

## ASSESSMENT OF A SIMPLIFIED EQUILIBRIUM MODEL FOR WASTE GASIFICATION

by

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*The applicability is studied of a simplified equilibrium model for prediction of the composition and quality of producer gas from gasification of different waste. A simplified equilibrium model of stoichiometric type based on system thermodynamic equilibrium has been developed in the form of a stand-alone computer application. Standard numerical methods have been implemented for solving the mathematical problem formulation. The model's predicted results have been compared with the published results for biomass and some waste types – municipal solid wastes and refuse derived fuels. Results are included for a bubbling fluidized bed and downdraft fixed bed allothermal gasification, also for catalytic supported gasification. Producer gas predictions by calibrated and non-calibrated versions of the simplified equilibrium model have been studied. The accuracy of these predictions has been evaluated. The results obtained by the simplified equilibrium model have confirmed that such model is a very useful tool for studying the gasification process for municipal solid wastes and refuse derived fuels process parameters for two mostly implemented gasifier types.*

Key words: waste, gasification, equilibrium model

### Introduction

Modern gasification reactors operate near the atmospheric pressure with or without catalytic support of the gasification process but also pressurized up to 100 bar [1]. Arena *et al.* [2] stated in their review for municipal solid waste (MSW) and refuse derived fuel (RDF) gasification that except plants from Ebara Co. and Ube Industries Ltd. for mixed plastic waste, commercial scale gasification plants are operating at atmospheric pressure. Beside updraft and downdraft fixed bed, fluidized bed reactor is common, while entrained flow reactor which operates pressurized is generally suitable only for fine particle wastes (sewage sludge) [1]. Optimizing gasification process efficiency by preheating of gasification agent is common – gasification process is called allothermal [1].

Mathematical prediction of gasification end products by model of thermodynamic system equilibrium is very useful, because it helps to show tendencies on the working parameter variations of the gasification reactor, helps to assess efficiency of fuel chemical energy (heating value) conversion, helps to find conditions for the elimination of tar and soot from producer gas and is compared to kinetic prediction models, which are useful also to optimize reactor design, independent of the gasification reactor type.

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In literature, there are two basic approaches for equilibrium gasification models: stoichiometric and non-stoichiometric or Gibbs energy minimization approach. The latter gives the possibility to include more producer gas species into consideration, is more suitable to consider higher process pressures (real gas properties instead of ideal gas), but one is faced with a more complex system of non-linear equations that has to be solved, together with much bigger solver convergence stability problems.

Ptasinski *et al.* [3] showed that chemical exergetic efficiency as ratio of heating value of producer gas convertible to (technical) work to that of the fuel is reaching highest value near the carbon boundary point (CBP). The CBP describes boundary conditions for gasification parameters at which only part of feedstock's carbon is converted to gaseous product and the rest remains in form of solid (soot) and liquid (tar) carbon in the gasification product.

Karamarković *et al.* [4] showed that, in the case of equilibrium gasification model of stoichiometric type predictions,  $\text{CH}_4$  is underestimated, and CO is overestimated, so the mathematical modeling of this models should include some form of calibration possibility to overcome this weakness.

Altafini *et al.* [5] compared results for producer gas composition obtained from experimental tests and those predicted by using an equilibrium gasification model of non-stoichiometric type with no calibration possibility. The experimental test results refer to an average of 10 tests performed at fixed bed downdraft gasifier, where sawdust of Pinus Elliotis wood of approximately 11 wt.% moisture content (MC) is gasified at the gasification temperature near 832 °C and at atmospheric pressure. The prediction refers to gasification of feedstock of 10 wt.% MC at gasification temperature of 800 °C, at atmospheric pressure and heat loss in the gasifier equals to 1% based on the higher heating value (HHV) of the feedstock. The  $\text{H}_2$  prediction is high (+42.9%) and CO prediction low (-2.2%) relative to the average experimental tests values, the  $\text{CH}_4$  prediction is nearly zero. Although the  $\text{H}_2$ -CO content in the dry base (d.b.) producer gas predicted through the model was moderate higher (+16.5%) than the average value of the experiments, the absence of  $\text{CH}_4$  and higher hydrocarbons in the prediction determines lower heating value (LHV) close to experiment values (-4.5%). The higher values reported for the producer gas yield in the model prediction determine higher cold gas efficiency (CGE) value than that of the experiments.

