DETAILED DEM SIMULATION OF PARTICLE-WALL INTERACTIONS UNDER COAL GASIFIER CONDITIONS

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Abstract
Detailed DEM simulations of a simplified configuration, aiming at reproducing the conditions encountered by char and ash particles near the walls of a reactor during gasification, have been performed. A large number of parameters related to material properties and operative conditions were investigated. Results allowed to identify the parameters most affecting the effective conversion rates of entrained flow coal gasifiers.

Introduction
The entrained flow gasification is one of the main technologies for converting solid fuels into energy and basic chemicals. The process returns a product, the syn-gas, a gaseous mixture composed of H_2 and CO plus by-products, and a residue, the slag which, in the investigated process conditions (1900K, 30bar), is a viscous fluid that runs along the internal walls of the reactor and essentially consists of molten ash.
Although the entrained flow gasification is a widely used technology in the industrial field, the design and the sizing of the gasification reactors still present uncertainty points [1]. In particular, the description of the dynamics of the particles flow, as a result of their interaction with the gas flow and with the gasifier walls, as well as their self-interactions, is largely incomplete [2]. Several attempts to model, by means of computational simulations or theoretical studies, the particle-wall interactions are present in the literature [3]. However, most of these works adopt simplified models for the solid particle phase that are already the result of assumptions on the particle behavior in gasifiers, as the assumption of a critical viscosity discriminating the adherence and the consequent inclusion of impacting particles in the slag layer [4], leading to approximations that invalidate the design of the plants [5].
It was observed that the fate of char particles during gasification when they interact with a wall has a significant role in determining the final gasification degree depending on the coverage by slag, the presence of adhered particles on the surface and, not less important, the establishment of a dense-dispersed particle phase in the proximity of the wall [6]. Indeed, the buildup of a zone near the wall, where the

particles segregate and accumulate as a result of interaction with the wall, causes a lengthening of the average residence times of the char particles in the gasifier, which benefits the degree of conversion.
These interactions have been investigated by this research group, both in a phenomenological way [7] and by modeling analysis [8]. The present work aims to extend the modeling studies and to establish, through detailed DEM simulations, the most influencing mechanical and rheological properties of the particles (mainly determined by the progress of the reaction) and the role of the process variables (in particular the variation of the feeding flux of particles and the flow of oxidizing gas), to identify the conditions influencing the build-up and structure of the dense-dispersed phase near the wall. This information is essential to establish the effective average residence time of the particles in the gasifier.

Model setup
The particle and wall properties have been modeled assuming sticky and non-sticky limits: wall portions and particles covered by an exposed slag surface layer (characterized by a low restitution coefficient and the possibility of forming "liquid bridge") are considered as sticky, and wall portions not covered by slag or particles not sufficiently warm and converted as not sticky.

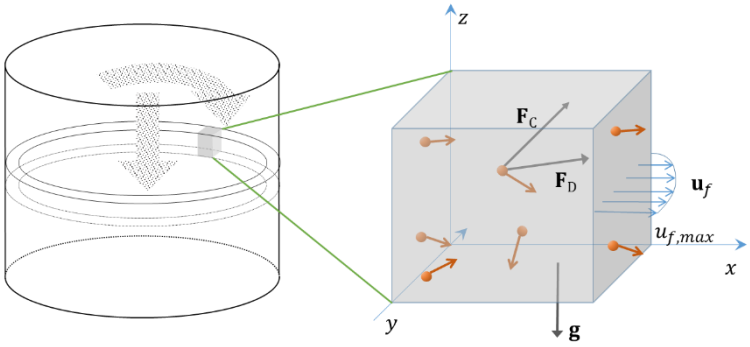

Figure 1. Geometrical setup of the computational domain.

The modeling analysis was carried out using an open-source software named LIGGGHTS [9], a very efficient and parallel DEM solver suitable to face the considerable computational effort required by this complex model. Several submodels were selected to describe in detail particle-particle and particle-wall collisions, starting with the soft-sphere model from the Hertzian theory. Submodels for rolling friction, cohesion and the possibility of formation of liquid bridge were included. The resulting model is computationally very demanding, requiring to greatly simplify the computational domain while keeping the particle phase fully described as single lagrangian elements. A very small portion of a cylindrical reactor, adjacent to the confining wall, as illustrated in Fig. 1, is considered. To further simplify the setup, the domain is represented by a hexahedron. Proper centrifugal forces are added to represent the effect of the curvature of the wall. Periodic

conditions are assigned along the x and z direction. All particles move under the action of this body force and of the drag forces determined by a fictitious gas flow field with prescribed velocity profile, null at the wall, and then having only v_x not null, with a maximum at a fixed distance from the wall.

