Carbon conversion predictor for fluidized bed gasification

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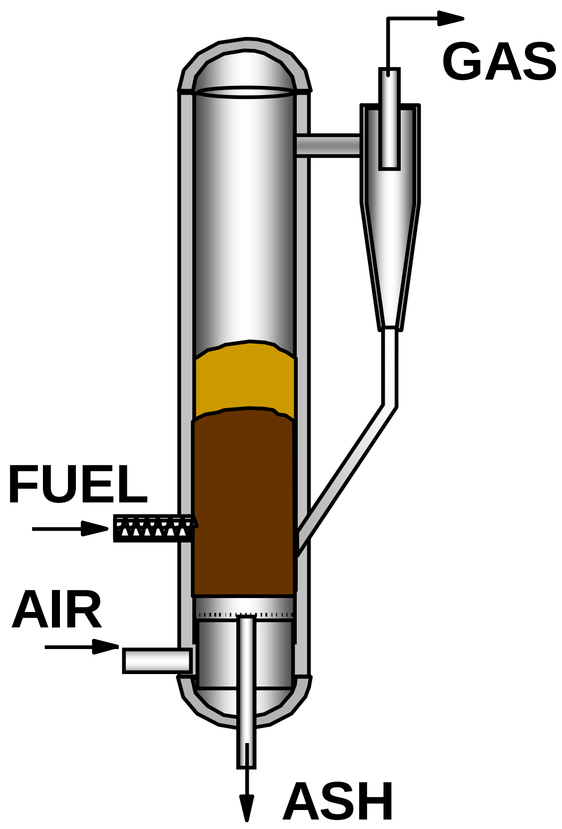
- Introduction
- Experimental / methodology
  - Converting kinetic parameters from TGA data (fluidized bed)
  - Fixed bed modeling
- Modeling
  - Fluidized-bed gasification
  - Fixed-bed gasification
- Conclusions

RECENT BOOK ABOUT BIOREFINERIES

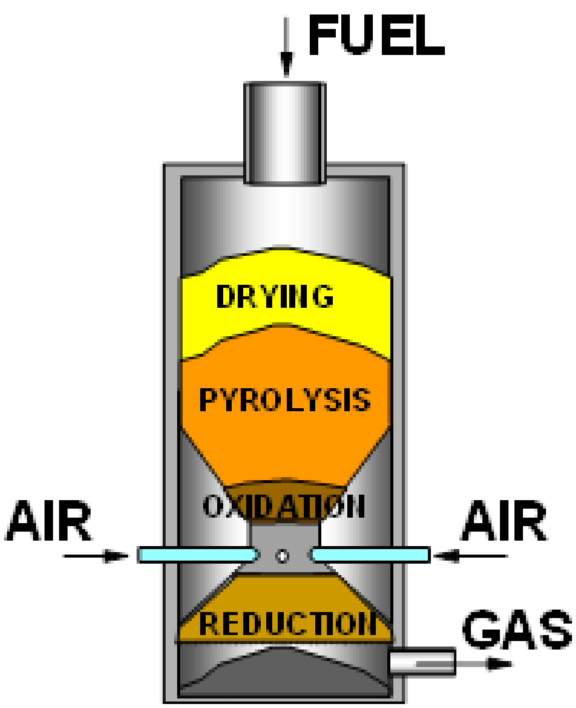
- Papermaking Science and Technology, Book 20: Biorefining of Forest Resources. Alén R. (ed.), Published by Paper Engineer's Association. Bookwell Oy, Porvoo, Finland 2011. ISBN 978-952-5216-39-4.
  - Chapter 8: Konttinen, J.; Reinikainen, M.; Oasmaa, A. and Solantausta, Y.: Thermochemical conversion of forest biomass Pp. 262-304

Gasification reactors to be modeled

Fluidized bed [1]



Downdraft fixed bed [1]