Zainal *et al.* [6] developed equilibrium gasification model of stoichiometric type for biomass gasification. Heat loss of the gasifier is not considered and calibration possibility of producer gas composition is not included in this model. The prediction values are compared to experimental test results for gasification of wood biomass of 20 wt.% MC at gasification temperature of 800 °C with air as gasification agent. Results show that  $\text{H}_2$  prediction by model is higher (+38.3%) and CO is moderate lower (-14.9%) than the experimental results. The  $\text{H}_2$ -CO content is predicted close to experimental results (+6.3%) while  $\text{CH}_4$  prediction value is lower than experimental results (-39.5%). The LHV prediction value for producer gas at d.b. is close to experimental value (-3.0%).

Jayah *et al.* [7] carried out experimental tests of rubber wood gasification and stated that heat loss for the updraft fixed bed reactor is between 5% and 15% of product gas enthalpy and has the greatest effect on the conversion efficiency because it lowers the reactor temperature and so reduces gasification reaction rates. So he stated that conversion efficiency of the reactor decreases approximately 11% for every 5% increase in heat loss.

The aim of this work is to develop a simplified thermodynamic equilibrium model of stoichiometric type and assess its applicability for MSW and RDF gasification's producer gas prediction. Predictions by non-calibrated and calibrated model version of the model will be

compared with experimental results for the two most implemented gasifiers – downdraft fixed bed and bubbling fluidized bed.

## Materials and methods

### Gasification model

A simplified equilibrium model of stoichiometric type has been developed for prediction of producer gas quality in the gasification process under conditions with remaining solid phase – solid carbon  $C_{(s)}$  – at and below the CBP and without solid carbon deposition – above the CBP. Air but also combinations of air with water steam or pure  $O_2$  can be considered as gasification agents in the model.

The model is based on the assumption that all the process conditions of the system are at steady-state and thermodynamic equilibrium of the system is achieved. Temperature and pressure are uniform across the observed system. Thus, the gasification reactions are regarded as completely finished. The  $N_2$  and ashes do not participate in chemical reactions. The content of sulfur is regarded as not high enough to influence the reaction and is counted as ash. The model is supposed to be valid for gasification temperatures between 800 °C and 1600 °C, and gasification pressure near to atmospheric pressure. All gases are regarded as ideal gases. Higher hydrocarbon gases are neglected, only  $H_2$ ,  $CO$ ,  $CO_2$ ,  $H_2O$ ,  $CH_4$ ,  $N_2$ , and  $C_{(s)}$  are taken into account as gasification products. The assumption of an adiabatic system is also fulfilled, but the model can be calibrated by means of including heat dissipation – heat loss of gasification reactor.

The model also has the capability of being calibrated by means of  $CH_4$  and  $CO$  content. To be able to predict allothermal gasification process outputs, additional heat supplied to the system other than by oxidation (autothermal gasification) can be considered (for example by thermal plasma torch or by gasification agent preheating).

### Modeling thermodynamic properties of predicted species

The temperature dependency of gases' specific heat capacity is calculated according to eq. (1):

$$c_{pj} = \sum_{i=1}^4 c_{pji} T^{(i-1)} \quad (1)$$

where  $c_{pj}$  is the specific heat capacity of a gas species,  $T$  [K] – the absolute temperature, and  $c_{pji}$  – the correlation coefficients obtained by Reid *et al.* [8] as presented in tab. 1. These polynomial correlations have been implemented, since they are more suitable for numerical formulation of the model.

**Table 1. Specific heat capacity correlation coefficients related to ideal gas temperature**

	$H_2$	$CO$	$CO_2$	$H_2O$	$CH_4$	$N_2$	$O_2$
$c_{pj1} [\times 10^3 \text{Jkmol}^{-1}\text{K}^{-1}]$	27.140	30.870	19.800	32.240	19.250	31.150	28.110
$c_{pj2} [\text{Jkmol}^{-1}\text{K}^{-2}]$	9.274	-12.850	73.440	1.924	52.130	-13.570	-0.004
$c_{pj3} [\text{J/kmol}^{-1}\text{K}^{-3}]$	-0.014	0.028	-0.056	0.011	0.012	0.027	0.018
$c_{pj4} [\times 10^{-6} \text{Jkmol}^{-1}\text{K}^{-4}]$	7.645	-12.72	17.15	-3.596	-11.32	-11.68	-10.65

Calculation of  $C_{(s)}$  specific heat capacity is showed by eq. (2):

$$c_{p7} = c_{p71} + c_{p72}T - c_{p73}T^{-3} \quad (2)$$

where  $c_{p7}$  is the specific heat capacity of  $C_{(s)}$ , and  $c_{p7i}$  are correlation coefficients obtained by Perry and Green [9], presented in tab. 2.

