Analytical and numerical modelling of biomass gasification in a lab scale downdraft gasifier

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Introduction

- Among the biomass conversion processes, gasification is a major technology to convert biomass into energy fuel.
- The gasification converts the solid material into a gaseous fuel called syngas mainly composed of CO, H_2, CH_4, O_2, N_2.
- Numerical simulation has been largely used to analyze biomass gasification in order to evaluate the process performance of different biomass under different operating conditions.

Numerical modelling approach.

- Kinetic rate models
- thermodynamic equilibrium models.
  - stoichiometric models
  - Non stoichiometric models

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Mathematical model

Jarungthammachote, S. and Dutta, A. Thermodynamic equilibrium model and second law analysis of a downdraft waste gasifier. Energy, ***2007****. 32(9): 1660-1669.*

- Global gasification reaction

$$CH_xO_yN_z + wH_2O + m(O_2 + 3.76N_2) = n_{H_2}H_2 + n_{CO}CO + n_{CO_2}CO_2 + n_{H_2O}H_2O + n_{CH_4}CH_4 + \left(\frac{z}{2} + 3.76m\right)N_2$$

- Carbon mass balance

$$n_{CO}CO + n_{CO_2}CO_2 + n_{CH_4}CH_4 - 1 = 0$$

- Hydrogen mass balance

$$2n_{H_2} + 2m_{H_2O} + 4n_{CH_4} - x - 2w = 0$$

- Oxygen mass balance

$$n_{CO} + 2n_{CO_2} + n_{H_2O} - w - 2m = 0$$

Water-shift reactions

$$CO + H_2O = CO_2 + H_2$$

$$K_2 = \frac{n_{CO_2} \cdot n_{H_2}}{n_{CO} \cdot n_{H_2O}}$$

$$\ln(K) = -\frac{\Delta G^0}{\bar{R}T} = -\frac{\sum_i v_i (\Delta \bar{g}^0_{f,i})}{\bar{R}T}$$

Mathematical model

Jarungthammachote, S. and Dutta, A. Thermodynamic equilibrium model and second law analysis of a downdraft waste gasifier. Energy, ***2007****. 32(9): 1660-1669.*

- The equilibrium constant calculation requires the knowledge of the gasification temperature

$$h^0_{f,CH_xO_yN_z} + wh^0_{f,H_2O} + \frac{\dot{n}_{O_2}}{\dot{n}_{CH_xO_yN_z}} h_{T_{IN},O_2} + \frac{\dot{n}_{N_2}}{\dot{n}_{CH_xO_yN_z}} h_{T_{IN},N_2} = n_{H_2} h_{T_{OUT},H_2} + n_{CO} h_{T_{OUT},CO} + n_{CO_2} h_{T_{OUT},CO_2} + n_{CH_4} h_{T_{OUT},CH_4} + n_{H_2O} h_{T_{OUT},H_2O}$$

- Enthalpy of organic matter $h^0_{f,CH_xO_yN_z} = LHV + \sum_{k=prod} \left[n_k \left(\bar{h}^0_f\right)_k\right]$

- Lower Heating Value $LHV = 0.3491 \cdot C + 1.1783 \cdot H - 0.1034 \cdot O - 0.0151 \cdot N - 0.0211 \cdot ash - 9 \cdot H \cdot h_{fg}$

