Underground Coal Gasification – Recent achievements and further developments through coupled modelling

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Presentation outline

• Underground Coal Gasification (UCG)
  – General aspects
  – Current Status

• Numerical modelling
  – Previous (international) work
  – Ongoing theoretical and numerical model development at the GRC (CU)& IIT Roorkee
    • Thermodynamic Model - Coal/biomass gasification
    • COMPASS Code - Coupled thermo-hydraulic-chemical-mechanical (THCM) model
  – Model Application and Discussion

• Conclusions
Underground Coal Gasification (UCG) – General aspects

• Process of converting coal in situ into a combustible gas
  - Injection of O₂/Air and H₂O, to obtain SYNGAS (H₂, CH₄, CO, CO₂)
  - Clean coal technology with significant economic and environmental benefits over conventional underground mining and surface gasification
  - Safe as no people underground, minimum surface impact and transportable product
  - Security of supply (reduced dependence on imported fuels)
  - Possibility to couple with CCS
Underground Coal Gasification (UCG) – Current Status

• Recent Improvements and Key positives
  - 50+ years of pilot projects
  - Nearly constant gas quality and heating value
  - High thermal efficiency and resource recovery
  - High process efficiency and equipment reliability
  - Improvements on identifying site specificity and preferable well spacing

• Key Issues – obstacles for Commercialisation
  - Public & Authorities Perception
  - Ground water contamination and depletion
  - Surface subsidence
  - Controlling water influx and gas leakage
  - Professional management of the environmental risks
Numerical modelling of UCG – Previous international work

Performance of UCG gasifier is determined by complex interactions

- Chemical reactions (coal gasification and gas production)
- Gaseous and liquid flows (water, gases and contaminants)
- Heat release during chemical reactions and heat transfer
- Geochemical reactions (gas, contaminants and solid)
- Geo-mechanical processes (cavity growth, coal & rock spalling, subsidence)

“Previous models have focused on studying these aspects separately through several simplifying assumptions...Regardless of the approach of the models, there is not a single model that includes all the important physical and chemical models for the successful prediction of UCG.” (Khan et al., 2015)

<table>
<thead>
<tr>
<th>Problem focus</th>
<th>Model class</th>
<th>Potential software</th>
</tr>
</thead>
<tbody>
<tr>
<td>Overall performance</td>
<td>Process</td>
<td>ASPEN Plus, ChemCAD</td>
</tr>
<tr>
<td>Cavity growth</td>
<td>Coal Block</td>
<td>Matlab</td>
</tr>
<tr>
<td>Processes in void space</td>
<td>CFD</td>
<td>ANSYS FLUENT</td>
</tr>
<tr>
<td>Resource recovery</td>
<td>Reservoir</td>
<td>CMG STARS, ECLIPSE, MRST</td>
</tr>
<tr>
<td>Subsidence</td>
<td>Geomechanical</td>
<td>FLAC 3D</td>
</tr>
</tbody>
</table>

Table: Promising simulation platforms for modeling underground coal gasification. (Perkins, 2018)

No established contaminant transport model for UCG
Ongoing work between GRC (CU) & IIT Roorkee – general concept

- COMPASS code has been previously developed at the GRC to study coupled thermo-hydraulic-chemical-microbiological-mechanical processes in porous media for a range of geoenvironmental applications (nuclear waste disposal, carbon sequestration in coal, ground source heat, etc.)

- The code has been already successfully extended by including the advanced geochemical model PHREEQC

- COMPASS is currently being extended to accommodate the thermodynamic model, high temperature-high pressure relationships and the cavity growth mechanisms

**COMPASS**

**Thermodynamic Model**
- Production of different species (gases and contaminants)
- Individual component concentrations
  - Gasification temperature

**THCM Model**
- Heat Transfer
- Multicomponent gas transport
- Liquid and vapour transport
- Dissolved chemical transport
- Deformation
- Cavity growth
- Enhancement of the model for high temperature, high pressure conditions

**PHREEQC**
- Chemical reactions in liquid and gas phases
  - Phase transformation
  - Mineral precipitation/dissolution reactions
    - Surface complexation
    - Ion-exchange reactions
### COMPASS Code – Theoretical formulation

<table>
<thead>
<tr>
<th>Process</th>
<th>Mechanisms</th>
<th>Primary variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>① Heat Transfer</td>
<td>Conduction, convection, latent heat of vaporisation</td>
<td>Temperature ($T$)</td>
</tr>
<tr>
<td>② Moisture transfer (liquid and vapour)</td>
<td>Driven by thermal, hydraulic and vapour gradients</td>
<td>Pore water pressure ($U_l$)</td>
</tr>
<tr>
<td>③ Air (gas) transfer</td>
<td>Bulk flow by air pressure gradients (advection), diffusion and dissolved air (ideal and real gas conditions)</td>
<td>Pore gas pressure ($U_g$)</td>
</tr>
<tr>
<td>④ Multicomponent reactive chemical transport</td>
<td>Advection, diffusion, dispersion and geochemical reactions (equilibrium and kinetic)</td>
<td>Dissolved concentration of chemical components ($C_d$)</td>
</tr>
<tr>
<td>⑤ Deformation</td>
<td>Elasto-plastic model of deformation due to applied stress, suction, sorption and temperature changes</td>
<td>Displacements in $x$, $y$ and $z$ direction ($u$)</td>
</tr>
</tbody>
</table>