Results

A parametric investigation was first conducted to establish the mechanical properties of particle most influencing the dynamic behavior of the system. Starting from the injection of a fixed number of particles randomly dispersed in the domain, the system evolves with all particles remaining in the domain and eventually reaches a statistically asymptotic behavior, characterized by a certain level of total kinetic energy, as shown in Fig. 2.

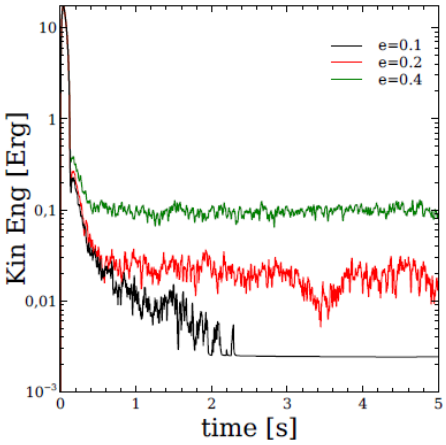

Figure 2. Total kinetic energy of particles versus time at different $\boldsymbol{e}$. $\boldsymbol{N_p = 7500}$.

This analysis confirmed the prominent role of the normal coefficient of restitution e with respect to other material relevant properties, like the Young's modulus, the friction coefficient and the rolling friction coefficient. Following the findings reported in [7], this parameter has then been varied between 0.4 (for not sticky particle) and 0.1 (for sticky particles). It is evident that the asymptotic state is an equilibrium between the kinetic energy gained under the action of the forces acting on the particles and the energy dissipated by collisions. The important feature of the system is the distribution of residence times that the particles realize in the domain upon their stratification structure is stabilized. These are reported in Fig. 3 for the same condition of Fig. 2. It is found that a roughly bimodal profile is realized, with the two main peaks separating apart by reducing e: a layer of particles with short residence time forms on top of the layer of particles almost lying on the walls. The time required to establish this structure (see Fig. 2) reduces with increasing e and becomes of order of magnitude comparable with the average residence time of coal particles in swirled gasification reactors.

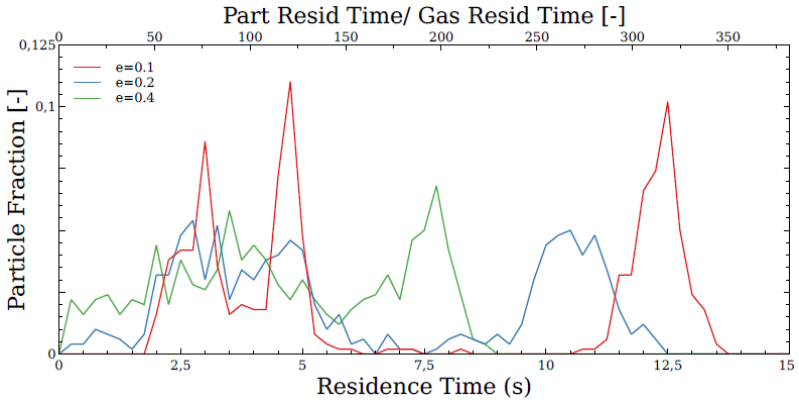

Figure 3. Distribution of particle fractions versus residence times for $\boldsymbol{N\_p = 7500}$ and $\boldsymbol{v_{max} = 40}$ cm/s.

Two operative parameters were found to mostly influence this dynamics: the particle number density and the gas flow velocity. The corresponding profiles of total kinetic energy versus time are reported in Fig. 4.

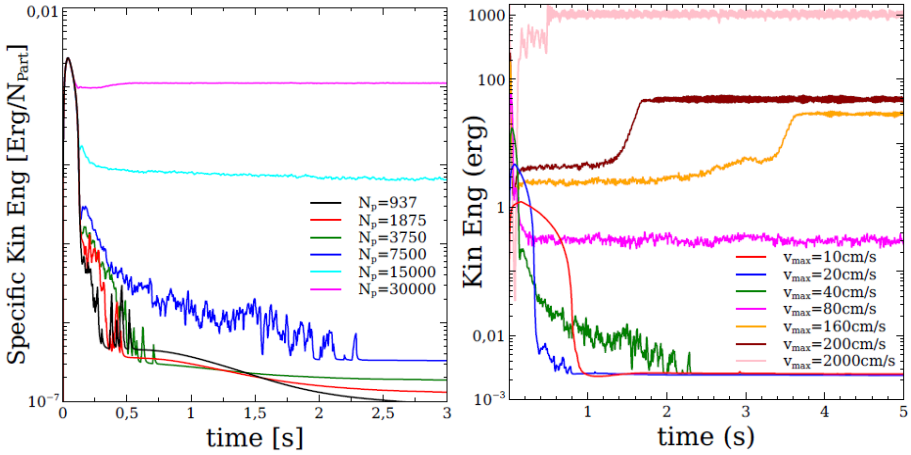

Figure 4. Total kinetic energy vs. time. On the left at varying the total particle number with0 $v_{max} = 40$ cm/s; on the right at varying the gas flow maximum velocity with $N_p = 7500$ and $e = 0.1$.

