SLAGGING COAL GASIFIERS: MODELLING OF THE MECHANISMS OF PARTICLES-SLAG INTERACTION

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Abstract
In pilot entrained-flow slagging gasifiers, high conversion efficiency and low level of pollutant emissions have been observed, but the mechanism leading to this behavior is not fully understood, limiting the capability to scale up their design.
In this paper, after a review of the principal mechanisms and modelling approaches already proposed, a new interpretation of the particle-slag interaction is given and some results of the modelling activities are presented to illustrate the main features that can be envisaged in the particle-slag interaction.

A not so brief literature survey
The investigation of the particle-slag interaction is not new, and can be linked to the development of particles deposition models. Indeed, almost all early models proposed in the literature assume that the particles impinging onto the slag, or more in general onto the combustor surface, are isolated. This assumption naturally makes the particle properties the dominant variables in the possible interaction regimes: viscosity and sticking probability become the most important parameters. This is the line proposed by several investigators in the '90s and successive years. Richards et al. [1], Wang and Harb [2], Seggiani [3], Tominaga et al. [4], Barroso et al. [5], Degereji et al. [6], proposed that particulate deposition on the wall or the slag surface occurs if either the char/ash particles or the layer already deposited on the wall have a viscosity lower than a critical viscosity. Therefore the role of the char and ash composition, as well as that of the degree of carbon conversion before the impact, is recognized in the ability to rule the viscosity of the particles and the state of the slag formed by the melting of the formerly accumulated particles. Some indexes were then proposed, like the sticking probability or the slagging index that, for a given impaction rate, furnish the rate of particle accumulation and then the accretion of the slag [7,8]. The micromechanical interaction of the single particle

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with the slag layer has been also deeply investigated by several authors. Wang et al. [9] extended the modelling to take into account the burning of suspension and deposited particles. Shannon et al. [10] described the different regimes that can occur after the impaction of the particle with the slag. Conditions of immediate entrapment or settling are separated by an oscillating behavior that can eventually lead to settling or to rejection. Li et al. [11], studying the micro-structure of different coal particles at different stage of burning, related the levels of stickiness probability to the conversion rate. Then, Akiyama et al. [12] established a connection between the residence time and the changes in the deposition mechanism leading to slagging or fouling. Ni et al. [13] reconstructed the very complex interaction of a single droplet of molten slag with the wall, and identified the maximum spread diameter of the slag droplet, the Reynolds and Weber number, and the impact and contact angles, as the key parameters determining rebound, shatter or sticking. However, it became soon evident the need to include parameters independent from the characteristics of the material forming the particles. Lee and Lockwood [14] and Costen et al. [15] recognized that smaller particles are dragged by the flow and then can be able to penetrate the boundary layer only if the magnitude of their velocity component normal to the wall is sufficiently high. Therefore, the impaction rate is related to a critical velocity, independently from the critical viscosity for the entrapment at impaction. Following this observation, Benyon [16] proposed an a-posteriori model: rate of particle accumulation is computed after the solution of the gas flow phase and the transport of solid particle phase. Pyykonen et al. [17] raised the role of the turbophoresis. They analyzed inertial impaction and turbulent impaction separately, and expressed the impact rate proportionally to the main parameter of the turbulent boundary layer, i.e. the wall shear stress τ_w. Shimizu and Tominaga [18] where among the first to recognize a possible role of the particle-particle interaction. They proposed a model of char capture by the slag partially covered by the unreacted char, elucidating the different response of the impaction of particles over an uncovered slag surface and a surface covered by settled particles. Montagnaro and Salatino [19] addressed the possibility that a new regime, called of “segregation and coverage”, can establish for the flying particles, different from entrapment, repulsion or simple settling onto the surface. Indeed, a strong intra-particle interaction, due to the increasing particle concentration inside the boundary layer, occurs in a very dense layer of flying particles close to the surface. The particles velocity in this layer is lower than that in the dispersed phase, increasing the particle residence times inside the gasifier. This observation was actually promoted by the discrepancy between the predicted combustion efficiencies and those measured in pilot/full-scale gasifier plants, that can be justified only allowing a longer residence time. From the picture delineated by this review, it arises that particle-slag interaction has been mostly investigated to predict the formation/accretion of the slag and its properties, instead that for the study of the effects of this interaction on the gasifier fluid-dynamic behavior, probably assuming that the gasifier performances could not be significantly affected by the structure of the small regions close to the boundaries of the gas-solid phase.

