

GASDS: a Kinetic-Based Package for Biomass and Coal Gasification

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In this paper, a simulation package called GASDS is introduced. It is particularly suited to evaluate the pyrolysis, gasification and combustion of biomass and coal feedstocks. The aim of this work is to describe the package from a numerical point of view and its interface. Additionally, experimental results for a countercurrent fixed-bed biomass gasification reactor are reproduced. The influence of reactor and particle discretizations are investigated with respect to accuracy and computational time. Some differences are present between experimental and simulation results. In order to improve the agreement between simulation and experimental results it is suggested to improve the kinetic scheme of the solid phase and gas-solid reactions. The negligible differences in terms of predictions, instead, do not justify the adoption of finer discretizations for the particle and reactor, which imply longer computational times.

1. Introduction

The exploitation of biomass as a renewable raw material plays a relevant role for meeting the European development targets set by the Horizon 2020 strategy (Difs et al., 2010). Additionally, it contributes to the development of a bio-based economy, as green chemicals can also be produced from biomass feedstock (Mood et al., 2013). Due to their complex structures, second generation biomasses are efficiently exploited only after suitable transformation processes. This allows to convert agro-industrial residues (i.e., second generation biomass) into more appropriate fuels for industrial use (e.g., bio-syngas, bio-ethanol) (Demirbas, 2009). The conversion to bio-syngas can be performed via gasification of such residues. In the current work, the exploitation of second generation biomasses for energy and syngas production is investigated via an up-draft fixed-bed gasifier (Di Blasi et al., 1999). As described by Mandl et al. (2010), this reactor configuration requires a continuous feeding of fresh biomass from the top and an oxidizing agent (air or O₂ and possibly water vapor) from the bottom. The reactor is thus operating in countercurrent configuration. During the process, biomass volatilizes and syngas is obtained. This gaseous mixture is rich in H₂ and CO and it can be used for several different purposes, from energy generation in a combustion engine (Balat et al., 2009) to chemical synthesis processes, like the Fischer-Tropsch reaction (Demirbas, 2009). After entering the countercurrent reactor the incoming biomass encounters different sections. At first the biomass is dried by the hot air coming from the lower reactor layers. Then pyrolysis reactions start. These endothermic reactions break the biomass into gaseous compounds, tar (condensables) and char (solid) (Ranzi et al., 2008). Afterwards, the solid char undergoes gasification to CO and H₂, while the remaining char is further oxidized in the last reactor layer, leading to CO, CO₂ and H₂O. Additionally, secondary reactions take place in the gas phase, for instance water-gas-shift and combustion of complex volatile products, e.g., levoglucosan (Ranzi et al., 2008).

Different models have been presented to describe the behavior of the reactor. De Blasi et al. (2004) presented a Partial Differential Equations (PDEs) model, where both time and longitudinal dependencies are taken into

account. They also exploited a lumped kinetic scheme to describe the reactions taking place in the gasifier. A similar approach was adopted by Mandl et al. (2010), who solved a steady-state operation problem. The aim is to present GASDS, a kinetic-based package for the numerical simulation of the pyrolysis, gasification and combustion processes of biomass feedstock.

2. Materials and Methods

The dynamic model used in the GASDS package was already introduced and validated on both coal (Corbetta et al., 2015) and biomass feedstocks (Ranzi et al., 2014). It accounts for a detailed kinetic scheme and different scales. These are the particle, the reactor layer and the gasifier reactor scales.

The dynamic process is described by a PDEs system, where gradients should be evaluated with respect to time, longitudinal direction and radial coordinate. However, some approximations allow to reduce the system to an Ordinary Differential Equations (ODEs) system, where only gradients with respect to time are considered. In fact the plug-flow behavior along the longitudinal direction is approximated by several reactor layers in series, where the gas phase is assumed to be perfectly mixed. Moreover, in the case of non-homogeneous particles, intra-particle gradients are approximated via a second discretization along the radial coordinate.

The ODEs system is solved by using advanced numerical methods included in the BzzMath libraries (Buzzi & Manenti, 2012). The used methods are particularly suited for stiff ODEs system and based on the Gear multi-value method (Gear, 1971).