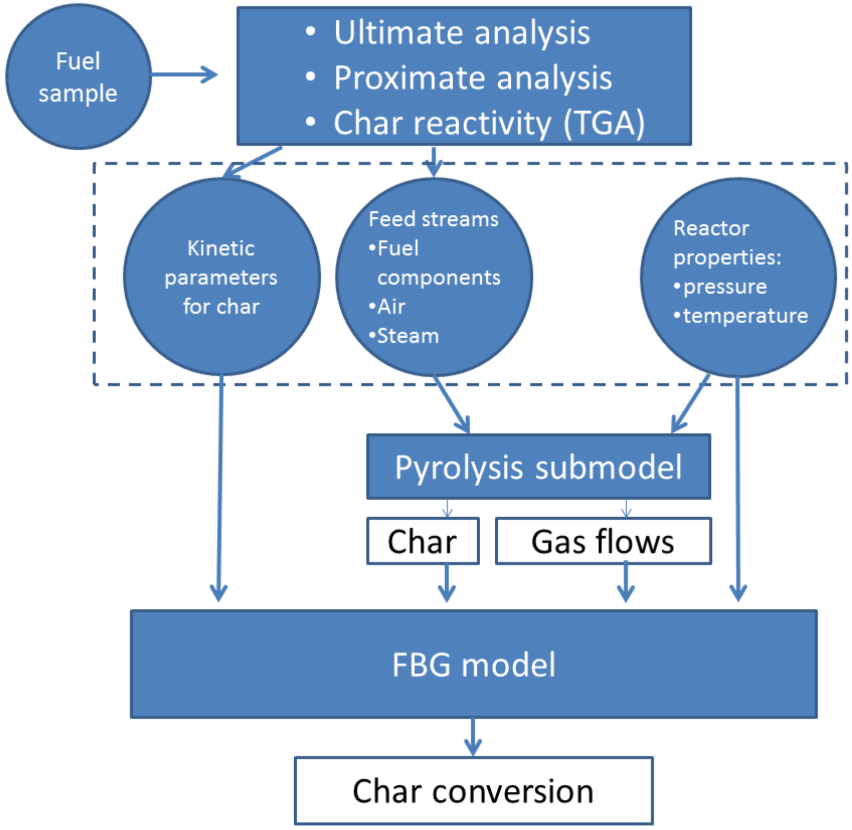


Carbon conversion predictor

- Oxidation of char carbon is the slowest step in the gasification of solid fuels
  - Contributes to gasifier efficiency (overall fuel conversion)
  - Contributes to the quantities and properties of ashes
- Gasification reactivity of waste and biomass chars is different from that of solid fossil fuels [2, 3]
  - Particle size
  - Rate of pyrolysis
  - Catalytic properties of ash (inhibition by CO/H_2)
- Should not just be another curve-fitting exercise…
  - Simple and transparent parameter fitting and modelling
  - With reasonable cost and effort

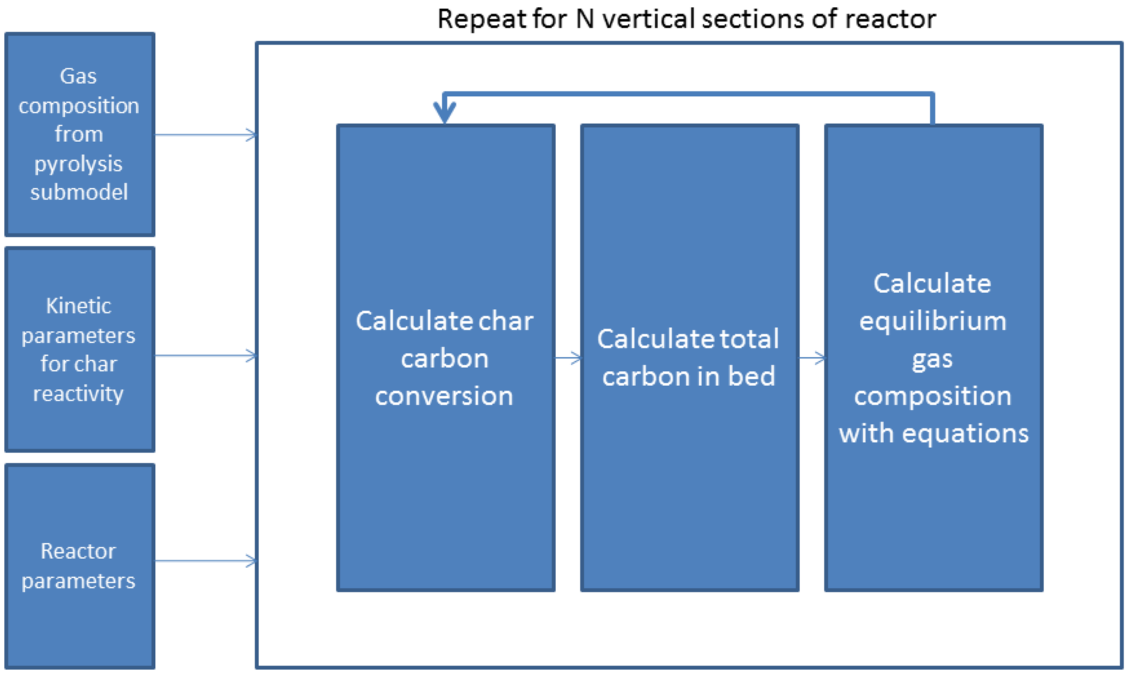
Carbon conversion predictor

- Schematic diagram of the overall carbon conversion predictor model [3]
- Inputs are intended to be based on relatively simple experimental tests on fuel samples (e.g. TGA)



