Hydrogen Rich Syngas Production via Underground Coal Gasification (UCG) from Turkish Lignite

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Outlines

1. Introduction and Aim(s)
2. Experimental Setup and Plan
3. Experimental Results
4. CFD Modeling and Results
5. Conclusions
Introduction and purpose

Aims:
• To investigate hydrogen rich syngas production from Turkish lignite by UCG.
• To determine appropriate/optimum UCG process parameters for Turkish lignite.
• To develop a UCG mathematical model to optimize the UCG process and to predict produced syngas properties.

The work presented in this paper has been performed in the frame of “Development of Underground Coal Gasification Technology For Turkish Lignites” project and supported by TURKISH -TUBITAK-ARDEB under the contract number 113M038.
What is UCG?

Underground coal gasification (UCG) is the gasification of coal in the seam. It is achieved by injecting oxidants, gasifying the coal and bringing the product gas to surface through boreholes drilled from the surface.
### UCG- Reactions

<table>
<thead>
<tr>
<th>Process</th>
<th>Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drying</td>
<td>Coal $\rightarrow$ Dried Coal + H$_2$O</td>
</tr>
<tr>
<td>Pyrolysis</td>
<td>Volatiles $\rightarrow$ a$_1$CO$_2$ + a$_2$CO + a$_3$H$_2$O + a$_4$H$_2$</td>
</tr>
<tr>
<td>Carbon Combustion</td>
<td>C + O$_2$ $\rightarrow$ CO$_2$</td>
</tr>
<tr>
<td>CO$_2$ gasification</td>
<td>C + CO$_2$ $\rightarrow$ 2CO</td>
</tr>
<tr>
<td>H$_2$O gasification</td>
<td>C + H$_2$O $\rightarrow$ CO + H$_2$</td>
</tr>
<tr>
<td>CO combustion</td>
<td>CO + 0.5O$_2$ $\rightarrow$ CO$_2$</td>
</tr>
<tr>
<td>H$_2$ combustion</td>
<td>H$_2$ + 0.5O$_2$ $\rightarrow$ H$_2$O</td>
</tr>
<tr>
<td>Water-Gas Shift</td>
<td>CO + H$_2$O $\leftrightarrow$ CO$_2$ + H$_2$</td>
</tr>
</tbody>
</table>

### UCG- Cavity Zones

- **Coal**
  - C + O$_2$ $\rightarrow$ CO$_2$
  - C + CO$_2$ $\rightarrow$ 2CO
  - C + H$_2$O $\rightarrow$ CO + H$_2$

- **Gasification Channel**
  - CO + $\frac{1}{2}$O$_2$ $\rightarrow$ CO$_2$ + HEAT
  - H$_2$ + $\frac{1}{2}$O$_2$ $\rightarrow$ H$_2$O + HEAT

- **Combustion**
  - Air, O$_2$
  - HEAT $>$ 900 °C

- **Drying + Pyrolysis**
  - HEAT 200-550 °C

- **Syngas**
  - HEAT
  - CO + H$_2$O $\rightarrow$ CO$_2$ + H$_2$

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The composition of the product gas and its calorific value depends on
1. Gasification agents
2. Temperature
3. Pressure
4. Hydrodynamic condition of process
Turkish Coal Reserves in Comparison with Europe (2012)

Source: Coal industry across Europe, EURACOAL, 2013
Lignite Basins in Turkey

Sample Lignite taken from this location
Sample Lignite Seam from Malkara Pirinççesme
## Analysis of the Malkara Lignite

<table>
<thead>
<tr>
<th>Approximate Analysis (%)</th>
<th>Analysis Type</th>
<th>Original Sample</th>
<th>Dry in Air</th>
<th>Dry Sample</th>
<th>Standard</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Moisture</td>
<td>25,17</td>
<td>15,27</td>
<td>-</td>
<td>ASTM D 7582-2012</td>
</tr>
<tr>
<td></td>
<td>Ash</td>
<td>17,95</td>
<td>20,33</td>
<td>23,99</td>
<td>ASTM D 7582-2012</td>
</tr>
<tr>
<td></td>
<td>Volatile Matter</td>
<td>28,74</td>
<td>32,55</td>
<td>38,41</td>
<td>ASTM D 7582-2012</td>
</tr>
<tr>
<td>Heating Value [kcal/kg]</td>
<td>Low Heating Value</td>
<td>3602</td>
<td>4151</td>
<td>4998</td>
<td>ASTM D-5865</td>
</tr>
<tr>
<td></td>
<td>High Heating Value</td>
<td>3894</td>
<td>4409</td>
<td>5203</td>
<td>ASTM D-5865</td>
</tr>
</tbody>
</table>

