CHAR-SLAG INTERACTION IN ENTRAINDED FLOW GASIFIERS:
MODELING OF EXPERIMENTAL EVIDENCES


marra@irc.cnr.it
* ENEA, CR Portici, Piazzale Enrico Fermi 1, 80055, Portici, Italy
** Istituto di Ricerche sulla Combustione, CNR, Via Diolezione 328, 80124, Napoli, Italy
*** Dipartimento di Chimica, Università degli Studi di Napoli Federico II, Complesso Universitario di Monte Sant’Angelo, 80126, Napoli, Italy
**** Dipartimento di Ingegneria Chimica, Università degli Studi di Napoli Federico II, Piazzale Vincenzo Tecchio 80, 80125, Napoli Italy

Abstract
This work describes the results achieved analyzing the complex phenomenology associated with interaction of a particle-laden turbulent flow with the slag-covered wall of an entrained flow gasifier. Two approaches are considered to address coal particle fate: experimental analysis of sample collected in operating gasifiers and a new numerical simulation approach based on a multilevel modeling. Results shed new insights on the effective mechanisms of coal particle conversion highlighting the role of the turbulence on the distribution of particles in gasifiers.

Introduction
IGCC (Integrated coal Gasification Combined Cycle) is a promising technology, allowing for an easier Carbon Capture and Sequestration while maintaining, or even increasing, the overall efficiency of the energy conversion process. An important unit of such plants is the gasifier, mostly realized in the form of entrained-flow. An high combustion efficiency is obtained by feeding pulverized coal, oxidant (air or oxygen) and steam into the furnace at high speed from tangentially placed injectors, to promote swirling flow and centrifugal motion of particles towards the walls. In this way the residence time is increased too. The gasification process, conducted at high pressure and temperature, is thus allowed to complete, especially for fine coal particles. Consequently the coal conversion efficiency can be very high, observed to range in pilot plants from 98 to 99.5 %. The combustion efficiency is influenced by several factors. Very small coal particle dimensions promote the heat up and the reaction of carbon with the surrounding hot oxidant and steam, as they flow through the gasifier but are immediately dragged by the flow, reducing the ability to separate the residual mineral matter. While thermal cracking reactions and pyrolysis can be considered weakly affected by the particle concentration, the oxidation of the volatile compounds released around the particles depends upon its mixing with the fresh oxidant mixture. Therefore combustion efficiency is influenced by the spatial distribution of the
particle phase, with an homogeneous distributions favoring a better mixing. Successive use of the flue gases in turbines for the electricity production or into units for CO2 sequestration and capture, require a very small particulate concentration. This is another reason why the design of new generation of entrained-flow coal gasifiers aims at favoring ash migration/deposition onto the reactor walls, whence the molten ash (slag) flows and is eventually drained separately at the bottom of the gasifier [1,2]. It clearly appears that a proper prediction of the fate of burning particles is crucial for proper design and scale up, especially in regions close to the gasifier walls [3], where large part of the oxidation process takes place under a competition between the release of a large amount of volatile compounds and the poor mixing conditions with the oxidant mixture due to the hindered flow motion, both effects due to the presence of the dense dispersed solid phase.

Most research efforts have been focused simply to determine the rate of particle deposition and the build-up of the molten slag layer [4]. Even with this respect, several authors already recognized the limits of models simply based on the number of particles impingements and on the ability to deposit and stick on the molten ash layer depending on particle viscosity [5]. Indeed, besides the effect of the temperature, also the effects of the flow turbulence on the motion of particles plays a fundamental role on the formation of clusters of particles and their aggregation or segregation. Usually, the flow turbulence is taken into account by incorporating models for turbulent particle dispersion [6]. These models are effective in the regime of high dilution, that actually occurs in the core region of a gasifier, and for the larger unburnt coal particles, weakly affected by the smallest scales of turbulent flow structures. However such models largely fail in two important situations. The first occurs when the finer ash particles are considered. They tend to be rapidly clustered by the vortical structures of turbulence. The second, of extremely importance in entrained coal gasifier, arises for all particles close to the walls, where the dilution levels can decrease of orders of magnitude, making questionable the assumption of not colliding particles and direct impingement with the slag layer [7]. Aim of this work is to study the possible occurrence of this regimes in entrained flow gasifier by coupling several levels of experimental and theoretical investigations.

**Experimental investigation**

An experimental evidence of this picture for the fate of particles has been recently assessed by analyzing the chemical composition of samples of coarse slag and slag fines generated in the ELCOGAS entrained-flow gasifier located in Puertollano, Ciudad Real (Spain) [7]. Cross-sections of coarse slag and slag fines particles were analyzed by Scanning Electron Microscopy/Energy Dispersive X-ray (SEM-EDX) analysis. Quantitative EDX analysis of the coarse slag, of which some samples are shown in Fig. 1, revealed the presence of small marks with a significant carbon content as high as 48.8–54.2%. This fact can be explained by assuming the entrapment of not fully burned coal particles into the slag.
This finding contributes to the assessment of the relevance of carbon entrapment in slag particles. The results of the SEM analysis performed on whole slag fines particles showed that the carbon content was larger than the value obtained from the inspection of coarse slag particles, in line with results of elemental analysis. Some samples of this analysis are shown in Fig. 2.