Carbon conversion predictor

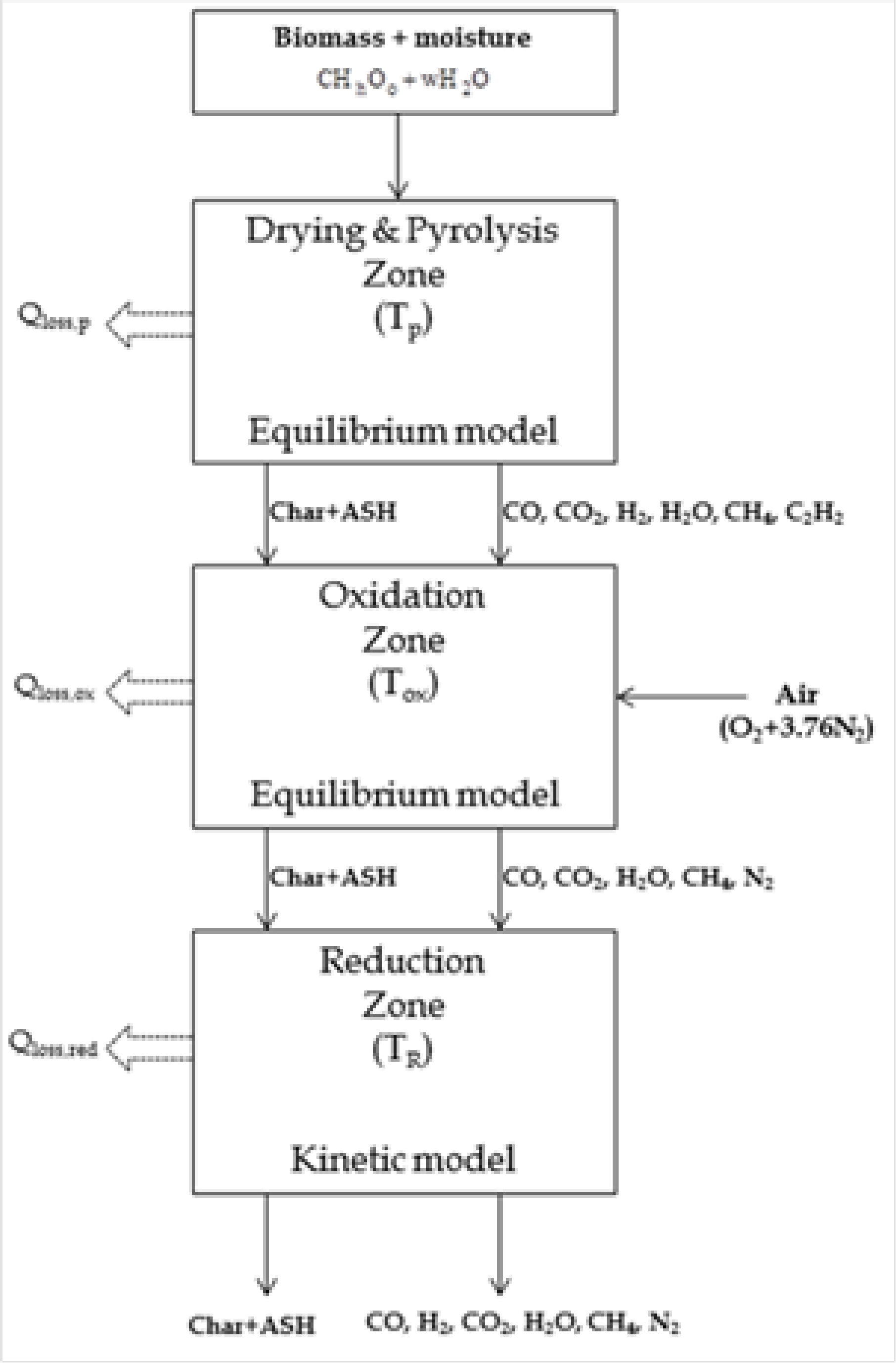
- Schematic diagram of the updated FBG component of the predictor model [3]
- Includes correlations for residence time and conversion calculations from Gómez-Barea and Leckner [7]



