Geophysical Research Abstracts
Vol. 13, EGU2011-5116, 2011
EGU General Assembly 2011


# Modelling tar pollutant production and solubility in the frame of UCG with combined CO2 storage

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Facing the ongoing depletion of traditional energy ressources underground coal gasification (UCG) with combined $CO_2$ storage is a sustainable approach with positive economic potential (KEMPKA et al. 2009). Industrial UCG applications focus the production of a high calorific product gas, simultaneously undesired by-products have to be minimized to maintain the environmental safety in the aboveground and underground ambience. Considering the underground system the estimation of in-process generated tar pollutant quantities and its discharge into the adjacent groundwater system under in-situ conditions is a major challenge that still remains unsolved by now (SURY et al 2004, FRIEDMAN et al. 2009). Tars generally comprise a complex pollutant spectrum with up to 10.000 single species (FRANK & COLLIN 1968). Information on tar data from past UCG field trials is rare and where available often precise data on single compound quantities generated in the pyrolysis and gasification zone are missing. Analyzing the bulk tar production quantitatively pyrolysis seems to be the dominant tar generating process (STEPHENS & THORSNESS 1985).

Against this environmental background a thermodynamic model for in-process generated tar single pollutant quantities under consideration of site specific UCG-reactor zones and trial conditions is currently developed and validated against past field trial data in the frame of the national joint project CO2SINUS, funded by the Federal Ministry of Education and Research (BMBF), Germany. In the frame of a multi parameter study the following input parameters are analysed regarding their influence on tar single pollutant output production:

- Coal chemistry and volume-streams
- In-situ pressure and temperature conditions
- Reactor water influx from the adjacent overburden
- Reactor heat losses

The results gained out of these scenario calculations are used as input data for the parameterization of a separately developed tar-groundwater-$CO_2$ solubility model considering single tar pollutant groups. In this context a special focus is set on pressure-dependent solubility changes for deep coal deposits (1 to 5 km), reflecting the European bituminous coal conditions.

The benefit of both model approaches together will allow a single pollutant precise aqueous tar solubility prognosis for planned UCG projects under consideration of site specific boundary conditions (coal type, (hydro-)geology, deposit pressure and temperature, water and heat streams) as well operative tasks, e.g. the scheduled product gas mix. A step ahead the environmental long-term groundwater risk of future UCG applications can be estimated using the pollutant distribution data as input stream for upcoming pollutant transport models.

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