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Prediction of feasible synthesis gas compositions at three European coal deposits

Christopher Otto[1] and Thomas Kempka[2]
[1]GFZ German Research Centre for Geosciences, Section 3.4 - Fluid Systems Modelling, Potsdam, Germany (otto@gfz-potsdam.de)
[2]University of Potsdam, Institute of Geosciences, Potsdam, Germany

In the present study, we apply our validated stoichiometric equilibrium model [1], based on direct minimisation of Gibbs free energy, to predict the synthesis gas compositions produced by in-situ coal conversion at three European coal deposits. The applied modelling approach is computationally efficient and allows to predict synthesis gas compositions and calorific values under various operating and geological boundary conditions, including varying oxidant and coal compositions. Three European coal deposits are assessed, comprising the South Wales Coalfield (United Kingdom), the Upper Silesian Coal Basin (Poland) and the Ruhr District (Germany). The stoichiometric equilibrium models were first validated on the basis of laboratory experiments undertaken at two different operating pressures by [2] and available literature data [3]. Then, the models were adapted to site-specific hydrostatic pressure conditions to enable an extrapolation of the synthesis gas composition to in-situ pressure conditions. Our simulation results demonstrate that changes in the synthesis gas composition follow the expected trends for preferential production of specific gas components at increased pressures, known from the literature, emphasising that a reliable methodology for estimations of synthesis gas compositions for different in-situ conditions has been established. The presented predictive approach can be integrated with techno-economic models [4] to assess the technical and economic feasibility of in-situ coal conversion at selected study areas as well as of biomass and waste to synthesis gas conversion projects.

[1] Otto, C.; Kempka, T. Synthesis Gas Composition Prediction for Underground Coal Gasification Using a Thermochemical Equilibrium Modeling Approach. *Energies* **2020**, *13*, 1171.

[2] Kapusta et al., 2020

[3] Kempka et al., 2011

[4] Nakaten and Kempka, 2019