Downdraft fixed bed gasification model [5, 6]

- The gasification process is conceived to follow a particular sequence of drying, pyrolysis, oxidation and reduction process
- Drying and pyrolysis that comprises of a sub-model is formulated based on empirical and stoichiometric equilibrium modeling approach.
- Oxidation (partial) process is also framed on stoichiometric equilibrium model
- The sub-model for reduction process is established on finite kinetic modeling approach.
  - Reduction process is accredited with an essential phenomenon during gasification process and encompasses several gasification reactions. [5, 6]
- Thus, the model can be used to
  - analyze the influence of moisture content and equivalence ratio on the product gas composition, heating value and carbon conversion.
  - the model may help in optimizing the gasification process in a downdraft gasifier.

Downdraft fixed bed gasification model [6]



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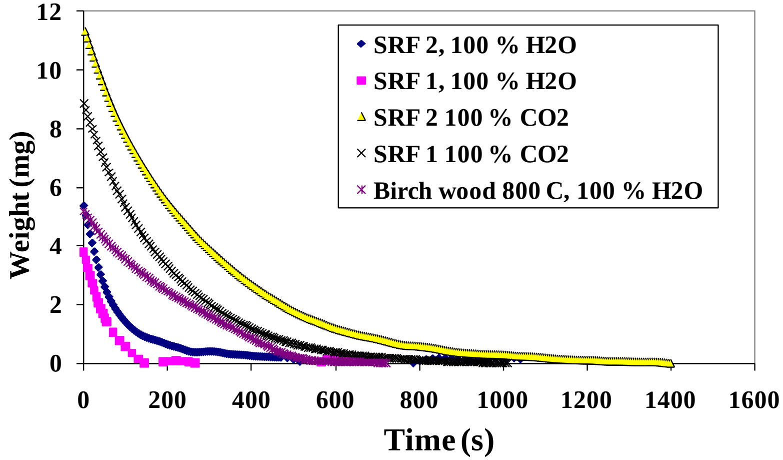
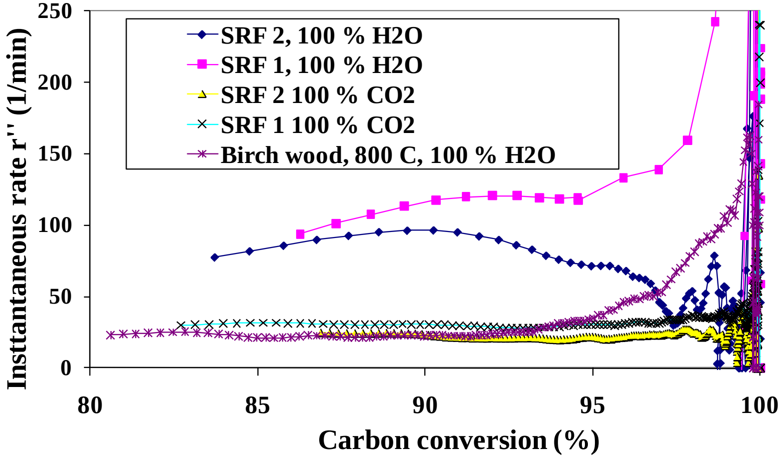
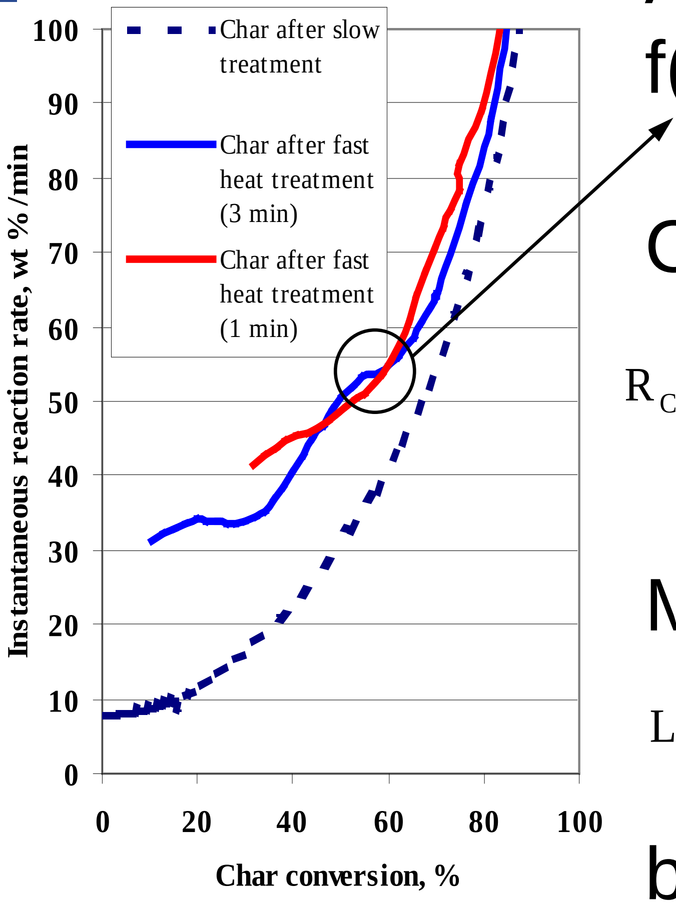
Char carbon gasification - conversion of TGA data [3]