**Table 2. Specific heat capacity correlation coefficients of solid carbon**

$c_{p71} [\times 10^4 \text{ Jkmol}^{-1}\text{K}^{-1}]$	$c_{p72} [\text{Jkmol}^{-1}\text{K}^{-2}]$	$c_{p73} [\times 10^6 \text{ Jkmol}^{-1}\text{K}^2]$
1.119	10.957	489.436

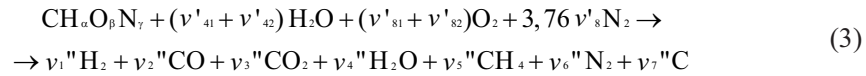
Specific heats of formation  $h_{ff}^0$  and specific Gibbs energies  $g_{ff}^0$  of species at standard pressure are obtained by Reid *et al.* [8] and presented in tab. 3.

**Table 3. Specific ideal gas standard enthalpy of formation, specific standard free Gibbs energy**

$j [-]$	CO	CO <sub>2</sub>	H <sub>2</sub> O	CH <sub>4</sub>
$j [-]$	2	3	4	5
$h_{ff}^0 [\times 10^6 \text{ Jkmol}^{-1}]$	-110.615	-393.769	242.000	-74.902
$g_{ff}^0 [\times 10^6 \text{ Jkmol}^{-1}]$	-137.400	-394.600	-228.800	-50.870

### Mathematical formulation of the model

Mathematical formulation of the model relies on three sets of equations: mass balance, thermodynamic equilibrium of the representative chemical reactions, and energy balance. A summarized reaction of gasification is presented by eq. (3):



where  $v'_j$  are stoichiometric coefficients of reactants, and  $v'_j$  the stoichiometric coefficients of gasification process products,  $v'_{41}$  is the coefficient for moisture,  $v'_{42}$  for water steam,  $v'_{81}$  for airborne and  $v'_{82}$  for pure O<sub>2</sub> as gasification agents.

Equation (4) represents the relation between stoichiometric coefficient,  $v'_{81}$ , of supplied airborne O<sub>2</sub> in the summarized reaction of gasification in connection to the equivalence ratio (ER) and hydrocarbon composition (CH<sub>α</sub>O<sub>β</sub>N<sub>γ</sub>) of dry ash free feedstock:

$$v'_{81} = ER(1 + 0.25\alpha - 0.5\beta) \quad (4)$$

Equation (5) represents the relation between stoichiometric coefficient,  $v'_{42}$ , of supplied water steam in the summarized reaction of gasification in connection to steam/fuel ratio (S/F), molar mass  $M_4$  of H<sub>2</sub>O and molar mass of the dry ash free feedstock  $M_{F\text{daf}}$ :

$$v'_{42} = S/F \frac{M_{F\text{daf}}}{M_4} \quad (5)$$

Equation (6) represents the relation between stoichiometric coefficient,  $v'_{82}$ , of supplied pure O<sub>2</sub> in the summarized reaction of gasification in connection to pure oxygen/fuel ratio (O/F), molar mass  $M_8$  of O<sub>2</sub> and molar mass of the dry ash free feedstock  $M_{F\text{daf}}$ :

$$v'_{82} = O/F \frac{M_{F\text{daf}}}{M_8} \quad (6)$$

### Mass balance

Mass balance considers atoms of C, H, O, and N from wet feedstock, gasification agent air, pure O<sub>2</sub> and water steam as presented by eqs. (7)-(13):

$$[a_{ij}][v_j''] = [b_{i0}] + [b_{i1}] + [b_{i2}] + [b_{i3}] \quad (7)$$

$$[a_{ij}] = \begin{bmatrix} 0 & 1 & 1 & 0 & 1 & 0 & 1 \\ 2 & 0 & 0 & 2 & 4 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \quad (8)$$

$$[b_{i0}] = [1, (\alpha + 2v_{31}'), (\beta + v_{41}'), 0.5\gamma]^T \quad (9)$$

$$[b_{i1}] = [0, 0, 2v_{81}', 3.76v_{81}']^T \quad (10)$$

$$[b_{i2}] = [0, 0, 2v_{82}', 0]^T \quad (11)$$

$$[b_{i3}] = [0, 2v_{42}', v_{42}', 0]^T \quad (12)$$

$$[v_j''] = [v_1'', v_2'', v_3'', v_4'', v_5'', v_6'', v_7'']^T \quad (13)$$

where  $[b_{i0}]$  is wet feedstock,  $[b_{i1}]$ ,  $[b_{i2}]$ ,  $[b_{i3}]$  are composition matrixes of the gasification agents air, pure  $O_2$ , and water steam, presented respectively, and  $[v_j'']$  is a producer gas composition matrix.

