**Multiscale circular economy process simulation and optimization**

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Treating solid materials such as biomass, coal, and municipal waste is an important challenge for the energy transition. To effectively address this problem, it would be useful to predict the outputs of the thermal treatment of the solid fuel, such as the gaseous species released over time, the temperature, and ultimately the energy that can be extracted from the fuel with a given reactor configuration and initial conditions. To this end, in this abstract, a framework for developing digital twins of reactors that treat solid fuels is presented. GasDS is a software tool developed at Politecnico di Milano for the dynamic modeling of the thermal treatment of solid fuels. GasDS models systems on a multi-scale level, including both particle and reactor scales. The solid feedstock is described as a linear combination of the properties of three reference components, based on a CHONS analysis of the material and the results are modeled over time for different reactor types, such as fixed-bed counter-current or co-current reactor, or batch reactor, using a kinetic scheme for the solid particles and one for the bulk reactions according to the type of fuel being treated. The resulting system of partial differential equations (PDEs) is transformed, through an appropriate discretization, into multiple reactor layers and particle volumes, into a system of ordinary differential equations (ODEs), which is integrated over time using appropriate numerical methods. The software has already been partially validated in literature for biomass [1] and coal [2], and used successfully with multiple industrial partners like A2A, Saipem, Gaironi Naval, Sintef, Capgemini, Acea, Techint, and Europower. The potential of GasDS lies in its ability to model all types of solid fuels whose properties and kinetics are known. This makes it useful for engineers and scientists working on digital twins of real plants or studying the impact and potential of a particular solid fuel.

**Keywords**: *Gasification, Pyrolysis, Digital model, Syngas, Optimization*

‌1 Ranzi, E.; Corbetta, M.; Manenti, F.; Pierucci, S. Kinetic Modeling of the Thermal Degradation and Combustion of Biomass. Chemical Engineering Science 2014, 110, 2–12. <https://doi.org/10.1016/j.ces.2013.08.014>.

2 Corbetta, M.; Bassani, A.; Manenti, F.; Pirola, C.; Maggio, E.; Pettinau, A.; Deiana,P.; Pierucci, S.; Ranzi, E. Multi-Scale Kinetic Modeling and Experimental Investigation of Syngas Production from Coal Gasification in Updraft Gasifiers. Energy & Fuels 2015, 29 (6), 3972–3984. <https://doi.org/10.1021/acs.energyfuels.5b00648>‌