$$r'' = \frac{1}{w}\frac{dw}{dt}$$





Average reactivity (1/s) = $f(T, p_{tot}, p_{H2O}, p_{CO2}, p_{CO}, p_{H2})$

Correlations (wood, small d_p) [3, 4]:

$$R_{C-CO_2} = \frac{k_{1f} P_{CO2}}{1 + \frac{k_{1f}}{k_3} P_{CO2} + \frac{k_{1b}}{k_3} P_{CO}} \qquad R_{C-H_2O} = \frac{k_{1f} P_{H2O}}{1 + \frac{k_{1f}}{k_3} P_{H2O} + \frac{k_{1b}}{k_3} P_{H2}}$$

Minimize:

$$L = \sum_j^N \left(R_{C\,exp} - R_{C\,model} \right)_j^2$$

To find:

$\Rightarrow k_{01f}, k_{01b}, k_{03}$
E_{1f}, E_{1b}, E_3

by Levenberg-Marquardt method

Kinetic parameters for Char Carbon Reactivity [3]

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Downdraft fixed bed gasification model

- The kinetic model for the gasification reactions are of Arrhenius type [5, 6]

Reactions	Reaction rate (mol/m^3.s)
Boudouard reaction: $C + CO_2 \leftrightarrow 2CO$	$r_1 = C_{RF} A_1 \exp\left(\frac{-E_1}{RT}\right) \cdot \left(y_{CO_2} - \frac{y_{CO}^2}{K_{eq,1}}\right)$
Water-gas reactions: $C + H_2O \leftrightarrow CO + H_2$	$r_2 = C_{RF} A_2 \exp\left(\frac{-E_2}{RT}\right) \cdot \left(y_{H_2O} - \frac{y_{CO} \cdot y_{H_2}}{K_{eq,2}}\right)$
Methane formation: $C + 2H_2 \leftrightarrow CH_4$	$r_3 = C_{RF} A_3 \exp\left(\frac{-E_3}{RT}\right) \cdot \left(y_{H_2}^2 - \frac{y_{CH_4}}{K_{eq,3}}\right)$
Steam reformation: $CH_4 + H_2O \leftrightarrow CO + 3H_2$	$r_4 = A_4 \exp\left(\frac{-E_4}{RT}\right) \cdot \left(y_{CH_4} \cdot y_{H_2O} - \frac{y_{CO} \cdot y_{H_2}^3}{K_{eq,4}}\right)$

- In the reaction rate equation, C_{RF} refers to char reactivity factor, A & E are the kinetic parameters, y_i is the mole fraction of the chemical species involved in the gasification process

- For example, the rate of formation or destruction of CO can be estimated as; $R_{CO} = 2r_1 + r_2 + r_4$. The reduction zone is partitioned into n number of compartments.