3. Presentation of the graphical interface

In this Section, the graphical interface of the GASDS package is introduced and described. Figure 1 shows the first tab of the package. Here the reactor configuration and its specifications are given by the user.

The screenshot shows the 'EQUIPMENT' tab of the GASDS software interface. The window title is 'Using: DiBlasi_beechwoodH104S4L2.inp'. The interface is divided into several sections:

- Equipment Selection:** A list of radio buttons for selecting the reactor type:
 - 1= Batch
 - 2= Semi Batch
 - 3= Continuous
 - 4= Moving Bed
 - 5= Drop Tube
 - 7= Steady Equi
 - 8= Double Room
- Flow and Temperature Parameters:**
 - Fresh solid top feed (kg/h):
 - 0= counter 1= cocurrent:
 - Feed Temperature (K):
- Reactor Specifications:**
 - Surface (m²):
 - Height (m):
 - Void fraction *100:
 - How many Volume Elements:
 - Initial Temperature (K):
 - Transfer_Line Height (m):
- Radiation:**
 - No
 - Yes
- Total analysis time (s):**
- Restart Option:**
 - Open Restart File:
 - Delay time (s):

Figure 1: Graphical interface of the GASDS package, Equipment tab. In the top box, the equipment type can be selected, specifying the initial temperature and the fresh biomass flow rate. In the second box, the equipment specifications are given. In this box, the reactor can be subdivided into multiple reactor layers (i.e., 'Volume elements' specification), to allow for a better resolution of the counter-current gasification process.