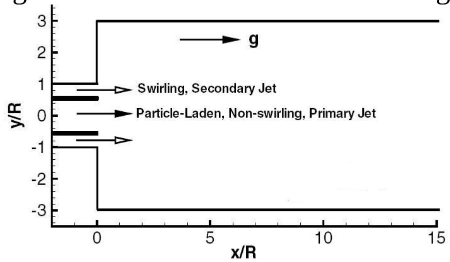

Figure 1. Sketch of the computational domain for RANS simulations; only a portion of the gasifier is reported.

The gasifiers modelling approaches developed up to now seem to confirm this observation. One-dimensional models, developed starting from the late ‘70s (see Refs from 1 to 4 reported in [20]), 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 performance (see Refs from 5 to 16 reported in [21]). Almost all of these models rely on the Reynolds Average Navier-Stokes (RANS) approach to take into account the effect of the turbulence on the flow field, actually solving for field variables averaged in time. This 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. Yong et al. [22] recently proposed a very complex model that incorporates a number of sub-models to take into consideration the properties of slag dependent upon temperature and composition, the contribution of momentum of captured particles and the possibility of slag resolidification. Special attention is given to the interaction of the particles colliding with the slag layer but, since only trapped particles are relevant to the slag layer build-up, just a particle capture criterion for colliding particles is introduced. The model predicts the local thickness of the molten and the solid slag layers, but still does not include the possibility to predict the occurrence of a segregation and coverage regime.

In the following, some results obtained by numerically investigating the particle-wall interaction are reported, to give an assessment of the major phenomena of particle-wall interaction that can affect the gasifier performances.

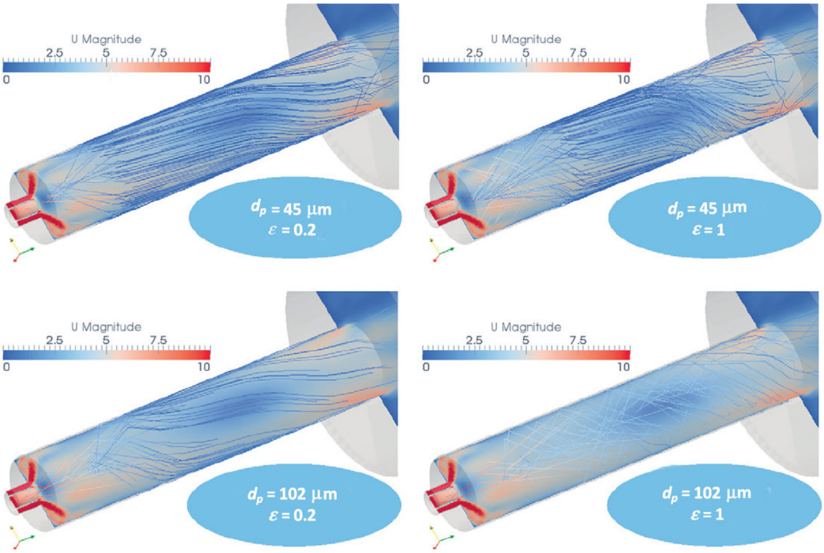

Figure 2. Particles pathlines in the gasifier for d_p = 45 μm (up) and d_p = 102 μm (down), with ε = 0.2 (left) and ε = 1 (right).

