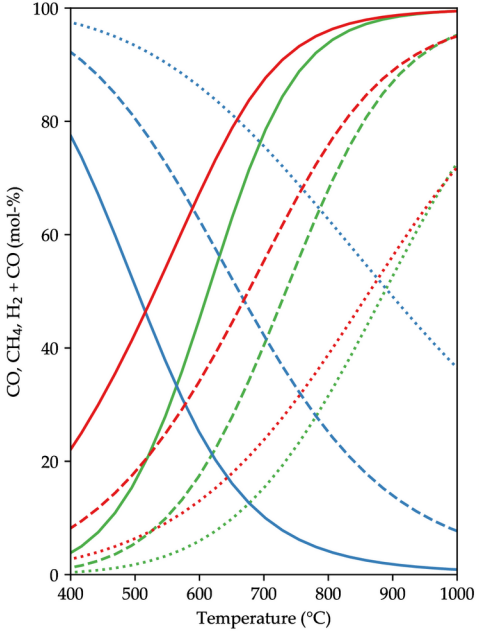
Simulating thermochemical conversion processes in context of Underground Coal Gasification (UCG)

- Estimation of equilibrium composition of synthesis gases produced by the gasification of carbon-rich feedstock (e.g., coal, municipal waste or biomass) with Cantera software package
- Stoichiometric equilibrium model is based on minimization of the Gibbs function (Villars-Cruise-Smith algorithm)



Considered equilibrium reactions for the equilibrium model are T/*p*-dependent

Boudouard $C + CO_2 \leftrightharpoons 2CO$

Methanation $C + 2H_2 \leftrightharpoons CH_4$

Water-gas shift $C + H_2O \leftrightharpoons H2 + CO$

p (MPa)
0.1
1.0
10.0

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Process quantification and modelling in subsurface utilisation
Thursday, May 7, 10:45 am CEST, Vienna, Austria

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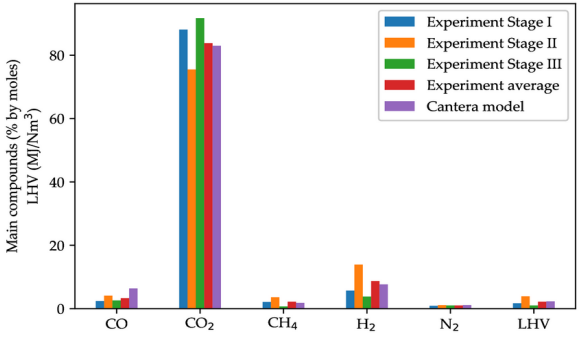
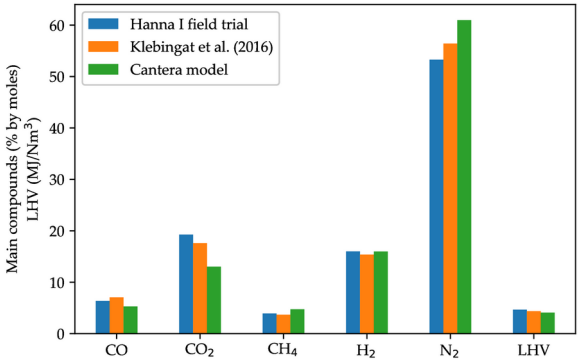
Broad range of end-use options available including fuels and chemical feedstock production

UCG ex-situ experiment
T = 580 °C
p = 1.0 MPa
SR = 0.35



UCG field-scale experiment
T = 600 °C
p = 0.48 MPa
SR = 0.12



SR = Stoichiometric ratio

- Modelling approach validated against thermodynamic models, laboratory gasification and demonstration-scale experiments
- Synthesis gas compositions have been found to be in good agreement under a wide range of different operating conditions
- Model coupling with multiphysics transport and process-unit level simulations ongoing

Otto, C.; Kempka, T. *Energies* **2020**, 13, 1171, https://doi.org/10.3390/en13051171.