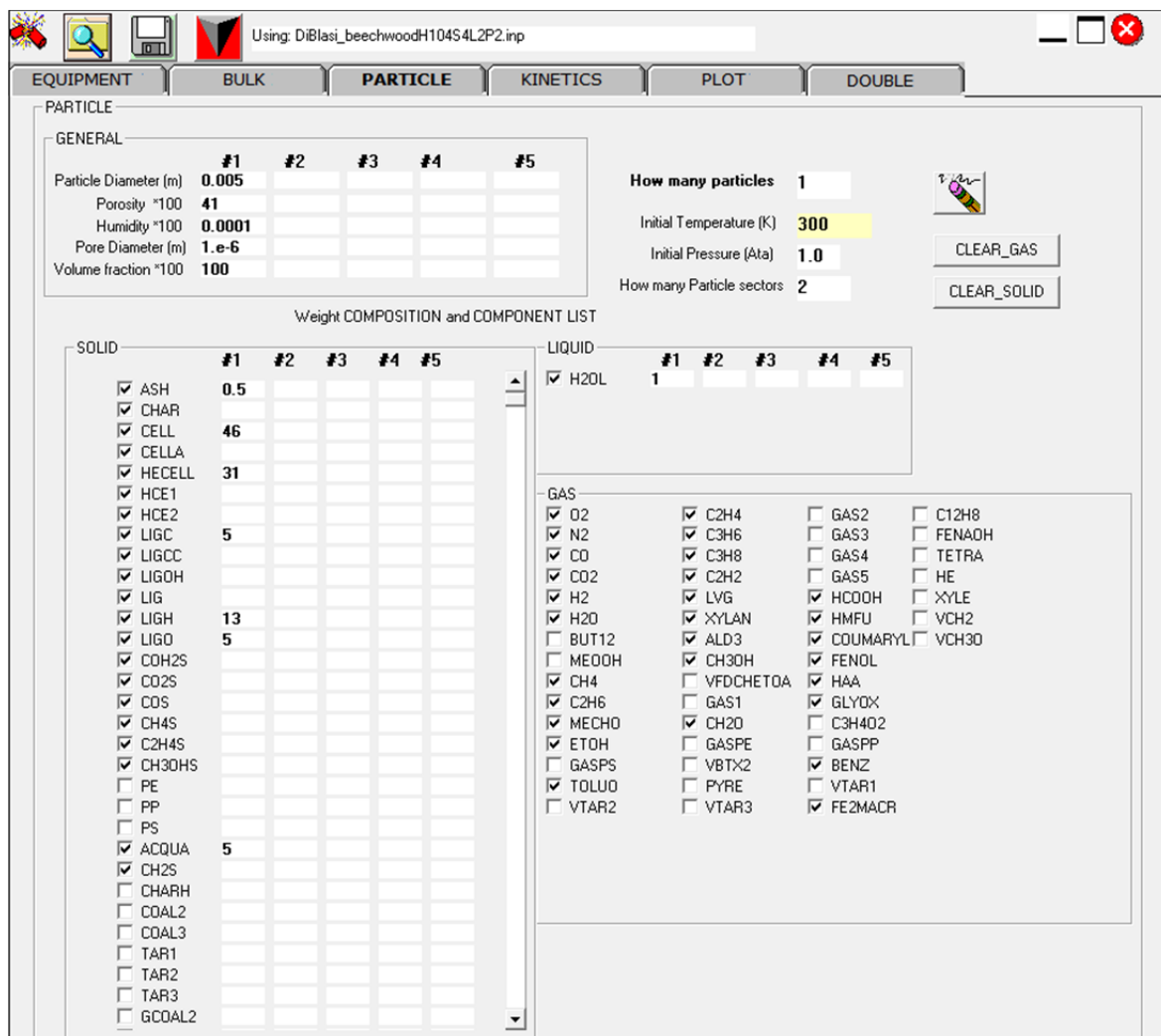


Figure 2: Graphical interface of the GASDS package, Particle tab. The particle is described from a physical point of view in the top left box. In the bottom left box, the composition of the biomass particle is given with respect to several pseudo components (Ranzi et al., 2014). Additionally, the components which are present in the gas phase (according to the kinetic scheme) are selected, while the operating pressure of the reactor and the discretization level of the particles are chosen on the right.

Also, in the case of long analysis time, it is possible to stop the simulation and restart it via the Restart Option box. It should be stressed that, in the case of a continuous (i.e., fixed bed) configuration, the biomass volume undergoes a shrinking process during the start-up operation, as highlighted by Corbetta et al. (2015). For this reason, the initial height of the continuous configuration is different from the one reached at the steady-state. In the example, an initial height of 10.4 m will lead to a final steady-state height of 0.55 m (Di Blasi et al., 1999).

Figure 2, instead, shows the Particle tab, where the user can input the biomass characteristics. Additionally, in this screen, the particle can be subdivided into several sectors, to take into account intra-particle mass and temperature profiles.

Figure 3 shows the kinetic scheme that is used to simulate the biomass pyrolysis and combustion. This scheme describes the kinetics of the solid phase and gas-solid reactions. The user can select reactions that are believed to be more relevant than others from the displayed list. The kinetic scheme is created in a secondary file where the reactions can be customized with respect to e.g., frequency factor, activation energy, reaction order and heat of reaction. These quantities are depicted on the right column of Figure 3. This file is then imported by the GASDS package. The gas phase reaction scheme (i.e., secondary reaction scheme) is instead imported from the DSMOKE tool (Bassani et al., 2015).

