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Prediction of gas composition in biomass gasifiers

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Content

- 1. Motivation and objective
- 2. Background: Existing evidence in gasification
- 3. Modelling
- 4. Experiments and application
- 5. Conclusions

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1. Motivation and objective

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- In the preliminary design of a FBG, the knowledge of the main components of the gas produced in the gasifier is a key factor
- Advanced models for FBG exist but require physical and kinetic inputs difficult to estimate and sometimes are not available to industrial applications
- Simple and reliable semi-empirical methods to predict gas composition and reactor performance are not common in literature, and there is a need for such modelling tools

Difficulty in modelling (complex Chemestry and transport phenomena at particle level)



Difficulty in modelling (complex flow pattern and transport phenomena at reactor level) $CO \Leftrightarrow H_2$ CO H₀ **Producer GAS** $\mathsf{CO},\,\mathsf{H}_{2}^{},\,\mathsf{CH}_{4}^{},$ C С С $CO_2, N_2, H_2O, C_xH_yO_z$ CO₂ Freeboard H₂O Char particle Volatiles (H_2, CO, C_xH_y) Boundary layer Char emulsion Bed bubble Fuel 0 0 air

1. Motivation and objective



- Equilibrium models (EM)
- Quasi-Equilibrium models (QEM)
- Empirical models

Equilibrium models (EM)

Advantages

- Simple to apply
- Independent of gasifier design
- Widely used

Failures

- Overestimates yields of H₂ and CO
- Underestimates the yield of CO₂
- Prediction of gas nearly free of CH_4 and tar
- No char in the gas phase over 1000 K

Quasi-Equilibrium models (QEM) (Gumz, 1950)

Advantages

- Improvement of EM
- Simple to apply

Failures

- Need correlations
- Dependent of gasifier design
- Most cases do not predict tar and/or char
- Sometimes recommendations can avoid correlation but this make QEM non-predictive

Empirical models

Advantages

- Simple to apply
- The best predictions

Failures

- Needs a lot of experimental data
- Only valid for a given facility and biomass

Example

 Maniatis et al (1994) → Correlations based on one parameter (ER)

Objective

To develop a model (method):

- -Based on QEM (simple)
- -With predictive capability
- Free from correlations
- -Able to estimate tar and char
- -Based on established evidences

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- Heterogeneous or homogeneous equilibrium?
 - In EM no solid carbon in the gas phase over 1000 K
- Steam Reforming of Methane (SRM) in equilibrium?
 - Steam reforming of methane is kinetically limited below 1300 K
 - methane in the exit stream of the gasifier ~ that formed in devolatilisation

- Water Gas Shift Reaction (WGSR) in equilibrium?
 - Equilibrium for the WGSR reached at 1273 K and residence time about 1 s
 - Between 1073 K and 1273 K the attainment of equilibrium has to be confirmed
 - This confirmation depends on the use of catalysts and steam presence:
 - Synthetic (Ni) vs. minerals (dolomite, olivine, etc) catalyst
 - Steam vs. air gasification



Conclusions from the existing evidence for the model

- Homogeneous equilibrium is enough for practical applications
- Modified equilibrium based on WGSR and SRM is convenient
- Kinetic rates of SMR should be included in the model
- CH₄ in the exit is nearly that formed during devolatilisation (air gasification without catalyst)
- Equilibrium of WGSR is nearly attained: an approach to equilibrium method based on T, t_{res}, type of catalyst and the presence of steam seems to be convenient

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3. Modelling

Simplified model of a FB gasifier ($N_{seg} >>1$)



3. Modelling

Steps in modelling

- 1. Estimation yields of light gases, char and tar from FPZ $(CH_4, tar and char are estimated as function of T)$
- 2. Estimation tar, methane and char conversion in CRZ by application simple kinetic models
- 3. QE model:

- Unconverted CH_4 , tar and char are removed from this analysis formulation of $C-H_2-O_2-N_2$ mass balances
- Mass balances with corrected C-H-O inputs

- two equilibrium (or approach to equilibrium) relationships (WGSR and SRMR)

4. Restoration of unconverted CH_4 , tar and char Application of heat balance over the corrected exit streams

Model concept adopted



Char conversion sub-model

- Based on a recent simple method for non-catalytic gas-solid reactions for one reaction
- Reaction: Char + R \rightarrow P, being R = H₂O + CO₂ and P = H₂ + CO
- Population balance and any kinetic models with any structural behavior and nth order kinetics respect to R is solved in one-envelope calculation

Tar and CH₄ conversion sub-model

- Calculated by single-flow kinetic models (CSTR, PFR)
 - Initial conditions established by solution of FPZ
- Adequate selection of tar and methane model could be challenge:
 - Tar: mainly depends on the biomass nature, operating conditions (T, t), presence of catalyst
 - Methane: The use of catalyst and the presence of steam

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10 kW_{th} Lab and pilot scale experiments



4. Experiments and application

Devolatilisation studies



Char reactivity studies



4. Experiments and application



150 kW_{th} pilot scale experiments



4. Experiments and application

Scaling-up



3 MW_{th} BFB Gasifier

4. Experiments and application

Applications

- Optimisation for gasification with wood and orujillo at 150 kW_{th} pilot scale
- Test programme for the 3 MW_{th} BFB gasifier
- Preliminary design of BFB gasifier for processing MBM
- The tool developed improves significantly the capability of equilibrium

Validation: Gasification of wood pellets at 150 kW_{th} pilot gasifier (ER=0.28)

	Units	This method	Equilibrium	Pilot results
СО	% vv	15.0	24.5	14.3
CO ₂	% vv	17.2	7.1	18.5
H ₂	% vv	12.5	25.5	11.9
H ₂ O	% vv	12.5	5.5	11
CH ₄	% vv	4.5	0.0	5.1
N ₂	% vv	51	40	52
C _k H _l O _m (tar)	g/Nm ³	12	0.0	12.5
F _{gp,d} (Gas yield)	mole gas/kg fuel daf	2.1	2.4	2.1
X _{C,ash}	kg _C /kg _{da}	0.32	_	0.28
CC (tar included)	%	91.5	100	92.5

4. Experiments and application



- 1. The development of a model based on QEA with predictive capability and easy to apply
- 2. Used as tool for design and optimisation: improves significantly equilibrium predictions
- 3. Valid for preliminary design
- 4. Yields of char, methane and tar during devolatilisation steps need to be estimated
- 5. Proper selection of kinetic parameters for tar and CH₄ may be critical



Thank you for your kind attention