- Use of the finite element method for spatial discretisation
- Finite difference method used for temporal discretisation
Thermodynamic model of coal gasification

- Development of a thermodynamic equilibrium (stoichiometric) model to predict the maximum achievable yield of products from a reacting system:

$$CH_xO_yN_z + m(O_2 + 3.76N_2) + nH_2O + wH_2O \rightarrow x_1H_2 + x_2CO + x_3CO_2 + x_4H_2O + x_5CH_4 + \left(\frac{z}{2} + 3.76\right)N_2$$

- Basic assumptions
  - Gasification occurs in steady-state conditions
  - Temperature and pressure are uniform throughout the system
  - All gases behave ideally
  - Model is zero-dimensional (geometrical variations are not considered)

- A set of non-linear equations solved by the Newton-Raphson method
- Model was successfully verified and validated against literature data $^{3,4}$
Coupled Model Application – Problems background

- Under some conditions of permeability and pressure history, a “shoulder” of unreacted coal may exist in the upper part of the coal seam, surrounding the cavity that is not water saturated (filled with gas).
- In case of dipping coal seams, the shoulder of unsaturated pore space can potentially extend a long distance.
- In such cases, gas could flow up away from the process area even though water is flowing down into the cavity.

a) Horizontal coal seam

a) Dipping coal seam
Coupled Model Application – Simulation Scenarios

- South Wales Coalfield – analysed data (borehole logs, x-ray diffraction patterns, etc.) show that samples from various depths exhibit mineralogical characteristics of shale deposits and locations of sandstone stratum above “big” (thick) coal seams and water level is around 350 m below surface.

- Using the model and taking into account unsaturated (dry) conditions, heat propagations and transport of UCG gaseous products through: (a) coal, (b) mudstone/shale, (c) sandstone are investigated.

- As CH\(_4\) and CO\(_2\) are the most potent greenhouse gases, it is also investigated whether sorption of those gases on coal and rock strata can retard their transport.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Coal</th>
<th>Mudstone/Shale</th>
<th>Sandstone</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity [%]</td>
<td>3.0</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>Permeability [mD]</td>
<td>0.1</td>
<td>0.01</td>
<td>1.0</td>
</tr>
<tr>
<td>Density [kg/m(^3)]</td>
<td>1376</td>
<td>2316</td>
<td>2650</td>
</tr>
<tr>
<td>Thermal conductivity [w/m.K]</td>
<td>f(T)</td>
<td>f(T)</td>
<td>f(T)</td>
</tr>
<tr>
<td>Heat capacity [J/kg.K]</td>
<td>f(T)</td>
<td>f(T)</td>
<td>f(T)</td>
</tr>
<tr>
<td>Langmuir Pressure (CO(_2)) [MPa]</td>
<td>0.61</td>
<td>2.83</td>
<td>1.0</td>
</tr>
<tr>
<td>Langmuir capacity (CO(_2)) [mol/kg]</td>
<td>1.73</td>
<td>0.49</td>
<td>0.285</td>
</tr>
<tr>
<td>Langmuir pressure (CH(_4)) [MPa]</td>
<td>1.2</td>
<td>3.86</td>
<td>1.71</td>
</tr>
<tr>
<td>Langmuir capacity (CH(_4)) [mol/kg]</td>
<td>1.52</td>
<td>0.175</td>
<td>0.184</td>
</tr>
</tbody>
</table>

Temperature, UCG gas products (CH\(_4\), CO\(_2\), H\(_2\), CO, N\(_2\)).
Coupled Model Application – Boundary Conditions through Thermodynamic Equilibrium Model

- Proximate and Ultimate Analyses data for the 9ft coal (anthracite) from the South Wales Coalfield are used as an input for the Thermodynamic model.
- Constant air supply of 0.5 kmol at 20bar, variable steam supply (0.3-1.5 kmol)

<table>
<thead>
<tr>
<th>Characterisation test</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Proximate Analysis</strong></td>
<td></td>
</tr>
<tr>
<td>Moisture content</td>
<td>0.91%</td>
</tr>
<tr>
<td>Ash content</td>
<td>4.62%</td>
</tr>
<tr>
<td>Volatile matter</td>
<td>5.73%</td>
</tr>
<tr>
<td>Fixed carbon content</td>
<td>88.7%</td>
</tr>
<tr>
<td><strong>Ultimate Analysis</strong></td>
<td></td>
</tr>
<tr>
<td>Total carbon content</td>
<td>89.5%</td>
</tr>
<tr>
<td>Sulphur content</td>
<td>0.87%</td>
</tr>
<tr>
<td>Hydrogen content</td>
<td>3.16%</td>
</tr>
<tr>
<td>Nitrogen content</td>
<td>1.31%</td>
</tr>
<tr>
<td>Oxygen content</td>
<td>0.33%</td>
</tr>
</tbody>
</table>