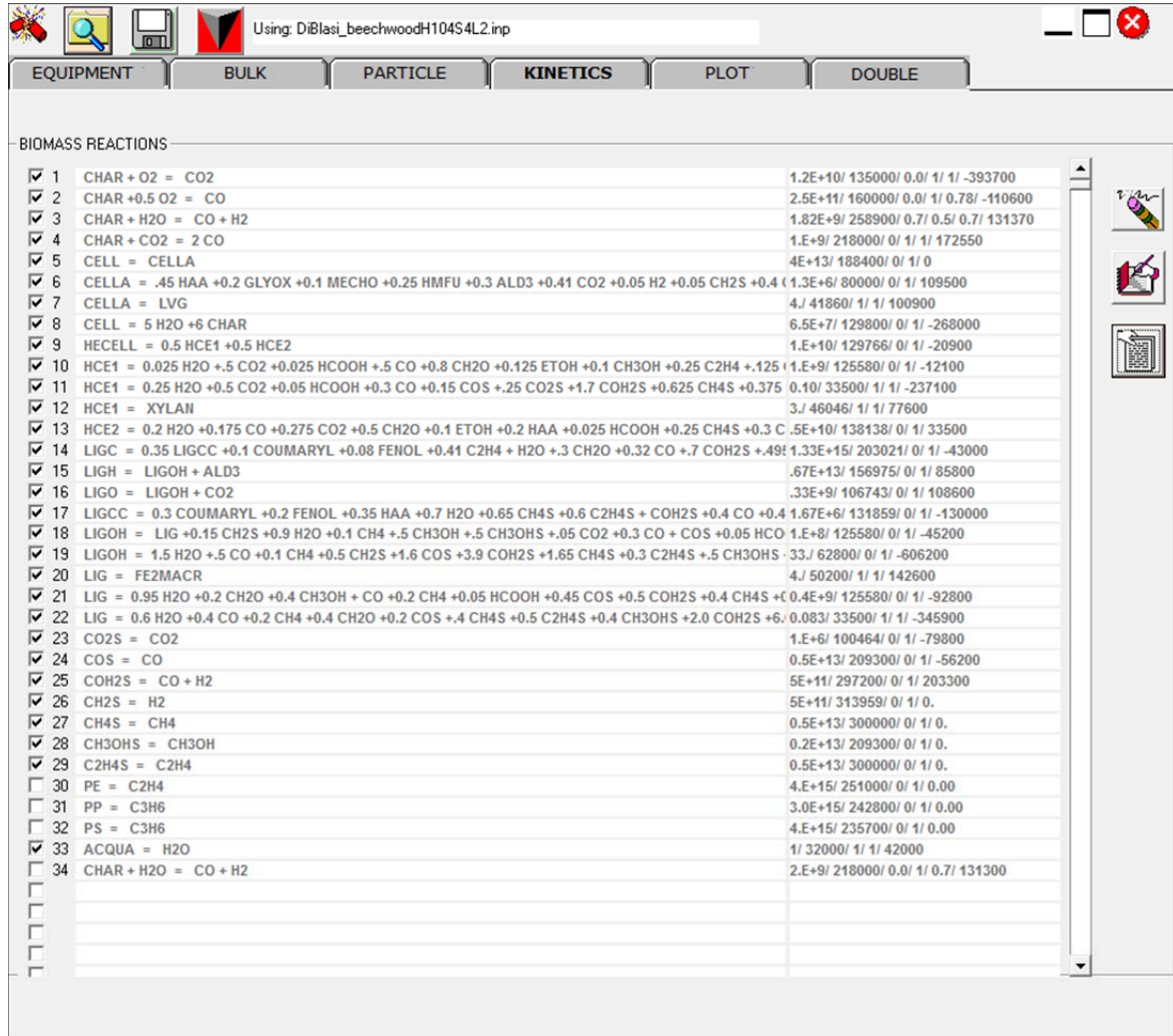


Figure 3: Graphical interface of the GASDS package, Kinetics tab. In this tab the user can customize the solid phase kinetic scheme.

In order to correctly simulate the mass and thermal transfer for each of the components that are present in the kinetic scheme, their properties are also specified in secondary files. These files, one for each phase, contain information about e.g., specific heat capacity at constant pressure, density, thermal conductivity, mass diffusivity or viscosity.

The Bulk tab is used to describe the inlet composition and properties of the gaseous combusive agent, which, for the current work, is taken as air at 300 K and 1 atm. The Plot tab, instead, allows to display the evolution of the process, even if calculations are not yet finished.

Table 1: Comparison between GASDS simulation prediction and experimental data (Di Blasi et al., 1999). Outlet dry gas molar fractions of relevant components.

Component	GASDS – 3 reactor layers	GASDS – 4 reactor layers	Di Blasi et al. (1999)
H ₂	13.12 %	13.09 %	7.00 %
CO	26.39 %	26.39 %	28.60 %
CO ₂	10.27 %	10.26 %	7.00 %
CH ₄	3.24 %	3.24 %	1.80 %