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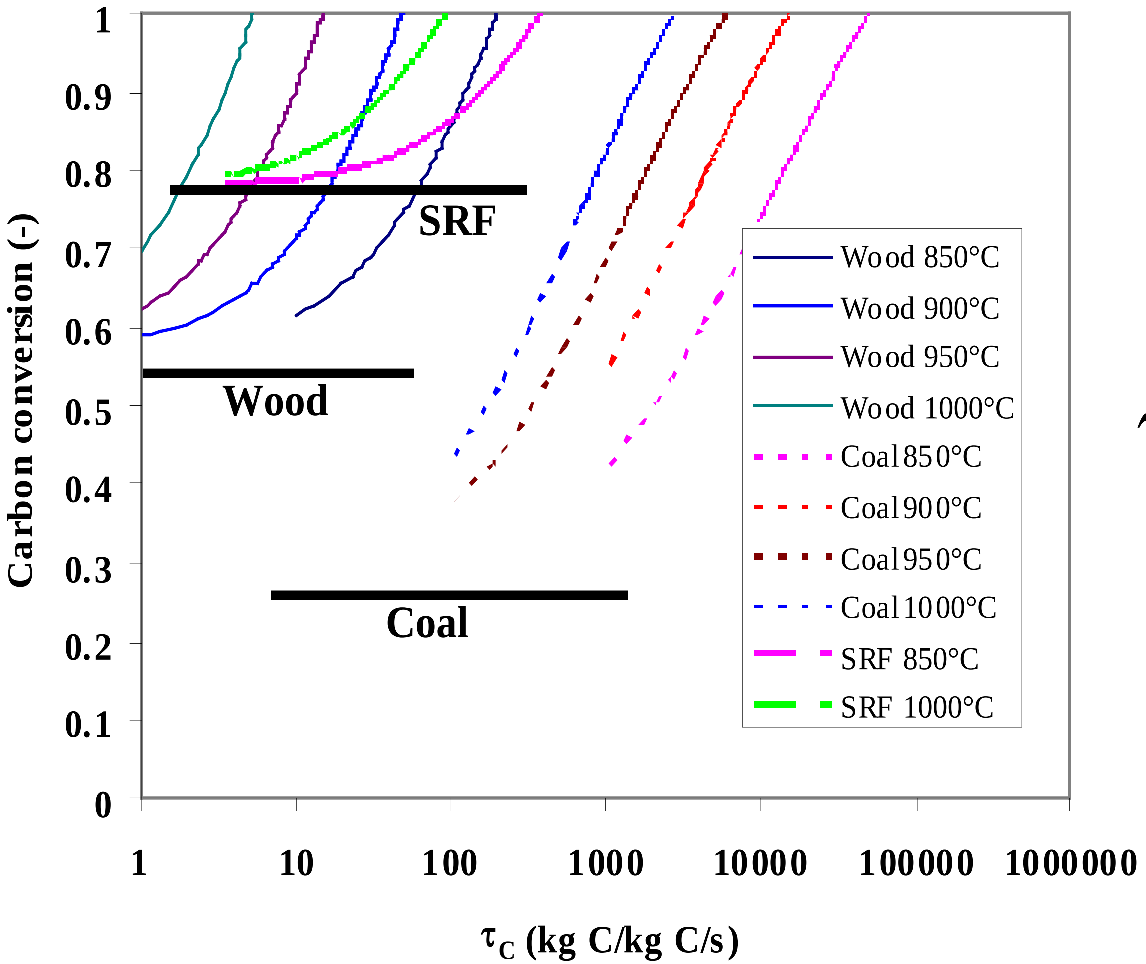
Carbon conversion predictor results