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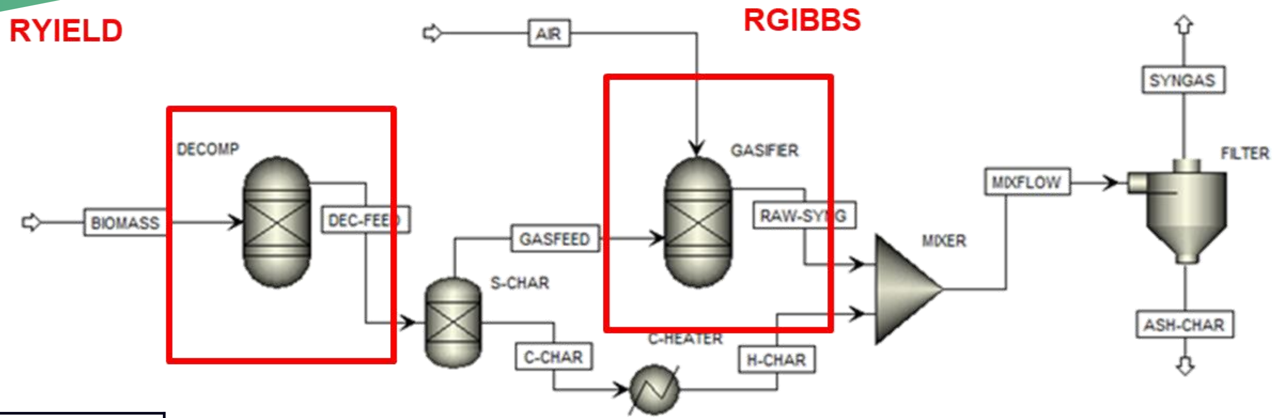
Aspen model



DECOMP (Ryield)	Decomposes the biomass into its constituent elements requiring yield distribution of the biomass into its components
GASIFIER (RGibbs)	Simulates gasification of biomass and modes the chemical equilibrium by minimizing Gibbs free energy
S-CHAR (Ssplit)	Separates unconverted char from syngas

C-HEATER (Heater)	Heats the unconverted char to the gasification temperature
MIXER (Mixer)	Mixes the syngas stream leaving the gasifier with unconverted char
FILTER (Ssplit)	Separates ash and char from syngas

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Aspen model

DECOMP (RYield)

Biomass $\rightarrow$ a Char + b N_2 + c H_2O + d CO + e CO_2 + f H_2+ g CH_4 + h O_2+ Ash

Calculator block in FORTRAN statement

```
H2O = WATER / 100
ASH = ULT(1) / 100 * FACT
CHAR = ULT(2) / 100 * FACT
H2 = ULT(3) / 100 * FACT
N2 = ULT(4) / 100 * FACT
O2 = ULT(7) / 100 * FACT
```

GASIFIER (RGibbs)

Gasification reactions that occur in RGibbs

R1. $C + 2H_2 \rightarrow CH_4$ Methanation
R2. $CO + H_2O \rightarrow CO_2 + H_2$ CO shift
R3. $C + O_2 \rightarrow CO_2$ Carbon Combustion
R4. $H_2 + 0{,}5\ O_2 \rightarrow H_2O$ Hydrogen Combustion

Restricted Chemical Equilibrium is chosen to specify the chemical reactions with different Temperature approach

Tapp1 = -167.6 °C
Tapp2 = 305.4 °C
Tapp3 = - 59.4 °C
Tapp4 = 0 °C

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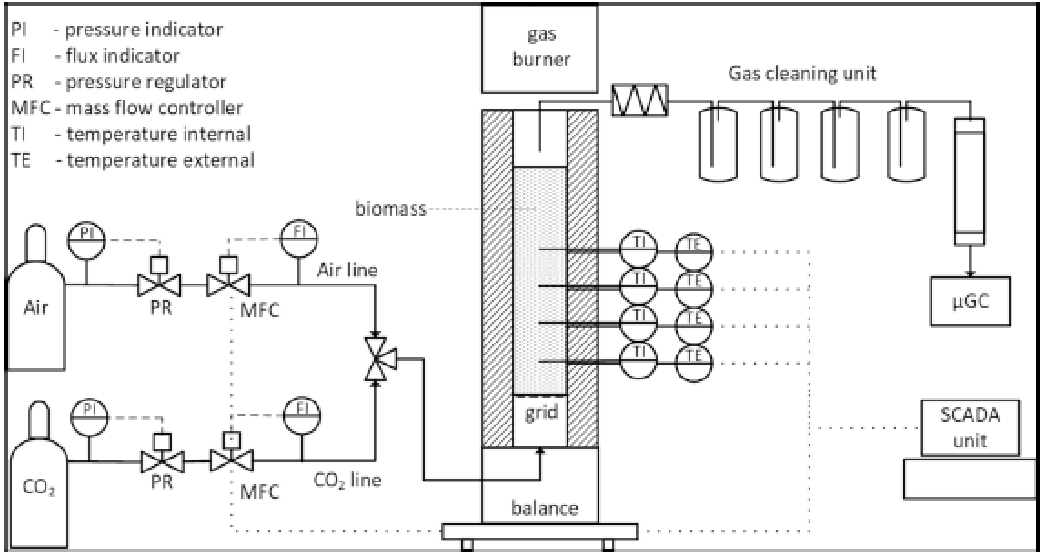
Pilot Gasification Plant

- Pilot plant installed in the Bioenergy Laboratory of the Free University of Bozen-Bolzano.
- Fixed bed reactor comprised of stainless steel cylindrical vessel with an internal diameter of 54 mm and a height of 1250 mm.

