Gasification of Athabascan asphaltenes in a drop tube furnace: experimental and modeling results

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Asphaltenes:
Melting temperature
150 – 250°C

Proximate Analysis, kg/kg
Fixed carbon: 0.28
Volatile matter: 0.71
Ash content: 0.01

Ultimate analysis, kg/kg:
C: 82.17;
H: 8.18;
N: 1.17;
S: 7.45;
O: 1.03

[1] Alberta geology survey
ags.gov.ab.ca
Content

1. Experimental setup
2. CFD Modeling
3. Subgrid Modeling
4. Conclusion
Reactor design

Drop tube furnace:
- Length: 1.5 m
- Diameter: 6.5 cm
- Electrical wall heated: 1573 K
- Atmospheric pressure
- Nitrogen as carrier gas for the asphaltene particles

Fig.: Reactor scheme [2]

Reactor design

Fig.: Nozzle

Inlet: fuel

Inlet: gasification agent

Nozzle

Reactor wall

Fig.: Cross section of the reactor top
Particle size determination

Data generation:
Image processing with pulsed LED source

[3] Figures from Brochure:
Retsch Technology, CAMSIZER XT,
Particle size of the feed particles

![Particle size histogram](image)

- **Probability density function, %, μm**
- **d, μm**

- **X-Fall**
- **X-Jet**

- **Agglomeration effects!**
Particle size of the feed and char particles

Probability density function, %, µm

Feed (X-Fall): λ = 0.34, X = Fall;
Feed (X-Jet): λ = 0.34, X = Jet

λ = 0.13, X = Fall; λ = 0.13, X = Jet

Particle size of the feed and char particles:

- Feed (X-Fall): λ = 0.34
- Feed (X-Jet): λ = 0.34
- λ = 0.13 (X-Fall)
- λ = 0.13 (X-Jet)
CFD model

- Ansys Fluent 14.0
- 2D-axisymmetric geometry
- k-ω-SST turbulence model
- P-1 radiation model
- Incompressible ideal gas
- Euler-Lagrange approach

Heterogeneous reactions:

\[ 2\text{C} + \text{O}_2 \rightarrow 2\text{CO} \]
\[ \text{C} + \text{CO}_2 \rightarrow 2\text{CO} \]
\[ \text{C} + \text{H}_2\text{O} \rightarrow \text{CO} + \text{H}_2 \]

Homogeneous reactions:

\[ \text{CO} + 0.5\text{O}_2 \rightarrow \text{CO}_2 \]
\[ \text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2 \]
\[ \text{CH}_4 + 0.5\text{O}_2 \rightarrow \text{CO} + 2\text{H}_2 \]
\[ \text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2 \]
\[ \text{H}_2 + 0.5\text{O}_2 \rightarrow \text{H}_2\text{O} \]
\[ \text{C}_6\text{H}_6 + 3\text{O}_2 \rightarrow 6\text{CO} + 3\text{H}_2 \]
Gas profile in the reactor

Fig.: Contour of oxygen in kg/kg, with $\lambda$ as stoichiometric air-fuel ratio. The left represents the top and the right the bottom of the reactor. Reactor length is 1.5 m.
Gas profile in the reactor

Fig.: Contour of methane in kg/kg, with $\lambda$ as stoichiometric air-fuel ratio. The left represents the top and the right the bottom of the reactor. Reactor length is 1.5 m.
Gas profile in the reactor

Fig.: Contour of carbon monoxide in kg/kg, with \( \lambda \) as stoichiometric air-fuel ratio. The left represents the top and the right the bottom of the reactor. Reactor length is 1.5 m.
Subgrid model: Mass transfer

Advanced model concept

Heterogeneous reactions:

\[ 2 \text{C} + \text{O}_2 \rightarrow 2 \text{CO} \]
\[ \text{C} + \text{CO}_2 \rightarrow 2 \text{CO} \]
\[ \text{C} + \text{H}_2\text{O} \rightarrow \text{CO} + \text{H}_2 \]

Homogeneous reactions:

\[ \text{CO} + 0.5 \text{O}_2 \rightarrow \text{CO}_2 \]
\[ \text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2 \]
\[ \text{CH}_4 + 0.5\text{O}_2 \rightarrow \text{CO} + 2\text{H}_2 \]
\[ \text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2 \]
\[ \text{H}_2 + 0.5\text{O}_2 \rightarrow \text{H}_2\text{O} \]
\[ \text{C}_6\text{H}_6 + 3\text{O}_2 \rightarrow 6\text{CO} + 3\text{H}_2 \]
Subgrid model: Heat transfer

Standard model concept

Advanced model concept

Eulerian grid cell

Eulerian grid cell
Particle conversion steps: Temperatures

- **Heating**
- **Melting**
- **Pyrolysis**
- **Burnout**

![Graph showing particle conversion steps and temperatures](image)
Particle conversion steps: Temperatures
Energy balance:
Virtual homogeneous reaction Zone
Energy balance: Particle

![Energy balance diagram]

The figure illustrates the energy balance for a particle in different stages: Pyrolysis and Burnout. The energy fluxes include:

- \( \dot{Q}_{\text{fu}} \): Frictional heating
- \( \dot{Q}_{\text{pyro}} \): Pyrolysis heating
- \( \dot{Q}_{\text{rad}} \): Radiative heating
- \( \dot{Q}_{\text{con,p}} \): Conduction to the particle
- \( \dot{Q}_{\text{con,\infty}} \): Conduction to infinity
- \( \dot{Q}_{\text{sen}} \): Sensible heat
- \( \dot{Q}_{\text{R,s}} \): Radiation from the particle

The diagram shows four distinct periods (I to IV) in the particle's thermal history, each represented by different energy flux profiles.

1. **Pyrolysis (I)**: This period is characterized by a sharp increase in the pyrolysis heating rate, followed by a decrease as the volatile matter ignites and the particle transitions to the next phase.
2. **Inert period (II)**: The heating rate slows down significantly, indicating the particle is losing energy to the surroundings.
3. **Pyrolysis (III)**: The heating rate increases again, possibly due to the onset of a new reaction or increased heating effects.
4. **Burnout (IV)**: This period shows a gradual decrease in the heating rate as the particle reaches ambient temperature and the energy flux stabilizes.

The surrounding gas temperatures are represented by \( T_{\infty} \), and the particle's temperature is denoted by \( T_p \). The diagram also illustrates the virtual homogenous reaction zone (TH) and the reaction rate \( \dot{Q}_{\text{R,h}} \).

The figure is a graphical representation of the energy balance equations and their application to the thermal behavior of a particle undergoing pyrolysis and burnout processes.
Validation: Carbon conversion at the reactor end

Fig: Carbon conversion

Fig: Particle residence time
Summary and Outlook

• The experimental gasification of Athabascian asphaltenes can be simulated with CFD and stand-alone subgrid models with good agreement.

• Particles enters the drop to furnace as clusters of single particles.

• Advanced particle transformation model for size and shape are needed.

• The “virtual homogeneous reaction zone model” shows a significant energy feedback from the vicinity around the particle onto the particle.
Thank you for your attention!

**Literature** concerning previous VHRZ subgrid model development steps:
