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Thermochemical equilibrium modeling approach for carbon-rich feedstock gasification validated against laboratory and large-scale experiments

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In the present study, a pre-existing stoichiometric equilibrium model based on direct minimization of Gibbs free energy has been further developed and applied to estimate the equilibrium composition of synthesis gases produced by the gasification of carbon-rich feedstock (e.g., coal, municipal waste or biomass) in a fixed-bed reactor [1]. Our modeling approach is validated against thermodynamic models, laboratory gasification and demonstration-scale experiments reported in the literature. The simulated synthesis gas compositions have been found to be in good agreement under a wide range of different operating conditions. Consequently, the presented modeling approach enables an efficient quantification of synthesis gas compositions derived from feedstock gasification, considering varying feedstock and oxidizer compositions as well as pressures and temperatures. Furthermore, the developed model can be easily integrated with numerical flow and transport simulators to simulate reactive transport of a multi-componentgas phase.

[1] Otto and Kempka, Synthesis gas composition prediction for underground coal gasification using a thermochemical equilibrium modeling approach, Energies (in review)