F.S., Troiano, M., Montagnaro, F., Salatino, P., Solimene, R., "Particle–wall interaction in entrained-flow slagging coal gasifiers: granular flow simulation and experiments in a cold flow model reactor", *Int. J. Multiphase Flow* 91: 142–154 (2017).

[5] Yong, S.Z., Gazzino, M., Ghoniem, A., "Modeling the slag layer in solid fuel gasification and combustion – Formulation and sensitivity analysis", *Fuel* 92: 162–170 (2012).

[6] Seggiani, M., "Modelling and simulation of time varying slag flow in a Prenflo entrained-flow gasifier", *Fuel* 77: 1611–1621 (1998).

[7] Montagnaro, F., Salatino, P., "Analysis of char-slag interaction and near-wall particle segregation in entrained-flow gasification of coal", *Combust. Flame* 157: 874–883 (2010).

[8] Troiano, M., Salatino, P., Solimene, R., Montagnaro, F., "Wall effects in entrained particle-laden flows: the role of particle stickiness on solid segregation and build-up of wall deposits", *Powder Technol.* 266: 282–291 (2014).