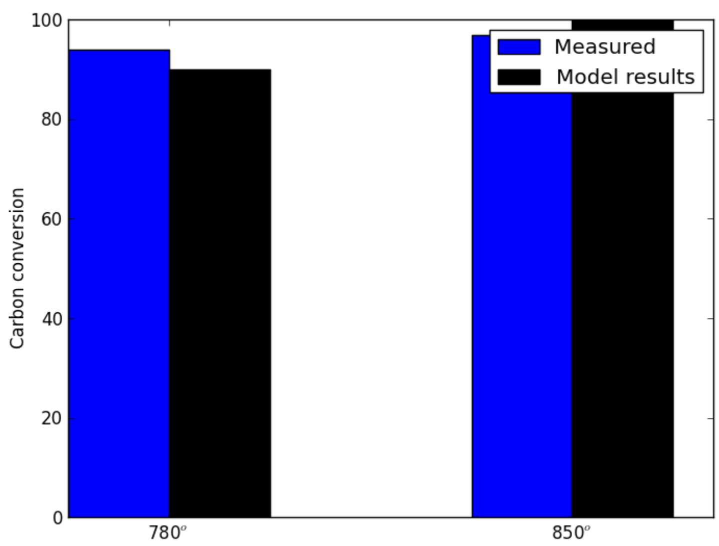


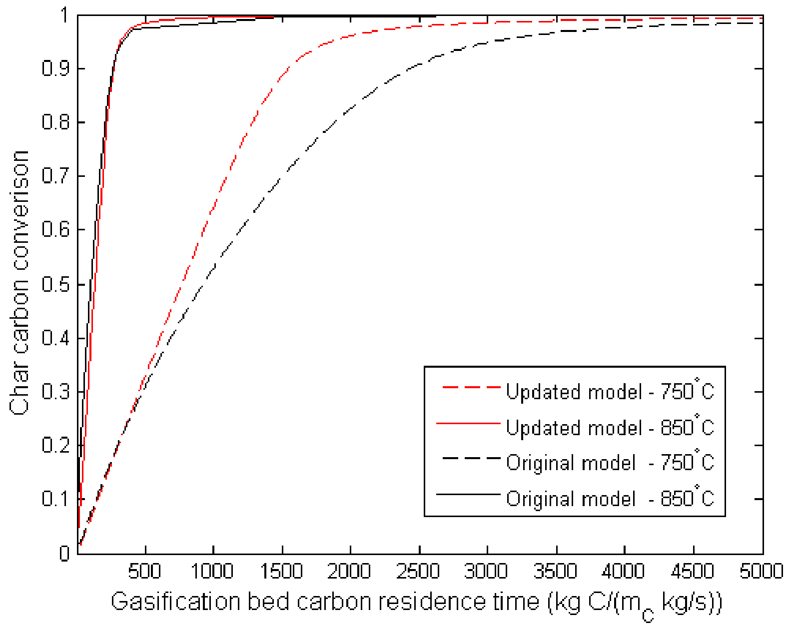
$$\tau_C = \frac{M_{Cbed}}{m_{Cf}}$$

Konttinen et al. [3]

Carbon conversion predictor

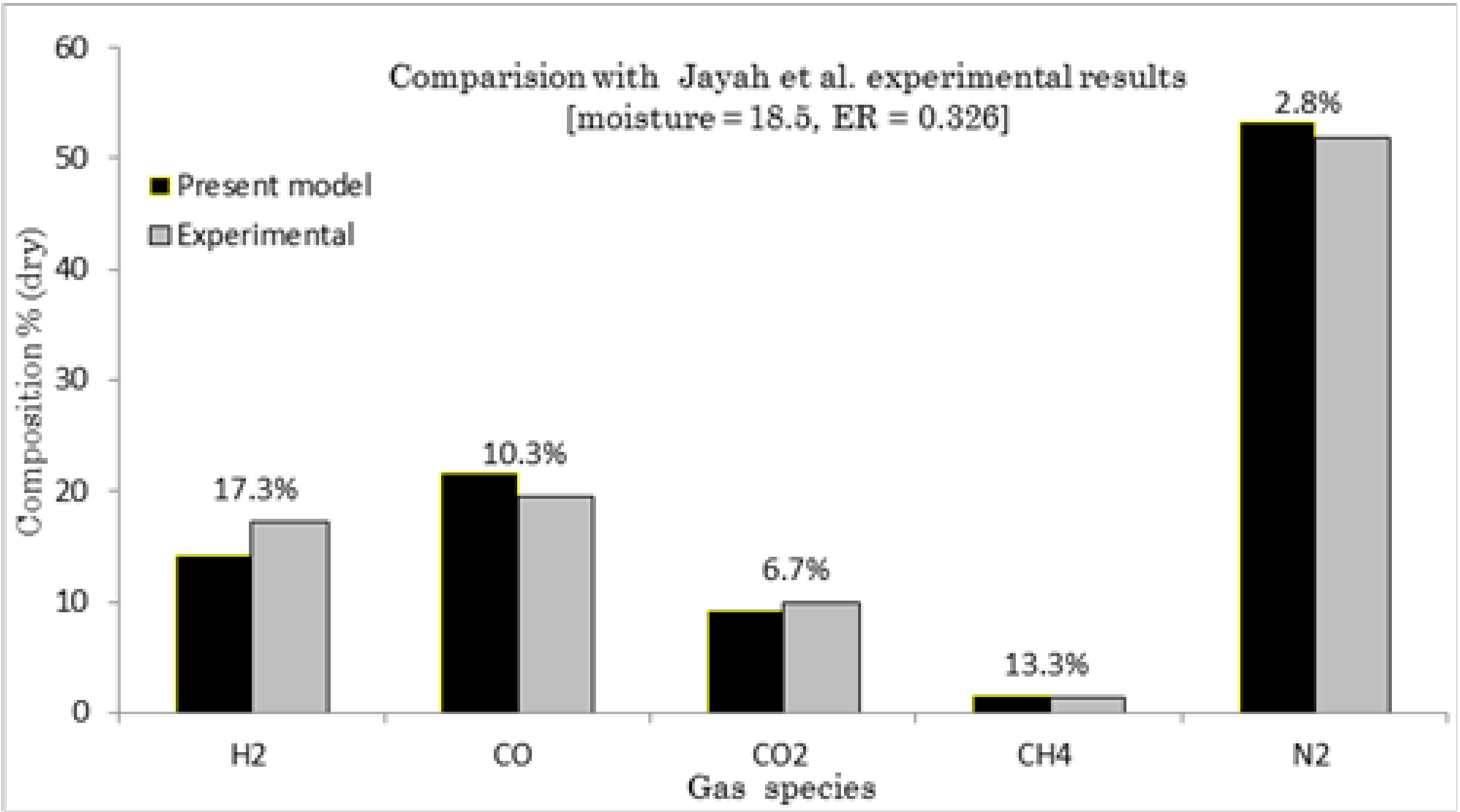
- Results based on preliminary modeling work
- Updated model results show good similarities with previous work
- Results match well with pilot scale data