### Ultimate Analysis (%)

<table>
<thead>
<tr>
<th>Ultimate Analysis (%)</th>
<th>Unit</th>
<th>In Dry Sample</th>
<th>Standard</th>
</tr>
</thead>
<tbody>
<tr>
<td>C (Carbon)</td>
<td>% mass.</td>
<td>57,02</td>
<td>ASTM D 5373-14</td>
</tr>
<tr>
<td>H (Hydrogen)</td>
<td>% mass.</td>
<td>3,99</td>
<td>ASTM D 5373-14</td>
</tr>
<tr>
<td>N (Nitrogen)</td>
<td>% mass.</td>
<td>1,44</td>
<td>ASTM D 5373-14</td>
</tr>
<tr>
<td>S (Sulphur)</td>
<td>% mass.</td>
<td>5,41</td>
<td>ASTM D 4239-14</td>
</tr>
<tr>
<td>Ash</td>
<td>% mass.</td>
<td>23,99</td>
<td>ASTM D 7582-12</td>
</tr>
<tr>
<td>Oxygen</td>
<td>% mass.</td>
<td>8,15</td>
<td>ASTM D 3176-09</td>
</tr>
</tbody>
</table>

- Sulphate Sulphur: % 0.113
- Pyritic Sulphur: % 2.520
- Total Sulphur: % 5.41
- Organic Sulphur: %2.777
Reactor was designed and constructed to simulate in ex-situ conditions of coal seam.
Thermocouple Locations on Ex Situ Reactor

reactor: 0.5x0.7x1.8 m
Coal Seam Placed in the Ex Situ Reactor

- Coal: 0.4x0.7x1.7 m (reactor: 0.5x0.7x1.8 m)
- Coal: 522 kg
Coal Seam Placed in the Ex Situ Reactor
Results: Flow rate of syngas and gasification agents

Gasification Agent Supply Rate and Syngas Rate

<table>
<thead>
<tr>
<th>Time (h)</th>
<th>Volumetric Flow Rate (m³/h)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>5</td>
</tr>
<tr>
<td>4</td>
<td>10</td>
</tr>
<tr>
<td>5</td>
<td>15</td>
</tr>
<tr>
<td>6</td>
<td>20</td>
</tr>
<tr>
<td>7</td>
<td>25</td>
</tr>
</tbody>
</table>

- Syngas
- Oxygen
- Steam
- Air
Coal Seam After Experiments (Cavity)
Results: Temperature in the coal seam

Temperature Level Inside The Coal Block

- Tr6
- Tr11
- Tr2
- Tr16
- Tr10

Temperature (°C)

Time (h)
Results: Syngas composition and its calorific value in the Oxygen Gasification Phase

Oxygen Phase – Syngas Composition and Syngas Calorific Value

Supply Rate: 3 m$^3$/h, $O_2$

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Results: oxygen and steam consecutive gasification phase (Char combustion/char gasification)
Mathematical models for UCG

• Underground Coal Gasification is a process, where the parameters change over time and within the space of the reactor.

• Consequently, it is necessary to develop appropriate mathematical models, which simplify the optimization and forecast of producing syngas properties.

• Unfortunately, experiments carried out directly in underground reactors are expensive and in same cases impossible to perform.

