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**
  \[ C + CO_2 \rightleftharpoons 2CO \]

- **Methanation**
  \[ C + 2H_2 \rightleftharpoons CH_4 \]

- **Water-gas shift**
  \[ C + H_2O \rightleftharpoons H_2 + CO \]

\[ p \text{ (MPa)} \]
- 
  \[ \begin{array}{c|c}
  \text{Temperature (°C)} & 400 & 500 & 600 & 700 & 800 & 900 & 1000 \\
  \hline
  p = 0.1 & \text{solid line} & \text{dashed line} & \text{dashed line} & \text{dashed line} & \text{dashed line} & \text{dashed line} & \text{dashed line} \\
  p = 1.0 & \text{dotted line} & \text{dotted line} & \text{dotted line} & \text{dotted line} & \text{dotted line} & \text{dotted line} & \text{dotted line} \\
  p = 10.0 & \text{dashed-dotted line} & \text{dashed-dotted line} & \text{dashed-dotted line} & \text{dashed-dotted line} & \text{dashed-dotted line} & \text{dashed-dotted line} & \text{dashed-dotted line} \\
  \end{array} \]

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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
- $SR = 0.12$

- 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