Downdraft fixed bed gasification model

Composition comparisons with experimental data of Jayah el al. [5, 6].
The data label refers to absolute error in prediction of corresponding gaseous species. (ER = equivalence ratio).



Carbon conversion predictor, future work

- Implement conversion dependent reactivity equations into reactor model
- Time dependendent, non-steady state/dynamic behavior

References

1. Konttinen J, Reinikainen M, Oasmaa A, and Solantausta Y Thermochemical conversion of forest biomass (Chapter 8). In: *Papermaking Science and Technology, Book 20*: Biorefining of Forest Resources. Alén R. (ed.), Published by Paper Engineer's Association. Bookwell Oy, Porvoo, Finland 2011. Pp. 262-304. ISBN 978-952-5216-39-4.

2. Moilanen A, Thermogravimetric characterisations of biomass and waste for gasification processes. *Academic dissertation*, Abo Akademi University. Espoo 2006. VTT Publications 607. 103 p. + app. 97 p.

3. Konttinen, J.; Moilanen, A.; DeMartini, N and Hupa, M.: Carbon conversion predictor for fluidized bed gasification of biomass fuels – from TGA measurements to char gasification particle model. *Biomass Conversion and Biorefinery*, 2 (2012) 3, pp. 265-274.
http://dx.doi.org/10.1007/s13399-012-0038-2

4. Barrio, M Experimental investigation of small-scale gasification of woody biomass. *Academic dissertation*, The Norwegian University of Science and Technology, Faculty of Engineering Science and Technology, Department of Thermal Energy and Hydropower. Trondheim., Norway, May 2002.

5. Jayah, TH, Aye, L, Fuller RJ, Stewart DF, "Computer simulation of a downdraft wood gasifier for tea drying," *Biomass Bioenergy*, vol. 25, pp. 459-469, 10, 2003.

6. Budhathoki, R, Three zone modeling of Downdraft biomass Gasification: Equilibrium and finite Kinetic Approach. *Master's Thesis*. University of Jyväskylä, Department of Chemistry, Finland, April 2013.

7. Gómez-Barea A, Leckner B, Estimation of gas composition and char conversion in a fluidized bed biomass gasifier, *Fuel* 107 (2013), pp. 419–431. http://dx.doi.org/10.1016/j.fuel.2012.09.084

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Conclusions

- High system efficiency requires good carbon conversion in the gasifier
- The reactivity of the char in gasification reactions (between char carbon and steam and CO_2 as well as the inhibiting reactions of product gases H_2 and CO) play a significant role in reaching good carbon conversion in a hot fluidized bed
- The gasification reactivity data of biomass chars, as measured in TGA experiments, is used for the determination of kinetic parameters for char carbon gasification reactivity correlations

Conclusions

- Laboratory measured reactivity values from TGA experiments are used in the Carbon Conversion predictor to simulate carbon conversion in a real scale fluidized bed gasifier
- The predictor is a relatively simple and transparent tool for the comparison of the gasification reactivity of different fuels in fluidized bed gasification
- Also a three-zone model for fixed bed gasification has been developed, based on models and parameters from the literature.
- Simulations with the models against some pilot-scale results show reasonable agreement

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