Optimal Tuning of a Thermo-Chemical Equilibrium Model for Downdraft Biomass Gasifiers

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A thermo-chemical equilibrium model is applied to predict the released syngas composition, char, tar content and temperature in biomass gasifiers. The accuracy of the model results is improved by proper calibration, namely by modifying the equilibrium constants through correction factors that represent the degree of approach of the analyzed system to equilibrium. To this aim, the developed model is coupled with a genetic algorithm (MOGA II), to search for the optimal correction factors able to minimize the error between the computed and the experimentally measured product yields and temperatures. The approach is repeated to simulate the thermal treatment of different biomasses with increasing carbon content, from straw to sawdust. The possibility to resort to a unique set of correction factors for different biomasses is explored, that would allow the model being of particular interest for engineering applications, to trace the design guidelines for gasification systems.

1. Introduction

According to Basu (2010), simulation models of biomass gasifiers can be classified in the following categories:
• Models based on the thermo-chemical equilibrium hypothesis;
• Kinetic models;
• Phenomenological models;
• Models based on artificial neural networks.
The thermodynamic equilibrium models predict the maximum yield attainable by a reagent system. In other words, if the reagents are allowed to react for an infinite time, they reach equilibrium and the conversion occurs to the maximum yield. In this perspective, equilibrium models reproduce the ideal performance of a gasifier. Due to their simplicity and the reduced computational time, they are suitable of being employed in a first phase of study or within optimization procedures, where the influence of a certain number of parameters has to be investigated or a choice of the optimal biomass to be treated for a certain scope is to be made.
The main assumptions of thermo-chemical equilibrium models are indeed quite restrictive: the gasifier is seen as zero-dimensional and perfectly insulated, all gases are assumed as ideal, without residual and tar, perfect mixing and uniform temperature are assumed, the reaction rates are fast enough and residence time is sufficiently long to reach equilibrium. In the practice, gasifiers have heat losses to the environment, the gas behavior may be far from the ideal gas assumption and the chemical reaction rate be enough slow to not allow reaching equilibrium. Also it is to be kept into account that gasifiers are different in shape and dimension.
To increase the accuracy of the equilibrium models results, calibration is necessary for each specific considered operating case. Equilibrium constants must be modified in order to account for the actual rate of approach to equilibrium. Based on this consideration, a procedure is here developed to improve the predictive capability of a model developed by Costa et al. (2014) on the ground of the work of Jarungthammachote and Dutta (2007). The novelty of this work consists in the coupling between the developed thermo-chemical equilibrium model with an optimization software calculating the optimal correction factors able to minimize the error between computed and experimentally measured yields and temperatures. The optimal tuning of the
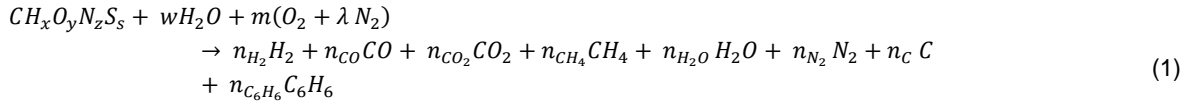
model is repeated for different biomasses in order to search for a set of correction parameters suitable of being used under different circumstances, so to give to the model an objective prediction capability, independent on the considered system or the kind of treated material.

In order to greatly reduce the calculation time, the Design Of Experiment (DOE) space, where to search for the optimal tuning coefficients, is initially reduced in size through the Response Surface Method (RSM).

The model considers the syngas as composed of H_2, CO, CO_2, CH_4, H_2O and N_2, and tar. This last is modeled as benzene C_6H_6, according to Abuadala et al. (2010) and Vera et al. (2011).

2. Mathematical model characterized by a different carbon content

The gasification model is based on the overall reaction of gasification in the presence of air:

$$CH_xO_yN_zS_s + wH_2O + m(O_2 + \lambda N_2)$$
$$\rightarrow n_{H_2}H_2 + n_{CO}CO + n_{CO_2}CO_2 + n_{CH_4}CH_4 + n_{H_2O}H_2O + n_{N_2}N_2 + n_C C$$
$$+ n_{C_6H_6}C_6H_6 \tag{1}$$

where the tar formation is also considered, differently from the previous work of Costa et al. (2014), as a function of the gasification temperature [K]:

$$n_{C_6H_6} = 35.98 \exp(-0.0029\,T). \tag{2}$$

The unknowns of the problem are $n_{H_2}, n_{CO}, n_{CO_2}, n_{CH_4}, n_{H_2O}, n_C, n_{C_6H_6}$ and the gasification temperature T.