Numerical simulations and main results

To study the effect of the presence of the slag on the impinging surface of the particles, RANS simulations with a Lagrangian particle tracking (LPT) algorithm have been performed. The trajectories of particles after the impact with different values of the kinetic energy restitution coefficient ε were simulated. The geometry of the prototype gasifier is reported in Fig. 1. Details can be found in Ref. [20]. Two gas streams are coaxially injected into the main cylindrical chamber. The outer stream feeds gas, while the inner stream feeds gas loaded with particles. The main chamber extends for 0.96 m, corresponding to 5-times its diameter (0.192 m). The OpenFOAM [23] code is adopted to compute the numerical solutions. Spatial discretization of the gas phase equations is performed with a FV discretization. The algorithm implemented for the LPT is the so-called TrackToFace method described in Macpherson et al. [24]. Fig. 2 reports the influence of ε and of the particle size on the patterns of particle flow. The switch from inelastic to elastic impacts and the size of particles clearly determine quantitative and qualitative features of particles trajectories. Lighter particles are drawn by the flow field after few rebounds following their first impact with the walls. Heavier particles are much less affected by drag, undergoing multiple rebounds all along the gasifier length, again with a pronounced influence of ε. Two different asymptotic conditions arise for the trajectories of the different particles: circumferential trajectories with particles repeatedly bouncing along the walls, and able to penetrate and leave the boundary layer, and axial trajectories with particles slowly moving very close to the wall, thus forming a dense layer over the surface. A more detailed study of the particle-wall interaction has been conducted adopting a LES approach to fully account for turbulence effects in the gas phase. Two prototypal configurations have been conceived to represent the asymptotic conditions before recalled: a planar channel flow and a curved channel flow. Details can be found in [21]. Here for the sake of brevity only major conclusions are recalled. Both turbulence and large scale vortical motion promote the migration of particles towards the wall, favoring the formation of regions with dense particle concentration. In both cases, the level of particle concentration, especially for the curved channel configuration, becomes very high close to the surface, making questionable the assumption of particles moving independently from each other. Intra-particle collision (4-way coupling) need to be included to correctly predict the structure of the dense layer close to the surface. For this reason, and to appreciate the role of different levels of stickiness of both the surface and the particles themselves, a DEM granular simulation [25] has been set up for a configuration similar to the curved channel flow. This approach fully take into account the particle-particle and particle-wall interaction with an Hertzian approach. Influence of the gas phase is only roughly represented by prescribing a field of body forces acting on the particles, that imposes a motion similar to the motion due to the swirled flow. The main results are reported in Fig. 3, where the influence of the matrix of binary condition “sticky-nonsticky” for wall and particles is documented.

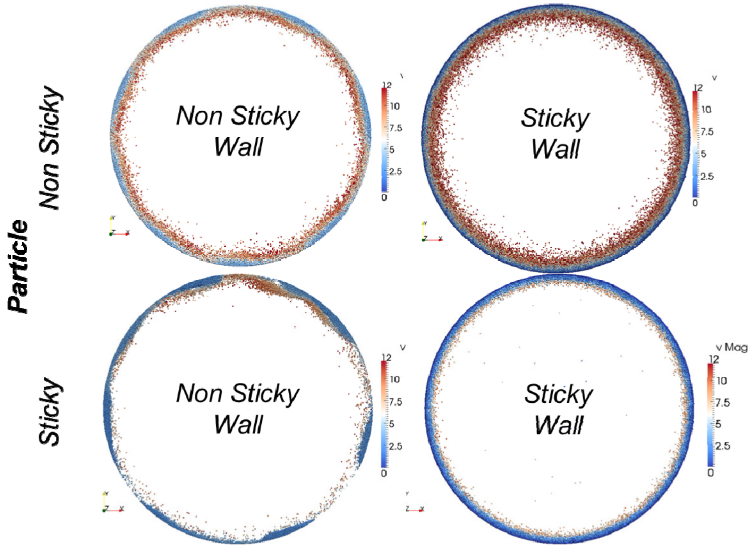

Figure 3. Snapshots of particles distribution during the equilibrium phase with the DEM granular simulations.

Acknowledgements

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References

[1] Richards, G. H., Slater, P. N. & Harb, J. N., “Simulation of ash deposit growth in a pulverized coal-fired pilot scale reactor”, *Energy Fuels,* 7:774-781 (1993)

[2] Wang, H. & Harb, J. N., “Modeling of ash deposition in large-scale combustion facilities burning pulverized coal”, *Prog. Energy Combust. Sci.,* 23:267-282 (1997)

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

[4] Tominaga, H., Yamashita, T., Ando, T. & Asahiro, N., "Simulator development of entrained flow coal gasifiers at high temperature and high pressure atmosphere", *IFRF Combust. J.,* 200004 (2000)

