Biomass gasification in updraft gasifier: Experiments and numerical modelling

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ASCI minisymposium
28/02/2022
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**Introduction: Motivation**

- In 2019 over 80% of the world primary energy was provided from the fossil fuel
- Climate changes caused by fossil fuel combustion
- World population growth
- Rising energy demand
- Development of renewable energy resources with an aim to implement it as a main energy resource in the future – possibility of 100% renewable energy by 2050?
- Biomass as an energy resource – wide distribution of raw materials and good exploitation conditions, currently, 10% share of total world primary energy
- Mathematical models are widely used to reduce the expensive experimental researches and for process optimization
Introduction: Biomass gasification

Biomass gasification – thermochemical process of partial combustion with a final product of hydrogen-enriched syngas suitable for further energy conversions.

4 chemical processes of an updraft gasifier:
- drying, pyrolysis, gasification and oxidation

Biomass gasifier designs:
- Fixed bed gasifier:
  - Downdraft
  - Updraft
- Fluidized bed gasifier
- Gasifier with entrained flow

\[
\begin{align*}
\text{Primary gas-phase reactions} & : \\
\text{drying, pyrolysis, gasification, and oxidation} & \\
\text{Secondary gas-phase reactions} & :\\
\text{tars} + \text{heat} & = \text{char} + \text{gases} \\
\text{CO} + \text{H}_2\text{O} & = \text{CO}_2 + \text{H}_2
\end{align*}
\]
• Introduction

• **Experiments**
  
  • Gasification modelling
  
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Experimental plant

- **ENEA Trisaia Research Center** (Italy) – Pilot scale uPdRAft GAsifier (PRAGA)
- **Biomass input** – 20-30 kg/h of lignocellulosic feedstock
- **Gasifying agents** – air, enriched air, steam, pure oxygen
- **Gas cleaning system** – biodiesel scrubber with two coalescence filters
- **11 thermocouples** in a steel probe
- **6 sampling points in the bed core** – for gas and liquids analysis
- **Gas Chromatography** – H₂, CO, CO₂, O₂, N₂, CH₃, C₂H₆, C₃H₈
- **Tar content**

![Sampling the gas and liquids](image1)

![Gasification reactor](image2)
Experimental cases and biomass feedstock

<table>
<thead>
<tr>
<th>Almond shells</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Cellulose, wt.%</td>
<td>31.2</td>
</tr>
<tr>
<td>Hemicellulose, wt.%</td>
<td>28</td>
</tr>
<tr>
<td>Lignin, wt.%</td>
<td>32.18</td>
</tr>
<tr>
<td>Ash, wt.%</td>
<td>1.2</td>
</tr>
<tr>
<td>Lig-C, wt.%</td>
<td>4.18</td>
</tr>
<tr>
<td>Lig-H, wt.%</td>
<td>21.67</td>
</tr>
<tr>
<td>Lig-O, wt.%</td>
<td>6.33</td>
</tr>
<tr>
<td>Hydrophobic extractives, wt.%</td>
<td>7.42</td>
</tr>
</tbody>
</table>

Experimental temperature profiles for a) air gasification, b) air+steam gasification
• Introduction
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Schematic representation of the numerical model

- Holocellulose
- Lignin
- Extractives

**Pyrolysis reactions** – Debiagi et al. 2016

- Gasifying agents
- Char
- Liquids
- Gases

**Gasification and oxidation zones** – TEM model

- Gases
- Liquids (including tars)
- Gases

**Secondary gas-phase reactions**

**Outflow from the reactor**: Syngas + liquids (including tars)

**Drying**

**Pyrolysis**

**Reduction**

**Oxidation**

Gasifying agents

Grate

Ash

Reduced: Goyal et al. 2017

Pyrolysis kinetic model

Biomass devolatilization: CRECK-S-BIO kinetic mechanism

51 species 27 Reactions

CELL ➔ CELLA
   | Char + H₂O
   | LVG + Char + Gases + Tars
HCE ➔ CELLA ➔ HCE 1 ➔ Xylan + Gases + Tars
   | Char + Gases + Tars
   | Char + Gases + HWMC
HCE 2 ➔ LIG-H ➔ Char + Gases + HWMC
LIGIN ➔ LIG-O ➔ LIG-OH ➔ Char + Gases + HWMC
   | Tars
   | Char + Gases + Tars
LIGNIN ➔ LIG-C ➔ LIG-CC ➔ Char + Gases + HWMC