In order to determine these eight unknowns, the following equations are written in addition to Eq. (2).

Balance of C

$$n_{CH_4} + n_{CO} + n_{CO_2} + 6\,n_{C_6H_6} + n_C - 1 = 0 \tag{3}$$
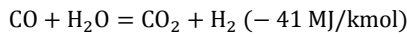
Balance of H

$$4\,n_{CH_4} + 2\,n_{H_2} + 2\,n_{H_2O} + 6\,n_{C_6H_6} - x - 2\,w = 0 \tag{4}$$
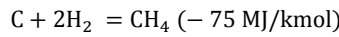
Balance of O

$$n_{H_2O} + n_{CO} + 2\,n_{CO_2} - w - 2\,m - y = 0 \tag{5}$$

Three further equations are derived by imposing the equilibrium the following reactions:
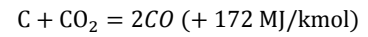
Water - gas homogeneous reaction	**Methane formation reaction**	**Boudouard reaction**
$CO + H_2O = CO_2 + H_2$ (-41 MJ/kmol)	$C + 2H_2 = CH_4$ (-75 MJ/kmol)	$C + CO_2 = 2CO$ $(+172\text{ MJ/kmol})$

$$K_1 = \exp\left[-\frac{\overline{\Delta G_T^0}}{RT}\right] = \frac{n_{co_2}\,n_{H_2}}{n_{co}\,n_{H_2O}} \qquad K_2 = \exp\left[-\frac{\overline{\Delta G_T^0}}{RT}\right] = \frac{n_{CH_4}}{(n_{H_2})^2}\left(\frac{P}{n_{tot}\,P_0}\right)^{-1} \qquad K_3 = \exp\left[-\frac{\overline{\Delta G_T^0}}{RT}\right] = \frac{(n_{co})^2}{n_{co_2}}\left(\frac{P}{n_{tot}\,P_0}\right) \tag{6}$$

The last equation necessary for calculating the gasification temperature is the energy balance as written by Costa et al. (2014), where also the contribution of tar is accounted for.

3. Validation of the model

The developed model is initially validated on the ground of the experimental data reported in Jayah et al. (2003). Table 1 reports the ultimate analysis of the processed biomass and the syngas composition and temperature, as measured an as numerically computed.

Table 1: Comparison between the numerical model results and the experimental data

Ultimate analysis	ASH	C	H	O	N	S	
	0.7	50.6	6.5	42	0.2	0	

Syngas composition	CH_4	H_2	CO	CO_2	N_2	H_2O	T_{gas} [K]
Experimental data	0.013	0.17	0.184	0.106	0.527	0.0	1100
Numerical data unoptimized	0.0118	0.230	0.217	0.120	0.419	0.0	924.64