Antolini, D., et al., Experimental investigations of air-CO2 biomass gasification in reversed downdraft gasifier. *Fuel*, **2019**. 253: 1473-1481.



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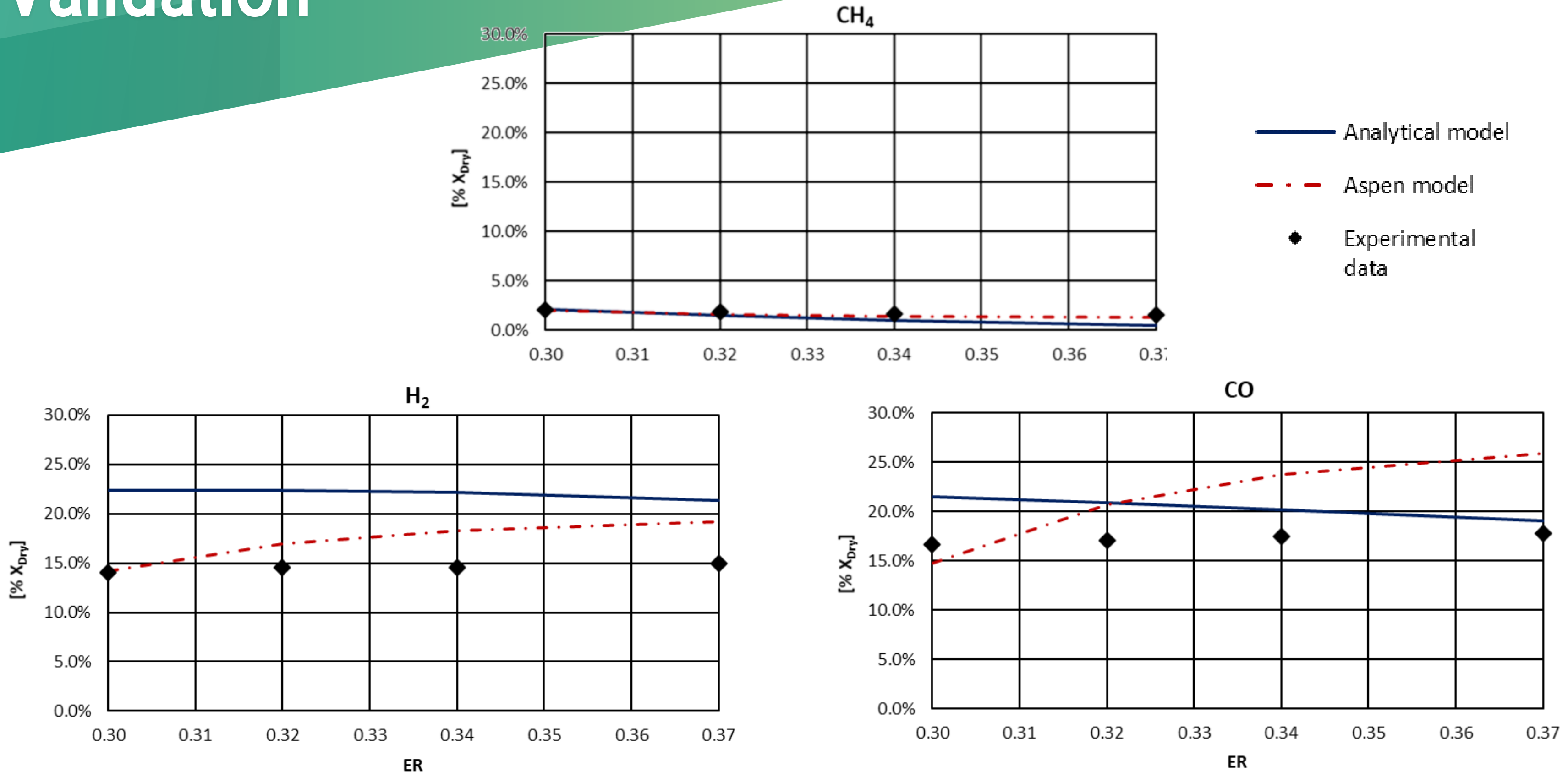
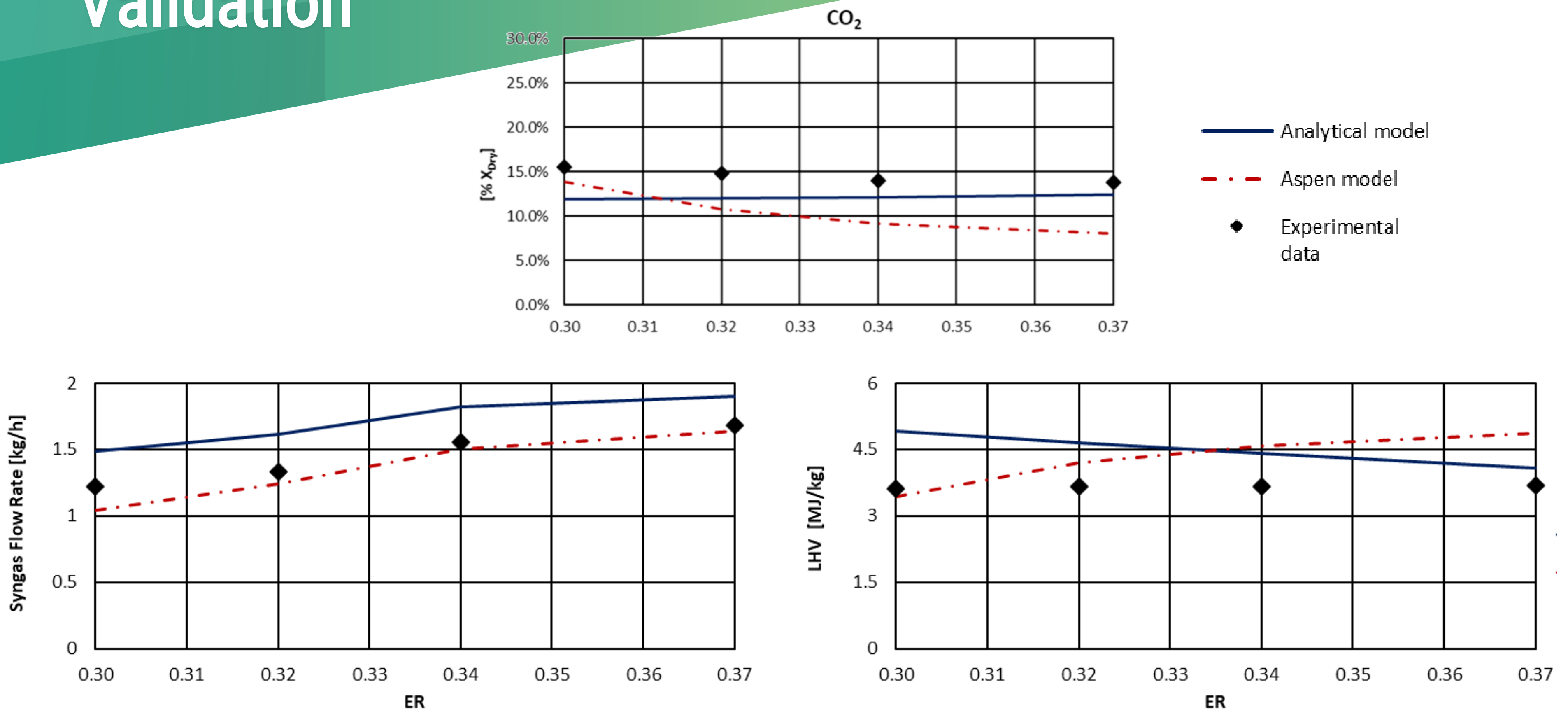
Validation



