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#### Fuel





# Entrained-flow gasification of coal under slagging conditions: Relevance of fuel-wall interaction and char segregation to the properties of solid wastes



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#### HIGHLIGHTS

- Results show that both C-entrapment inside and C-coverage of the slag can occur.
- A multilevel modeling approach is used to understand char segregation patterns.
- Compartmental, RANS- and LES-based models are developed.
- A dense-dispersed particle-laden flow establishes close to the gasifier wall.
- The relevance of near-wall particle segregation was confirmed.

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#### ABSTRACT

Entrained-flow slagging gasifiers are characterized by operating conditions that promote ash migration/ deposition onto the reactor walls, whence ash is drained as a molten phase. Experimental investigation on ashes generated by full-scale plants suggested that both char entrapment inside the melt and carboncoverage of the slag can occur. Because of the wide range of spatial and temporal scales involved in these phenomena, numerical simulation of the fate of the flying fine char particles is a very difficult task. This work illustrates how different numerical modeling approaches can be jointly used to understand segregation patterns of char particles in full-scale entrained-flow coal gasifiers operated in the slagging regime. A multilevel approach has been developed for this purpose. RANS-based simulations of the full-scale geometry with coal particle injection and tracking aimed to obtain the general behavior of the flow field and particle trajectories. Simulations enabled to estimate the effect of swirl and tangential flow on the bulk-to-wall char particle deposition rate. Then, RANS results were adopted in a more detailed numerical model based on the solution of the filtered Navier-Stokes equations. In this last model, a turbulence LES approach for the Eulerian gas phase was applied. The equations of particles motion were solved via a Lagrangian particle tracking algorithm with the TrackToFace method. Simulations were performed involving a level of detail that allowed to obtain a clear picture of the multiphase flow behavior responsible for char deposition phenomena. This multilevel approach enabled the assessment of the char particle deposition rates and the nature of char-slag interaction (segregation/entrapment) that are likely to occur in full-scale slagging gasifiers. Results of numerical simulations have been critically discussed in the light of experimental findings. They represent a useful source of information for the implementation of constitutive equations and parameters in design-oriented reduced compartmental models.

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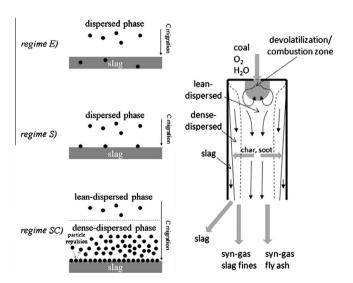
#### 1. Introduction

Modeling coal gasification under entrained-flow conditions is still a challenging goal with broad areas of uncertainty, despite the fact that several entrained-flow gasifiers have been in operation for decades. One-dimensional models, developed starting from the late seventies [1–4], are based on the assumption that the gas and solid phases both move in plug flow. More comprehensive models, supported by CFD-based detailed descriptions of flow, temperature and concentration fields, consider the relevance of complex hydrodynamics and multiphase flow to the gasifier

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performance [5-16]. Almost all of these models rely on the Reynolds Average Navier-Stokes (RANS) [17] approach to take into account the effect of the turbulence on the flow field, actually solving for field variables averaged in time. The RANS approach strongly limits the predictive capabilities of the simulations, because several closure models have to be adopted to introduce the effects of the unresolved time scales on the averaged fields. Unsteady phenomena like turbulent dispersion of particles, coal particle combustion, homogeneous gas phase reactions, turbulence-wall and particle-wall interactions are all modeled by a RANS method. Despite such limitations, the adoption of this approach is unavoidable to limit the computational power required. Entrained-flow gasifiers are indeed characterized by a wide range of turbulence scales. Typical integral dimensions are on the order of 10 m, while the Kolmogorov scale can be estimated on the order of 0.1 mm. being the bulk Reynolds number, computed with the plug-flow velocity and the gasifier diameter, on the order of  $10^6$ .