4. Modification of the model

In order to increase the accuracy of the results of the simulation model, the reasoning of Gumz (1950) is followed, stating that equilibrium constants may be corrected, to account for the actual distance from the ideal state, by considering multiplicative factors representing the degree of approach to equilibrium. An approach of this type is used by Jarungthammachote et al. (2007), Mendiburu et al. (2014), Barman et al. (2012) and Vaezi et al. (2011). The proper values of the multiplicative factors is found by solving a multi-objective optimization problem through the genetic algorithm MOGA II. The problem is formulated according to the scheme represented in Figure 1, were a properly design of experiment (DOE) space of values of the constants $costK_i$, for i=1,2,3, is explored in order to find the triple minimising the error between the numerically computed mass fractions of the syngas components and the experimentally measured ones.
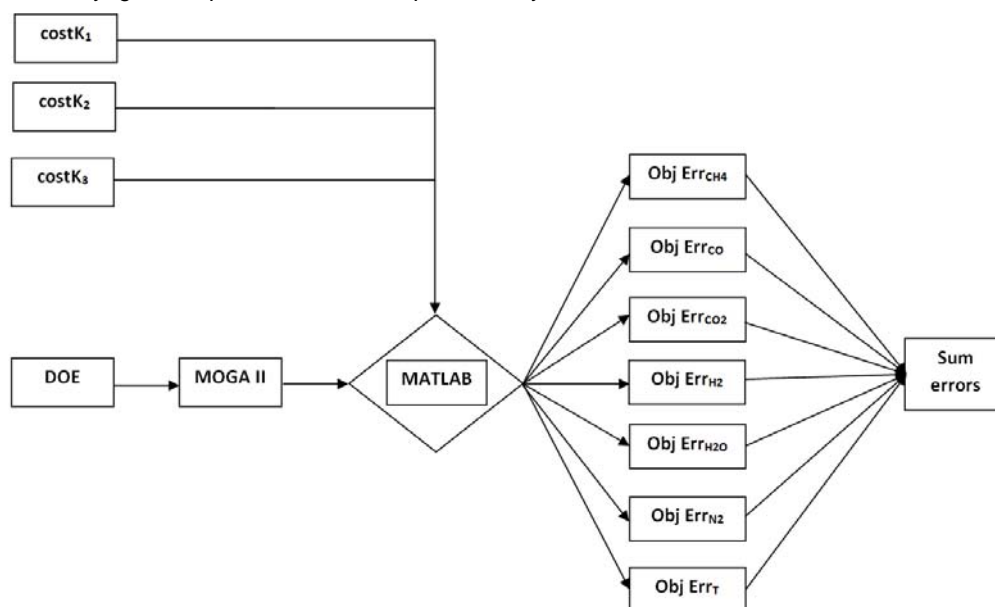

Figure 1. Scheme of the optimization approach followed for the optimal tuning of the thermo-chemical equilibrium model of biomass gasification.

The results of the optimization process for the biomass rubber wood are reported in Table 2, together with the multiplicative factors used by Jarungthammachote et al. (2007).

Table 2. Correction factors for the equilibrium constants (Eqs. (6)).

Rubber Wood	$costK_1$	$costK_2$	$costK_3$
Present Model	0.58	11.9	0.02
Jarungthammachote et al., (2007)	0.91	11.28	0.00

The effect of the optimal tuning of the equilibrium constants is shown in Figure2, where the syngas composition (top) and temperature (bottom) are represented as a function of the equivalence ratio. The experimental data reported by Jarungthammachote et al. are also represented, together with the curve obtained without any correction to the equilibrium constants. It is evident that the performed approach leads to more accurate results as regards the prediction of both the product yields and the gasification temperature.
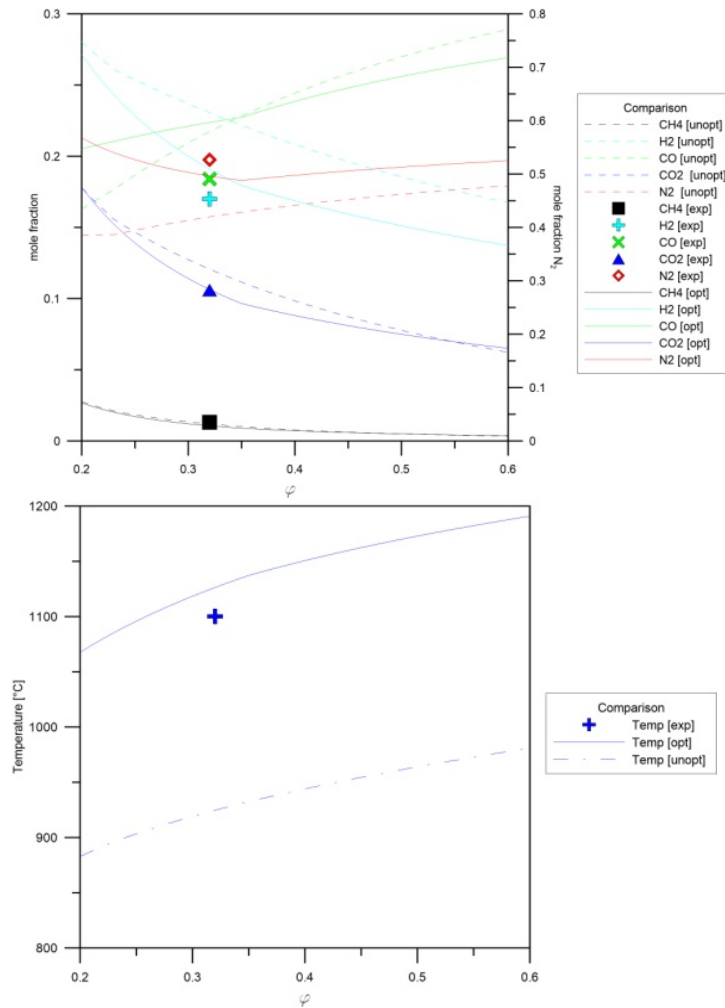
Figure 2: Effect of the multiplicative constants on the molar fraction and temperature for rubber wood.