Validation


CO2
[% XDry]
30.0%
25.0%
20.0%
15.0%
10.0%
5.0%
0.0%
0.30
0.31
0.32
0.33
0.34
0.35
0.36
0.37
Analytical model
Aspen model
Experimental data
Syngas Flow Rate [kg/h]
2
1.5
1
0.5
0
ER
LHV [MJ/kg]
6
4.5
3
1.5
0
ER

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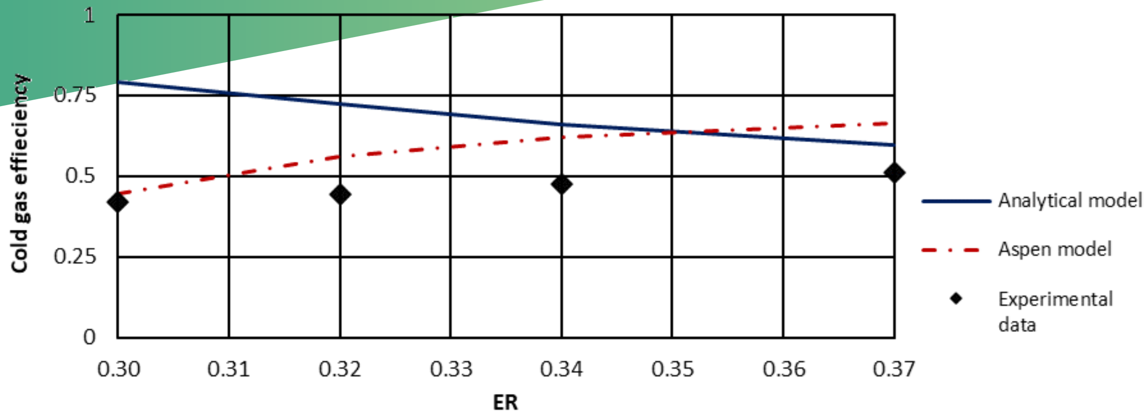

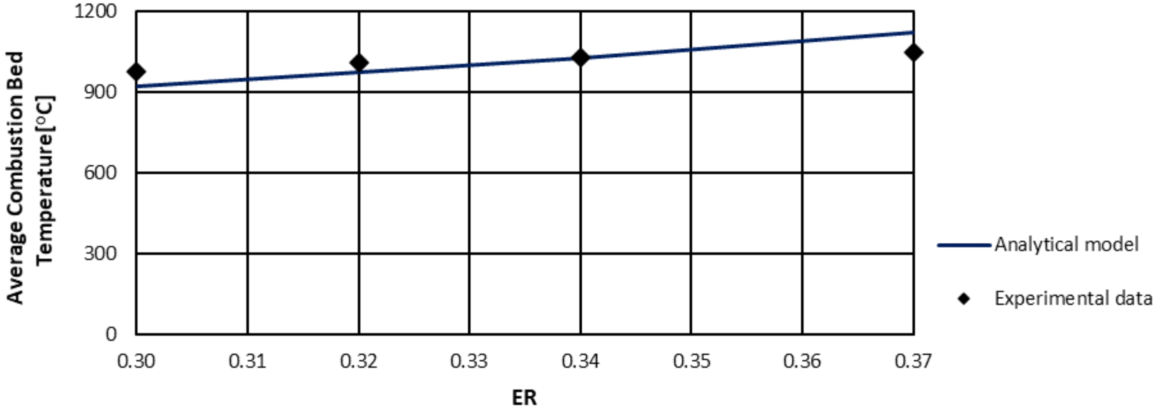

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Conclusions

- An analytical model based on the thermodynamic approach and a numerical model using Aspen Plus have been developed to investigate the process of biomass downdraft gasification using air as gasification agent. The analytical and Aspen models were validated with experimental data. The results of syngas composition are shown in relation with ER.
- Both model results present an overestimation of H2 and CO, in contrast, CO_2 is underestimated.
- The syngas composition results of both models are in quite good agreement with experimental data.

Future Development

- Model modification to take into account inlet air dilution with CO_2.
- Detailed 3D model using modern CFD techniques.