[5] Barroso, J., Ballester, J. & Pina, A., "Study of coal ash deposition in an entrained flow reactor: assessment of traditional and alternative slagging indices", *Fuel Process. Technol.,* 88:865-876 (2007)

[6] Degereji, M., Ingham, D., Ma, L., Pourkashanian, M. & Williams, A., "Numerical assessment of coals/blends slagging potential in pulverized coal boilers", *Fuel,*102:345-353 (2012)

[7] Fan, J. R., Zha, X. D., Sun, P. & Cen, K. F., "Simulation of ash deposit in a pulverized coal-fired boiler", *Fuel,* 80:645-654 (2001)

[8] Fang, Q., Wang, H., Wei, Y., Lei, L., Duan, X. & Zhou, H., "Numerical simulation of the slagging characteristics in a down-fired, pulverized-coal boiler furnace", *Fuel Process. Technol,* 91:88-96 (2010)

[9] Wang, X., Zhao, D., He, L., Jiang, L., He, Q. & Chen, Y., "Modeling of a coal-fired slagging combustor: development of a slag submodel", *Combust. Flame,* 149:249-260 (2007)

[10] Shannon, G., Rozelle, P., Pisupati, S. V. & Sridhar, S., "Conditions for entrainment into a FeO_x containing slag for a carbon-containing particle in an entrained coal gasifier", *Fuel Process. Technol.,* 89:1379-1385 (2008)

[11] Li, S., Wu, Y. & Whitty, K. J., "Ash deposition behavior during char-slag transition under simulated gasification conditions", *Energy Fuels,* 24:1868-1876 (2010)

[12] Akiyama, K., Pak, H., Takubo, Y., Tada, T., Ueki, Y., Yoshiie, R. & Naruse, I., "Ash deposition behavior of upgraded brown coal in pulverized coal combustion boiler", *Fuel Process. Technol.,* 92:1355-1361 (2011)

[13] Ni, J., Yu, G., Guo, Q., Zhou, Z. & Wang, F., "Submodel for predicting slag deposition formation in slagging gasification systems", *Energy Fuels,* 25:1004-1009 (2011)

[14] Lee, F. C. C. & Lockwood, F. C., "Modelling ash deposition in pulverized coal-fired applications", *Prog. Energy Combust. Sci.,* 25:117-132 (1999)

[15] Costen, P., Lockwood, F. & Siddique, M., "Mathematical modeling of ash deposition in pulverized fuel-fired combustors", *Proc. Combust. Inst.,* 28:2243-2250 (2000)

[16] Benyon, P. J., "Computational Modelling of Entrained Flow Slagging Gasifiers", PhD Thesis, *School of Aerospace, Mechanical & Mechatronic Engineering - University of Sydney* (2002)

[17] Pyykonen, J., Jokiniemi, J. & Jacobson, T., "Development of a Prediction Scheme for Pulverised Coal-Fired Boiler Slagging", in *Impact of Mineral Impurities in Solid Fuel Combustion, Springer US,* 735-752 (2002)

[18] Shimizu, T. & Tominaga, H., "A model of char capture by molten slag surface under high-temperature gasification conditions", *Fuel,* 85:170-178 (2006)

[19] 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)

[20] 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,* In Press (2013)

[21] Ambrosino, F., Aprovitola, A., Brachi, P., Marra, F. S., Montagnaro, F. & Salatino, P., "Investigation of char-slag interaction regimes in entrained-flow gasifiers: linking experiments with numerical simulations", *Combust. Sci. Technol.,* 184:871-887 (2012)

[22] 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)

[23] OpenCFD. OpenFOAM Programmers Guide ver. 1.7 (2008)

[24] Macpherson, G. B., Nordin, N. & Weller, H. G., "Particle tracking in unstructured, arbitrary polyhedral meshes for use in CFD and molecular dynamics", *Comm. Num. Meth. Eng.,* 25:263-273 (2009)

[25] Kloss, C., Goniva, C., Hager, A., Amberger, S. & Pirker, S., "Models, algorithms and validation for opensource DEM and CFD-DEM", *Prog. Comput. Fluid Dyn., An Int. J.,* 12:140-152 (2012)