5. Assessment of the predictive capability of the optimized model

In order to establish the reliability of the optimized model as a predictive tool for the design of gasifiers, the afore described procedure is applied to predict the conversion of various biomasses characterized by a different value of the carbon content, for which experimental data relevant to released syngas composition are available in the literature. Straw paper (Ptasinski et al., 2007), rubber wood (Jayah et al., 2003), treated wood (Ptasinski et al., 2007) and sawdust (Altafini et al., 2003) are considered. In order to identify the range of variation of costKi for all the biomasses, the idea is followed to use the RSM to reconstruct the objective function representing the sum of the errors between numerical results and experimental data, relevant to each specific component of the syngas. Figure 3 represents an example of the response surface as computed for rubber wood in the plane costK2 - costK3, where it is evident that the lowest errors pertain to the values of costK3 lower than 4. The sets of constants obtained as optimal for the four considered biomasses are reported in Table 3.

Table 3: Optimal multiplicative constants for different biomasses

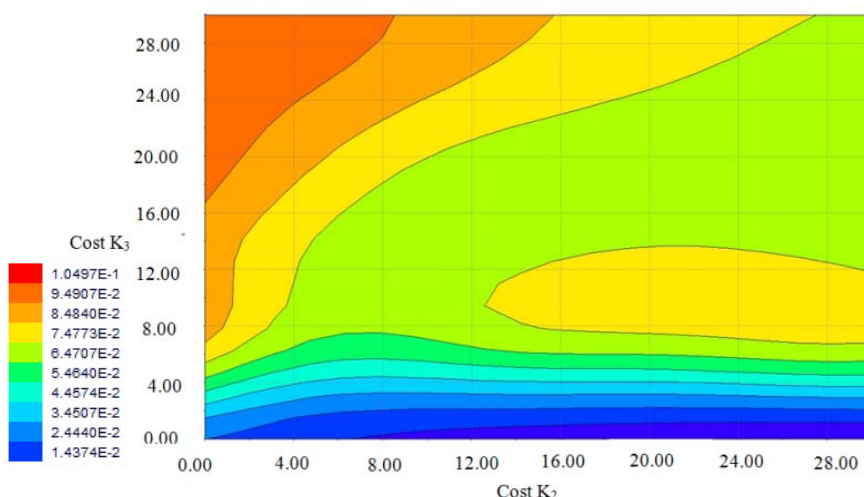| C	$costK_1$	$costK_2$	$costK_3$	Biomass	Sum errors
48.9	0.99	1.24	0.76	Straw	2.02E-03
50.6	0.58	11.9	0.02	Rubber Wood	3.54E-03
51.5	1.08	1.25	0.75	Treated Wood	6.57E-04
52	0.94	20	0.05	Sawdust	7.29E-03

Figure 3: RSM for rubber wood in the costK2 - costK3 (sum of errors)