Secondary gas-phase reactions:

• Reduced secondary gas-phase mechanism by Goyal et al. – 44 chemical species and 118 chemical reactions

• Detailed secondary gas-phase mechanism by Debiagi et al. – 137 chemical species and 4533 chemical reactions

Pyrolysis solver:

• Kinetics:

\[ E_{pyr} = \sum_{j=1}^{n} (k_j) \times \frac{dm_p}{dt} \]

\[ k_j = A_j T^\gamma \exp \left( - \frac{E_j}{RT_p} \right) \]

\[ \frac{dm_p}{dt} = \text{netProdRates()} \]

• Mass update:

\[ m_{p,i} = m_{p,i-1} + \frac{dm_p}{dt} \times \Delta t \]
Gasification and oxidation thermodynamic equilibrium model

Char gasification and oxidation model — thermodynamic equilibrium model through the minimization of Gibbs free energy:

- the total Gibbs free energy of a closed system at a constant temperature and pressure must decrease during an irreversible process
- minimum is reached at equilibrium state

\[ (dG^t)_{T,P} = 0 \]

\[ G^t = \sum_{i=1}^{N} n_i \mu_i \quad \mu_i = G_i^\circ + RT \ln \left( \frac{f_i}{f_i^\circ} \right) \]

Char gasification and oxidation solver — Cantera chemical equilibrium Gibbs solver

- equilibrate() function with fixed thermodynamic properties (pressure and temperature)
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Air gasification results

- Detailed mechanism
- Reduced mechanism
- Experiment

(a) $H_2$ vol\% vs. A21, A24_1, A24_2
(b) $C_{nH_m}$ vol\% vs. A21, A24_1, A24_2
(c) $CO_2$ vol\% vs. A21, A24_1, A24_2
(d) $CO/CO_2$ vs. A21, A24_1, A24_2
Air+steam gasification results
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Mechanism reduction: Secondary gas-phase reactions

Pyrolysis conditions specific for the updraft fixed bed gasifiers:

- Biomass is completely dried
- There is no oxygen in the process
- The temperature range is between 550 K and 1100 K
- The reactor operates at atmospheric pressure
- Both slow and fast pyrolysis is applied

Reduction – 8 cases

Validation – 3 cases

\[
\text{average error} = \frac{1}{n} \sum_{i=1}^{n} \frac{x_{\text{reference},i} - x_{\text{reduced},i}}{x_{\text{reference},i}}
\]

- \( X_i \) - CO, CO\(_2\), CH\(_4\), H\(_2\) and syngas yield

Run simulation with reference mechanism

- \( R_{\text{max}} \)

Sort \( R_{\text{max}} \)

Reduced number of reactions

Update species

Create reduced mechanism

Run simulation with reduced mechanism

Post-processing

Reduced mechanism

error > 5%

error < 5%
Mechanism reduction: Model validation

Reduced mechanism: 240 chemical reactions (94.7% reduction), 73 chemical species (46% reduction)
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Conclusion

• The predictions obtained with the detailed secondary gas-phase mechanism generally showed a better agreement with measurements

• CO$_2$ predictions higher deviations were observed (around 20%), mostly due to the assumption of thermodynamic equilibrium in the gasification and oxidation zones

• The reduced mechanism showed generally higher deviations for the predictions of H$_2$, CO and CO$_2$ predictions, which is described to the lack of chemical reactions that consider the thermal-cracking of liquids with non-condensable gases

• Higher deviations were noticed for C$_n$H$_m$ predictions regardless the mechanism

• The modelling approach used in this present work is able to capture the gasification trends of the measurements obtained in an updraft gasifier and represents a good basis that can be further developed

• Newly developed reduced mechanism obtained high accuracy compared to the detailed mechanism with previously explained deviations with experimental data
Thank you for your attention!

Questions?

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