Even if different patterns are found varying these parameters, it arises that both the increasing of flow velocity and increasing of particles number act towards the increasing of total kinetic energy. The observation of the distribution of particles residence times reported in Fig. 5 reveals that a critical value exists (respectively $N_p = 15000$ and $v_{max} = 80$ cm/s) beyond which a large portion of particles has a very short residence time (less than 1 s), meaning that, if real char particles are

considered, their conversion would be significantly limited. Conversely, at the lowest particle number and gas flow velocities, a large portion of particles results practically deposited on the reactor wall, indicating that if real char or ash particles are considered, they will be promptly engulfed in the slag, again limiting the char conversion.

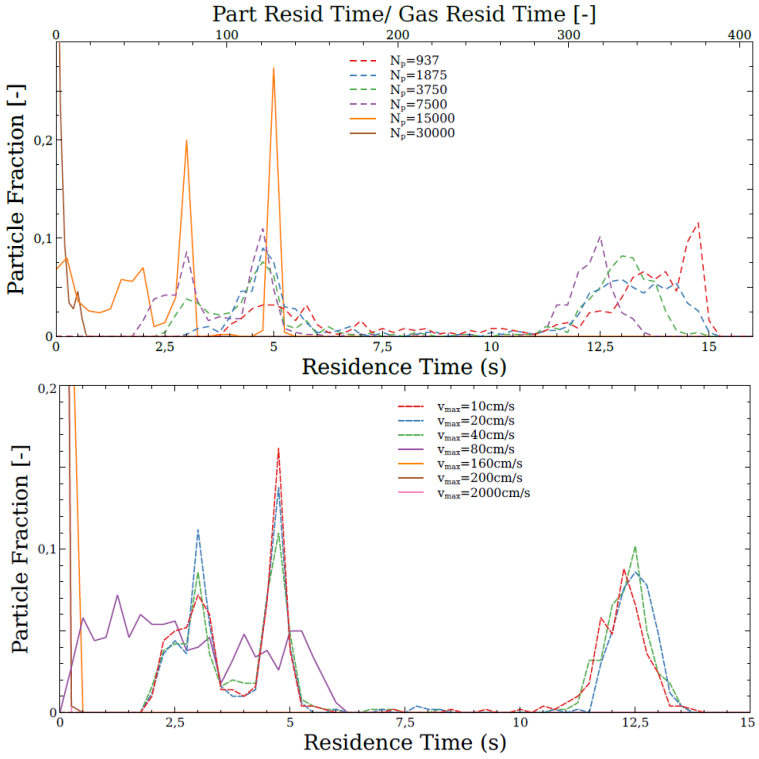

Figure 5. Distribution of particle fractions versus residence times. On top at varying $\boldsymbol{N_p}$ and $\boldsymbol{v_{max}} = \mathbf{40}$ cm/s. On bottom at varying $\boldsymbol{v_{max}}$ and $\boldsymbol{N_p} = \mathbf{7500}$.

Notably, in all cases the distribution of residence times is roughly bimodal, meaning that in any case the segregation and formation of a dense-dispersed phase is likely to establish on top of a surface covered by particles.

Conclusions

Results of simulations show that, among the mechanical and rheological properties investigated, the restitution coefficient alone is able to describe the variations of the particle and wall properties, causing major changes in the dynamic behavior of the particle phase.

An even greater effect on this behavior is given by the operating process conditions, expressed in terms of number density of particles flow and intensity of the bulk flow velocity of the gaseous phase. The formation of the segregated particle phase,

hypothesized by the reported studies, was reproduced by the present model. Several dynamic regimes have been observed indicating the limits of optimal conditions for operation of entrained flow gasifiers.
The results of this analysis have been further elaborated (here not shown for the sake of brevity) with reference to a kinetic gasification model [10], and considering the variation of residence times according to the different operating conditions as obtained from the modeling analysis. This allowed to obtain relations between: operating conditions, residence time, characteristic reaction time, Damköhler number, degree of gasification.

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