The use of the optimal multiplicative constants, calculated through the MOGA II algorithm, improves the model prediction capability in all the cases. This is demonstrated by the lower errors obtained between the numerically predicted and the experimentally measured syngas product yields with respect to the ones obtained through the unoptimised model. The syngas composition is represented in Figure 4. The gasification temperature is reported in Figure 5.
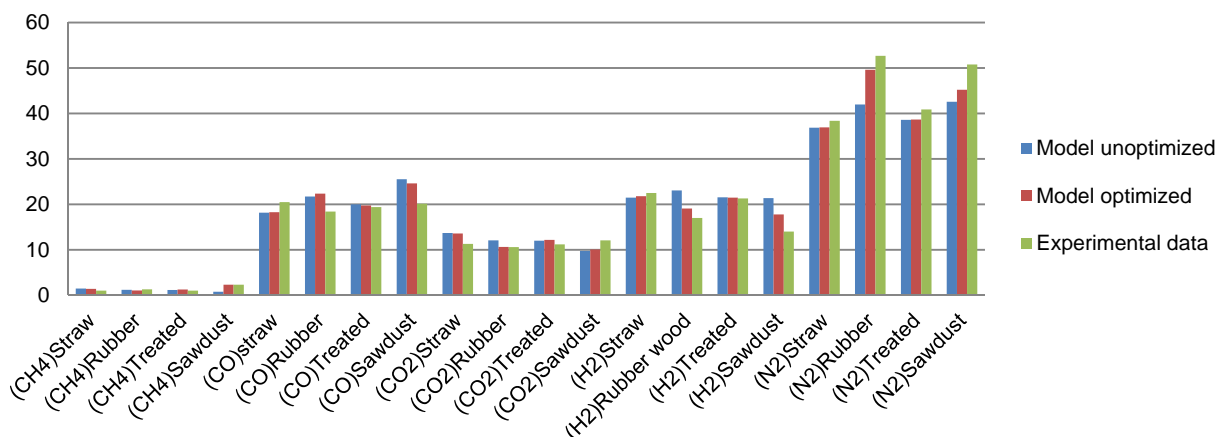

Figure 4: Gasification product yields as predicted by the unoptimized model, by the optimized model and as experimentally measured for different biomasses
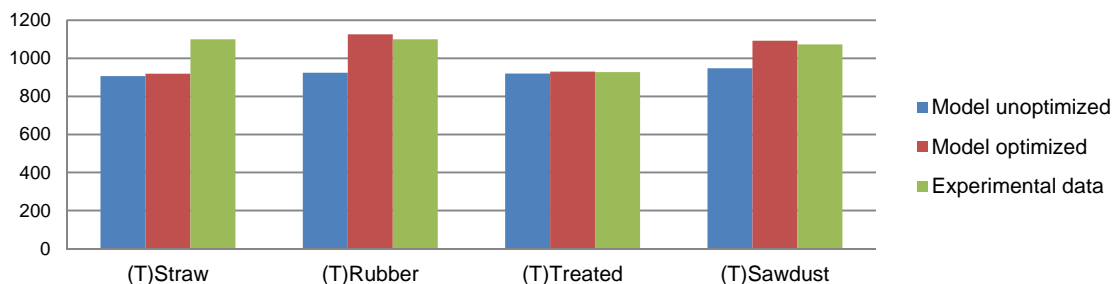

Figure 5: Gasification temperature as predicted by the unoptimized model, by the optimized model and as experimentally measured for different biomasses

The found constants of Table 3 may be not grouped in a unique triple of values suitable of being always used. In this sense, the model, even optimised, seems to fail in being predictive independently on the composition of the treated material. Nevertheless, the conducted analysis can be further extended to other kind of biomasses and may anyway may indicate a more recursive set of data, whose use can be demonstrated as leading to negligible errors also in situations where data of the correction factors different from the more recursive ones are found.

7. Conclusion

Modeling of gasification systems is today of great importance in the current research scenario in order to search for optimal methods of processing renewable energy sources. Gasification is one of the viable solution to exploit the energy content of biomasses or waste, especially as an alternative solution to landfill and for distributed power generation.
The design phase of gasifiers could be surely improved by resorting to virtual analyses based on the use of numerical methods, able to predict the system performance and trace hints regarding the best operating conditions, or even the more proper biomass to be treated to reach predefined objectives of heating value of the obtained syngas.
The present work introduces a thermo-chemical equilibrium model, accounting also for tar and char formation, and a procedure devoted to the improvement of its prediction capability. By assuming that a correction to the equilibrium constants is needed to account for the actual speed of approach to equilibrium, a multi-objective genetic algorithm is used to search for the correction factors able to reduce the error between the computed syngas composition and temperature and the available experimental data. Different biomasses are analysed.
Although a unique set of correction factors is not found, the procedure leads to quite reliable results under all the considered situations.
This effectiveness of the introduced technique would be increased by analysing a larger set of experimental data, in the attempt of individuating a relationship, if any, between the values of the corrected equilibrium constants and some relevant quantity, as may be the carbon content of the treated material. In any case, the optimised model is a reliable tool within decision making procedures aimed at dimensioning gasification systems.

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