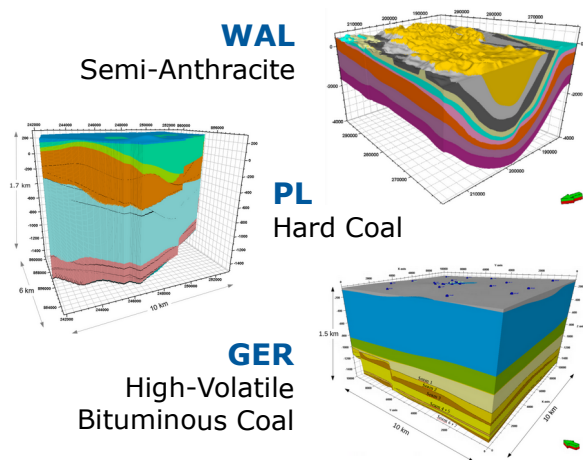


Simulating thermochemical conversion processes: Prediction of feasible synthesis gas compositions

Motivation

Estimation of **synthesis gases** produced by **in-situ coal conversion** for three different European sites

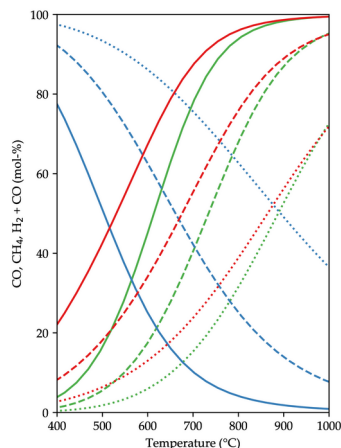


Methods

Stoichiometric equilibrium model based on **minimisation of the Gibbs free energy** with **Cantera** software package

Results

Modelling approach enables an **efficient quantification** of synthesis gas quality, considering **varying coal** and **oxidiser** at deposit-specific p/T



Boudouard
 $C + CO_2 \rightleftharpoons 2CO$

Methanation
 $C + 2H_2 \rightleftharpoons CH_4$

Water-gas shift
 $C + H_2O \rightleftharpoons H_2 + CO$

p (MPa)

— 0.1
- - - 1.0
..... 10.0