The design and operating conditions of entrained-flow gasifiers of new generation aim at promoting ash migration/deposition onto the reactor walls, whence the molten ash (slag) is drained and eventually collected as a melt at the bottom of the gasifier [18-23]. The recent literature on entrained-flow gasification has addressed the fate of char particles as they impinge on the wall slag layer [24-27]. Montagnaro and Salatino [28] highlighted the relative importance of the parallel pathways of coal conversion consisting of entrained-flow of carbon particles in a lean-dispersed gas phase vs. segregated flow of a dense curtain of char particles in the proximity of the gasifier walls. The establishment of this segregated dense-dispersed particle phase is promoted by particle migration and interaction with the molten slag. Taking into account properties such as char density, particle diameter and impact velocity, slag viscosity, interfacial particle-slag tension, theoretical criteria for both char particle entrapment inside and carbon-coverage of the wall ash layer have been developed. This is represented in Fig. 1, where the possible regimes of C-slag micromechanical interaction are outlined: regime E) (entrapment), in which char particles reaching the slag surface are permanently embodied into the layer and further course of combustion/gasification is hindered; regime S) (segregation), in which char particles reaching the wall adhere to the slag layer's surface without being fully engulfed, so that the progress of combustion/gasification is permitted; regime SC) (segregation and coverage), in which the



**Fig. 1.** Left: regimes of fuel slag micromechanical interaction (E = entrapment; S = segregation; SC = segregation and coverage). Right: schematic diagram of the entrained-flow gasifier.

coverage of the slag layer with carbon particles is extensive. In this last regime a dense-dispersed annular phase is established in close proximity of the wall ash layer, where the excess impinging char particles which cannot be accommodated on the slag surface accumulate. This phase is likely to be characterized by a velocity that is intermediate between that of the fast lean-dispersed phase and that of the slowly moving wall ash layer. This feature is beneficial to C conversion due to the longer mean residence times of carbon particles belonging to this phase. Consistently, a schematic diagram of the entrained-flow gasifier is presented in Fig. 1 in which, in particular, the presence of three different sources of solid wastes is underlined, that is: slag phase, yielding coarse slag granules upon interaction with the quench bath at the bottom of the gasifier; dense-dispersed phase, giving rise to slag fines upon interaction with the quench bath; lean-dispersed phase, giving rise to fly ash escaping the gasifier in the gas stream.

The aim of this study is to demonstrate the possibility to gather information from models developed at different scales and levels of approximation to numerically investigate phenomena occurring at the smallest scales in a gasifier. The model results are then critically discussed with reference to the properties of solid residues generated in an industrial-scale entrained-flow slagging gasifier. A particular emphasis is devoted to the char-slag interaction, for which a very detailed model, based on the Discrete Element Method (DEM) for the solid phase [29] and the Large Eddy Simulation (LES) approach for the gas phase [30], has been adopted. Due to the impossibility to perform a full-scale and comprehensive simulation of the whole gasifier at this level of detail, different models are employed to derive constitutive equations and parameters. These are then used in simplified design-oriented compartmental or CFD-based models aiming at the prediction of the gasifier performance. The critical processes and parameters deserving a more detailed scrutiny were suggested by a sensitivity analysis of a compartmental 1D model (level 1) of the gasifier [28]. This model includes all the main phenomena occurring in the gasifier, i.e. fuel feeding with gas, coal pyrolysis and gasification, homogeneous reactions, char migration to the wall and slag build-up. Constitutive parameters of this model require the knowledge of the flow field establishing in the gasification chamber. As far as processes associated with char-slag interaction are concerned, particle velocities and trajectories as they impinge the confining walls covered by the slag must be known. In the present study, a DEM-RANS CFD model (level 2), is adopted to provide this information. Clouds of parcels representing particles of different size and mass, given a proper distribution of Stokes numbers with respect to the average bulk gas phase as computed in the first model, are introduced in a realistic representation of the gasification chamber. At this level, the focus is on the assessment of the distribution of particles in the gasifier, on the identification of the average particles load in the different zones of the gasifier and of their velocity and angle of impact onto the confining surface. Therefore, an approach based on a RANS model for the gas phase and on a Lagrangian Particle Tracking (LPT) algorithm to evaluate the particle movement is considered pertinent. The last level (level 3) of approximation addresses the detailed simulation of the particle-wall interaction, performed at comparable conditions, in terms of particle loads, particle size distribution and relative importance between drag and inertia effects, using an accurate DEM-LES [29] model. In this model the real particles trajectories are affected by the interaction with an unsteady turbulent field and with the confining surface. Properties of this surface are varied to take into account the different mechanisms of particle deposition due to the presence of a bare wall, a molten slag, or a slag already covered by a layer of particles. This latter level enables the assessment of the particle deposition regimes that are likely to occur under the assigned boundary conditions. The procedure, that is still under construction, will be

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