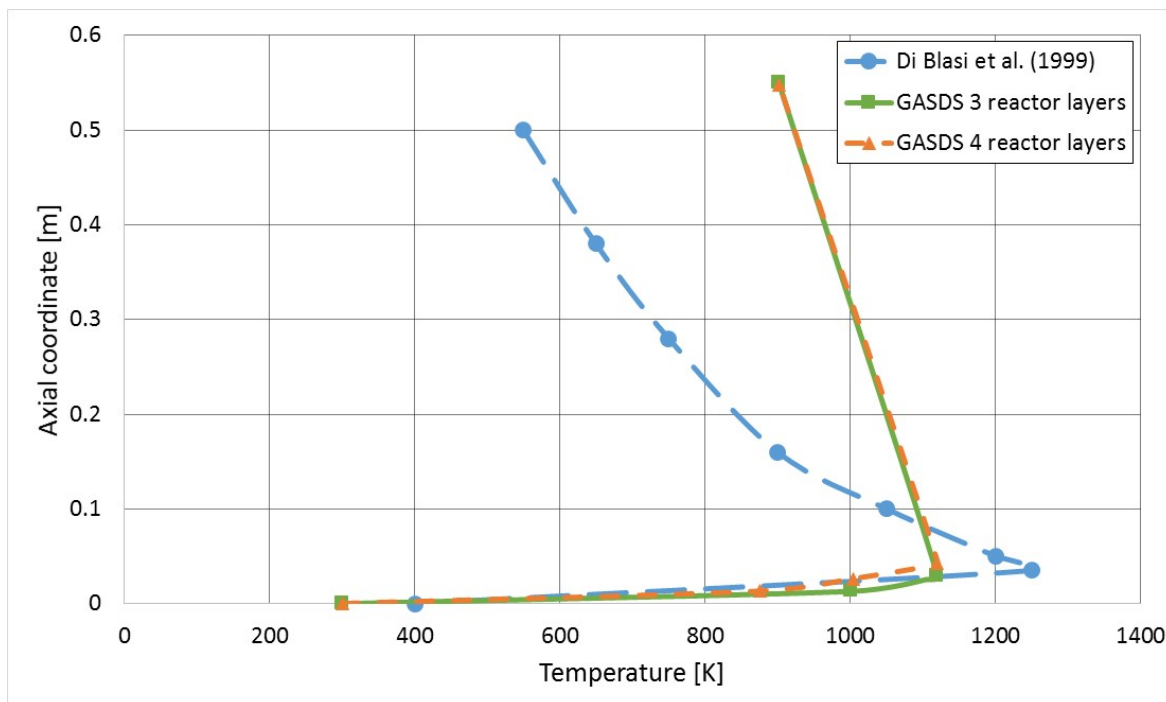


Figure 4: Comparison between GASDS simulation prediction and experimental data (Di Blasi et al., 1999). Gas phase temperature.

4. Results

In this Section, illustrative results are provided, to illustrate the validity of the GASDS package in predicting the behaviour of biomasses and coals during the gasification process. Table 1 and Figure 4 depict different comparisons between the experimental and simulation results. Despite a fair agreement in the outlet dry gas composition, especially concerning CO, it is possible to see that the simulation results still present relevant differences with the experimental data, in particular in the temperature predictions. The cause could be in the kinetic scheme of the solid phase and gas-solid reactions which needs further developments. Nevertheless, Table 1 and Figure 4 indicate that the simulation predictions, for the investigated case study is only slightly influenced by the amount of reactor layers that are considered. Table 2 instead shows the influence of multiple reactor layers and multiple particle sectors for the investigated case (Di Blasi et al., 1999). Finer discretizations in both axial and radial directions do not improve the prediction accuracy, leading, in essence, to the same simulation results. Thus the gain in terms of quality predictions does not justify the increase in terms of computational time. This result, though, is highly problem-dependent. For instance, in the case of a taller reactor or a bigger particle size, a finer discretization could lead to relevant improvements in terms of quality predictions. Due to the similarities between biomass and coal gasification, the tool is suitable also for describing coal pyrolysis, gasification and combustion processes. This was successfully done in Corbetta et al. (2015), to which interested readers are further referred.

Table 2: Influence of the multiple particle sectors on the outlet dry gas composition and computational time. Computational times were measured on an 8 GB RAM and an Intel® Core™ i7-4770S processor computer.