• Therefore computer simulations of gasification processes become increasingly significant in science and the industry in general.
UCG- CFD Simulations

ANSYS Fluent
Geometry of the ex-situ reactor

Coal – Porous Zone

Number of volumes = 30,000

Gasification Channel

Inlet

Outlet
ANSYS-Fluent Implementation

**INPUT**
- Ex-situ UCG reactor 2D geometry
- Supply rate and composition of gasification agent
  - Thermophysical properties
  - Reaction constants

**FLUENT**
- Momentum, heat, mass transfer calculations in time and space
- Calculation of turbulent quantities (k-ε Model)
  - Homogeneous reactions
- Time advancement for coal content
  - SIMPLE Algorithm
  - 2nd order discretization

**OUTPUT**
- Syngas composition
- Cavity formation
- Transient velocity field, temperature distribution, mass fraction of species
  - Reaction zones

**UDF**
- Source term calculations (heterogen reactions, pyrolysis and drying)
- Calculating varying thermophysical properties of coal (porosity, permeability, conductivity, heat capacity)

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CFD – Model (ANSYS-Fluent)

Conservation of Momentum

\[
\frac{\partial (\rho_f \vec{v})}{\partial t} + \nabla \cdot (\rho_f \vec{v} \vec{v}) = -\nabla p + \mu_f \nabla \cdot \tau + \rho_f \vec{g} - \left( \frac{\mu}{\alpha} \vec{v} \right)
\]

Conservation of Energy

\[
\frac{\partial}{\partial t} \left[ (\rho_f \phi C_{p,f} T + \rho_s (1 - \phi) C_{p,s} )T \right] + \rho_f C_{p,f} (\vec{v} \cdot \nabla T) = \nabla \cdot \left( k_{eff} \nabla T - \sum h_{i,j} \vec{j}_i \right) + \sum \text{rate}_i \Delta H_i
\]

Conservation of Species

\[
\frac{\partial}{\partial t} (\rho_f \phi_i) + \nabla \cdot (\rho_f \vec{v} \phi_i) = -\nabla \cdot (\rho_f D_i \nabla \phi_i) + \sum \text{rate}_i
\]

User Defined Scalars

\[
\frac{\partial}{\partial t} (\rho_f \phi_i) = S_{\phi_i}
\]

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Results: Comparison of experiment results with CFD results

Oxygen Gasification Phase

Steam Gasification Phase

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UCG -CFD Numerical Results

Coal Conversion (10\textsuperscript{th} hour)
Red zones indicates that coal (fixed carbon) content fully consumed
UCG CFD Numerical Results

Carbon Combustion \((C+O_2 \rightarrow CO_2)\) Reaction Rate (10\(^{th}\) hour)-ZONE
Carbon Dioxide Gasification (C+CO₂→2CO) Reaction Rate (10th hour)-ZONE
Steam Gasification (C+H₂O→CO+H₂) Reaction Rate (10^{th} hour)-ZONE
UCG CFD Numerical Results

Hydrogen Combustion ($H_2 + 0,5O_2 \rightarrow H_2O$) Reaction Rate (10th hour) - ZONE
Carbon Monoxide Combustion \((CO + 0.5O_2 \rightarrow CO_2)\) Reaction Rate \((10^{\text{th}} \text{ hour})\)-ZONE
UCG CFD Numerical Results

Temperature Distribution (10\textsuperscript{th} hour)
UCG CFD Numerical Results

Mole Fraction of Oxygen Specie (10\textsuperscript{th} hour)
Conclusion and outlook

- Turkish Malkara Pirinççeşme lignite with the moderate moisture appears to be very suitable for UCG,
- On average, 20% Carbon monoxide, 20% hydrogen and 2-3% methane gases of syngas are produced in the pure oxygen supplying phase.
- Produced syngas have heat values in the range of 5-6 MJ/m³.
- The average gas production rate was 5 and 15 m³/h for oxygen supply rates of 3 and 5 m³/h, respectively.
- After certain time, the syngas generation was deteriorated,
- In order to continue gasification, consecutive oxygen-steam gasification steps have to be applied.
- Only in the steam gasification step, it was possible to produce a hydrogen gas, whereas the pure oxygen phase was used to heat the coal seam to the gasification temperature. Therefore, such gasification phase can be called a char combustion/char gasification.
- In this steam phase, on average, 5% Carbon monoxide, 35-40% hydrogen are produced.
Conclusion and outlook

- CFD-Model - ANSYS FLUENT with UDF successfully simulated the UCG process of coal seam experimented here.
- The simulation results gave insight in the gasification parameters and gasification reaction rate and zone.
- Further studies are planned by using coal samples with different characteristics from different locations and by applying of UCG Methods of CRIP (Controlled retractable injection point).
Thank you for your attention

Acknowledgements
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