Selected as boundary conditions to the transport model (highest amount of CO$_2$ and CH$_4$)
### Coupled Model Application – Simulation conditions and material properties

**Boundary conditions (Left BC):**
- Temperature (K): 1062.64 °C ($T = 1335.79$ K)
- Gas concentrations (mol/m$^3$):
  - High pressure, 20 bar: 
    - $C_g (CO_2) = 28.25$
    - $C_g (CH_4) = 0.32$
    - $C_g (H_2) = 38.46$
    - $C_g (CO) = 20.46$
    - $C_g (N_2) = 92.54$

**Initial conditions (IC):**
- Temperature (K): 25 °C ($T = 298$ K)
- Gas concentrations (mol/m$^3$): Atmosphere pressure, 1 bar
  - $C_g (CO_2) = 0$
  - $C_g (CH_4) = 0$
  - $C_g (H_2) = 0$
  - $C_g (CO) = 0$
  - $C_g (N_2) = 32.31$
  - $C_g (O_2) = 8.59$

**Boundary conditions (Right BC):**
- Temperature (K): 25 °C ($T = 298$ K)
- Gas concentrations (mol/m$^3$): Atmosphere pressure, 1 bar, same as initial condition

**UCG gasification**
- $L = 30$ m
- $H = 1$ m

**Coal/rock**
- Discretised in 300 quadrilateral elements
Coupled Model Application – Temperature Results

The distribution of temperature after 30 days

- T-coal
- T-shale
- T-sandstone

Distance (m):
- 5.5 m
- 9.5 m
- 9.7 m
Coupled Model Application – Gas Concentration Results

CO2-coal
CO2-shale
CO2-sandstone

CH4-coal
CH4-shale
CH4-sandstone

H2-coal
H2-shale
H2-sandstone

CO-coal
CO-shale
CO-sandstone

N2-coal
N2-shale
N2-sandstone

Gas concentration (mol/m³)
Distance (m)

6.5 m
14.2 m

5.9 m
6.9 m
7.4 m
14.6 m
12.1 m
12.4 m
17.1 m

6.8 m
7.3 m
14.5 m

6.0 m
6.7 m
14.3 m
Coupled Model Application – Gas Sorption Results

Case 1: coal

The distribution of CO₂ and CH₄ concentrations after 30 days:

without vs. with adsorption

Gas pressure 2 MPa > 0.61 MPa
(Langmuir Pressure - \(P_L\))

\[ S = S_{max} \frac{u_g}{P_L + u_g} \]

Gas pressure 2 MPa > 1.2 MPa
(Langmuir Pressure - \(P_L\))
Case 2: shale

The distribution of CO$_2$ and CH$_4$ concentrations after 30 days: *without vs. with adsorption*

Gas pressure 2 MPa < 2.83 MPa \((\text{Langmuir Pressure} - P_L)\)

Gas pressure 2 MPa < 3.86 MPa \((\text{Langmuir Pressure} - P_L)\)
**Coupled Model Application – Gas Sorption Results**

Case 3: sandstone

The distribution of CO$_2$ and CH$_4$ concentrations after 30 days: *without vs. with adsorption*

\[
S = S_{max} \frac{u_g}{P_L + u_g}
\]

Gas pressure 2 MPa > 1.0 MPa *(Langmuir Pressure - $P_L$)*

Gas pressure 2 MPa > 1.71 MPa *(Langmuir Pressure - $P_L$)*
Conclusions

- **UCG** is an exploitation technology for *indigenous coal* which provides *security of supply* and possibility to be coupled with CO₂ capture and storage technology.

- **50+ years** of extensive trials have demonstrated the *viability of the technology* and made significant progress showing considerable promise for commercialisation as a *low cost carbon emission reduction technology* through UCG-CCS.

- **Environmental impact** and **UCG process control** are the *greatest public concerns*. UCG in deeper seams, more environmental knowledge in the public domain and *Government involvement and support* are crucial for commercialisation.

- Following proper **site selection** as a *crucial first step* for successful UCG, numerical modelling of coupled processes can ensure *good predictability* and *process control*.

- A **coupled thermodynamic and thermo-hydro-chemical-mechanical framework** has been presented here.

- Based on the results of this study, **advection is the dominant transport mechanisms in porous media with permeability >1mD** (sandstone), while the **contribution of diffusion increases in low permeability media** with permeability <0.1mD (coal and shale).

- Results suggest that **gas sorption** on the surrounding strata around the UCG cavity can **retard gas propagation** (depending on the sorption properties), with coal having stronger affinity for gas compared to shale and sandstone.
References


Thank you.

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