Component	GASDS – 3 reactor layers, 1 particle sector	GASDS – 3 reactor layers, 2 particle sectors	GASDS – 4 reactor layers, 1 particle sector	GASDS – 4 reactor layers, 2 particle sectors
H ₂	13.12 %	13.12 %	13.09 %	13.09 %
CO	26.39 %	26.40 %	26.39 %	26.39 %
CO ₂	10.27 %	10.27 %	10.26 %	10.26 %
CH ₄	3.24 %	3.25 %	3.24 %	3.25 %
CPU time [s]	826	1,707	2,072	5,600

5. Conclusion

In this paper, a package for biomass and coal gasification has been introduced and described. The gasifier model is derived from the PDEs system generated by energy and mass balances inside the equipment. Solution of the PDEs system involves its transformation into an ODEs system through discretization processes along the longitudinal and radial coordinate. These approximate the reactor in multiple consecutive reactor layers, where homogeneous conditions for the gas phase are assumed, while the biomass particles can be discretized in multiple concentric layers. The ODEs problem, is solved through advanced numerical methods (Buzzi & Manenti, 2012). A user-friendly graphical interface is also provided and explained which allows the user to customize the process simulation. In spite of showing some differences with the experimental data, the obtained results proved to be promising. As a future work, the kinetics of the biomass pyrolysis step should be investigated to improve the accordance between simulation results and experimental data. As an additional step, the package could be extended and improved to allow the control and optimization of the process.

Acknowledgments

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References

- Balat, M., Balat, M., Kirtay, E., & Balat, H. (2009). Main routes for the thermo-conversion of biomass into fuels and chemicals. Part 2: Gasification systems. *Energy Conversion and Management*, 50(12), 3158-3168.
- Bassani, A., Manenti, F., Ranzi, E., Lima, N.N.M., Zuniga Linan, L. (2015). Novel coal gasification process: Improvement of syngas yield and reduction of emissions. *Chemical Engineering Transactions*, 43, 1483-1488.
- Buzzi-Ferraris, G., & Manenti, F. (2012). BzzMath: Library overview and recent advances in numerical methods. *Computer Aided Chemical Engineering*, 30(2), 1312-1316.
- Corbetta, M., Bassani, A., Manenti, F., Pirola, C., Maggio, E., Pettinau, A., Deiana, P., Pierucci, S., & Ranzi, E. (2015). Multiscale Kinetic Modeling and Experimental Investigation of Syngas Production from Coal Gasification in Updraft Gasifiers. *Energy & Fuels*, 29(6), 3972-3984.
- Demirbas, M. F. (2009). Biorefineries for biofuel upgrading: a critical review. *Applied Energy*, 86, S151-S161.
- Di Blasi, C., Signorelli, G., & Portoricco, G. (1999). Countercurrent fixed-bed gasification of biomass at laboratory scale. *Industrial & Engineering Chemistry Research*, 38(7), 2571-2581.
- Di Blasi, C. (2004). Modeling wood gasification in a countercurrent fixed-bed reactor. *AIChE Journal*, 50(9), 2306-2319.
- Difs, K., Wetterlund, E., Trygg, L., & Söderström, M. (2010). Biomass gasification opportunities in a district heating system. *Biomass and Bioenergy*, 34(5), 637-651.
- Gear, C.W. (1971). Numerical initial value problems in ordinary differential equations. *Prentice Hall PTR*.
- Mandl, C., Obernberger, I., & Biedermann, F. (2010). Modelling of an updraft fixed-bed gasifier operated with softwood pellets. *Fuel*, 89(12), 3795-3806.
- Mood, S. H., Golfeshan, A. H., Tabatabaei, M., Jouzani, G. S., Najafi, G. H., Gholami, M., & Ardjmand, M. (2013). Lignocellulosic biomass to bioethanol, a comprehensive review with a focus on pretreatment. *Renewable and Sustainable Energy Reviews*, 27, 77-93.
- Ranzi, E., Cuoci, A., Faravelli, T., Frassoldati, A., Migliavacca, G., Pierucci, S., & Sommariva, S. (2008). Chemical kinetics of biomass pyrolysis. *Energy & Fuels*, 22(6), 4292-4300.
- Ranzi, E., Corbetta, M., Manenti, F., & Pierucci, S. (2014). Kinetic modeling of the thermal degradation and combustion of biomass. *Chemical Engineering Science*, 110, 2-12.