This is particularly evident for porous particles where C-content ranged between 82.3 and 86.5%. A considerable amount of unreacted coal is therefore entrapped into the slag matrix. From this observation emerges that a certain level of spatial non homogeneity of the solid phase distribution exists. In a recently published study by Montagnaro and Salatino [8], these data have been interpreted by assuming that different regimes of particles-slag interaction can occur: either char entrapment inside the melt or carbon-coverage of the slag may occur, depending on properties like char density, particle diameter and impact velocity, slag viscosity, interfacial particle-slag tension. Occurrence of char entrapment prevents further progress of combustion/gasification. On the contrary, if char particles reaching the wall adhere to the slag layer’s surface without being fully engulfed the progress of combustion/gasification is still permitted. The observed high rate of coal conversion can be therefore explained only if this second regime establishes on the slag surface. On the other hand, these results refers to a fixed set of gasifier
operating conditions. Thus a sensitivity analysis with respect to the gasifier operating condition could be performed only by assessing the parameters mostly affecting the particle-slag interaction.

**Numerical modeling**

The addressed considerations highlights the technological need to build up methods for the prediction of the mechanism of coal particles clustering and segregation. Actually a comprehensive numerical simulation of the whole range of spatial and temporal chemical and turbulent time scales involved in a full scale gasifier, is still unfeasible due to the high computational cost: the scales of turbulence involved in the gasification processes range from sub-micron scale up to the integral scale of a gasifier reactor chamber (of the order of tens of meters). To overcome this difficulty, the ongoing approach is based on the development of a multilevel approach [9]. A reduced order model based on a Plug Flow Reactor representation of the gasifier [8] is firstly adopted to obtain an order of magnitude estimate of the level of conversion rate of the particles that migrate towards the wall to form the slag layer.

![Figure 3. 3D-RANS simulation of a prototype gasifier. Particles pathlines in the gasifier for $d_p = 45 \, \mu m$ (left) and $d_p = 102 \, \mu m$ (right). U magnitude scale (m s$^{-1}$) refers to particle velocity, Umean Z scale (m s$^{-1}$) refers to mean flow axial velocity.](image)

In a second level, the motion of particles representing classes of partially converted coal in a 3-dimensional representation of the gasifier is modeled with a Computational Fluid Dynamic (CFD) approach [10]. Turbulence of the flow field is described adopting the RANS approach, while particle motion is resolved with a Lagrangian Particle Tracking (LPT) approach. The use of the RANS approach for the gas phase coupled with the LPT for the solid phase in this analysis is twofold. First it is used to address the behavior of coarse and fine coal particles trajectories when subjected to a swirl motion which induced a turbulent field. This model, while avoiding the great complexity and computational effort required by comprehensive numerical CFD models of gasifiers already proposed in the literature [5, 11], is sufficient to characterize the range of conditions, in terms of momentum possessed and direction, that the different particles show when approaching the gasifier walls, as shown in Figure 3. The second, aspect concerns
the identification of the regions where the coal clustering becomes foreseeable: distinct regions close to the wall have been in this way identified [9]. The obtained results confirmed the experimental evidence that finer particles could be mainly responsible of particle layering near the solid walls as they, after their first impinging on the wall, assumes a pathway parallel to the wall. In contrast, larger particles continue to bounce over the walls along the whole length of the gasifier.

**Figure 4.** Configurations of the 3D-LES computations and corresponding particle distribution. Top: plane channel flow, \(d_p = 102 \text{ \(\mu\)m} \) and \(\varepsilon = 0.2\). Bottom: curved periodic channel, \(U \text{ (m s}^{-1}\) refers to gas velocity, \(d_p = 102 \text{ \(\mu\)m}, \varepsilon = 0.2\) and 1.

The identification of these two different regions and the characterization of particle classes representative of partially burned coal particles, was the basis for the proper setup of numerical simulations based on a Large Eddy Simulation approach [10]. This level aims at a detailed investigation of the mechanisms of slag-particle interaction. Two different configurations have been considered. The first is a plane particle laden channel flow, that well represents the main features of the gasifier regions where particles move parallel to the wall. The second is a periodic particle laden curved channel flow, that best represent regions close to the wall but dominated by the external swirling flow. These configurations are shown in Figure 4, together with an example of the particle distributions that is obtained at steady state for different particle sizes or rebound restitution coefficient \(\varepsilon\).

Even if this model is still incomplete, a large amount of data is being collected regarding the time required to form a particle dense layer the level of segregation, the characteristic size of clusters, and many others, depending on particle diameter and weight and turbulence intensity levels [7,9].
Conclusions
A methodology to investigate numerically the occurrence of regimes of particle segregation and deposition onto the walls of an entrained-flow gasifier has been illustrated. The results allow to identify the operating conditions that lead to the occurrence of hypothesized coverage-segregation or entrapment regimes of ash-slag interaction, and to explain the level of carbon content in both coarse and fine slag collected at the bottom of the gasifier operated by ELCOGAS. The assessment of the mechanisms depending on the particles-turbulence interaction will made possible a better design of the future generation of gasifiers, needed to respect the protocols established for the reduction of pollutant emissions still adopting coal fossil fuel as primary source.

Acknowledgments
This work has been partially supported by the program agreement “MiSE – CNR Ricerca e sviluppo per il sistema elettrico nazionale”, project Carbone Pulito.

References