#### Thermodynamic equilibrium of representative chemical reactions

Because of different representative chemical reactions for gasification conditions above, at or below the CBP, the sets of thermodynamic equilibrium equations are different. The CBP is a condition when exactly enough gasification medium is added to avoid solid carbon formation from the gas phase (carbon saturated condition) and achieve complete gasification. Below, and at CBP, the gasification process is described by  $CH_4$  decomposition reaction (14) and eq. (17), water gas shift reaction (15) and eq. (18), and heterogeneous water gas shift reaction (16), eq. (19),



$$f_1 = \psi_1^3 \psi_2 - t_1 K_1 \psi_3 \psi_4 = 0 \quad (17)$$

$$f_2 = \psi_1 \psi_3 - t_2 K_2 \psi_2 \psi_4 = 0 \quad (18)$$

$$f_3 = \psi_1 \psi_2 - K_3 \psi_4 = 0 \quad (19)$$

$$\psi_j = \frac{v_j''}{\sum_{j=1}^6 v_j''} \quad (20)$$

where  $\psi_j$  is the mole fraction of the component in the gas phase,  $K_r$  – the temperature and pressure dependent equilibrium constant of the partial chemical reaction  $r$ ,  $t_r$  – the calibration coefficient,  $t_1$  – the reflecting underestimated  $CH_4$  prediction, while  $t_2$  – the reflecting overestimation of CO prediction.

The CBP gasification process is described by water gas shift reaction (15) and eq. (18) and  $CH_4$  formation reaction (21) and eq. (22), where  $t_4$  is reflecting underestimated  $CH_4$  prediction:



$$f_4 = \psi_5 - t_4 K_4 \psi_1^2 = 0 \quad (22)$$

Equation (23) is presenting the temperature dependency of equilibrium constant at standard pressure:

$$\ln K_r^0(T) = -\frac{\Delta G_r^0}{R_m T} \quad (23)$$

where  $R_m$  is the universal gas constant,  $K_r^0$  – the temperature dependent equilibrium constant at standard pressure,  $v_{rj}'$  and  $v_{rj}''$  are stoichiometric coefficients of products and reactants for the representative reaction  $r$ , respectively,  $\Delta G_r^0$  – the total Gibbs energy at standard pressure of the system for the observed partial gasification reaction given by eq. (24):

$$\Delta G_r^0 = \sum (v_{rj}'' - v_{rj}') g_{r,j}^0 + \sum (v_{rj}'' - v_{rj}') R_m T \ln \left[ \frac{(v_{rj}'' - v_{rj}')}{\sum (v_{rj}'' - v_{rj}')} \right] \quad (24)$$

which have to be solved for unknown values  $v_j$  to minimize  $\Delta G_r^0$ .

Equation (25) is presenting the pressure dependency of equilibrium constant  $K_r$ :

$$K_r = K_r^0 \left( \frac{p}{p_0} \right)^{\sum (v_{rj}'' - v_{rj}')} \quad (25)$$

where  $p$  is gasification pressure and  $p_0$  is standard pressure.

#### Energy balance

Equation (26) shows the energy balance for the reacting system under the assumption that the moisture of the waste is of standard temperature:

$$H_R + Q_{sup} - Q_{diss} = H_P \quad (26)$$

where  $H_R$  is the enthalpy of reactants,  $Q_{sup}$  – the heat supplied to the system (for instance: by plasma gasification),  $Q_{diss}$  – the heat dissipation (loss) of the gasification reactor, and  $H_P$  – the enthalpy of the producer gas.

Equation (27) presents the estimation of  $H_R$ :

$$H_R = H_{f,F}^0 + v_{41}' h_{f,41}^0 + v_{42}' \left( h_{f,4}^0 + \int_{T_0}^{T_{42}} c_{p,4} dT \right) + v_{81}' \int_{T_0}^{T_{81}} (3.76c_{p,6} + c_{p,8}) dT + v_{82}' \int_{T_0}^{T_{82}} c_{p,8} dT \quad (27)$$

where  $h_{f,41}^0$  is the heat of formation at standard pressure for liquid water (moisture),  $T_{42}$ ,  $T_{81}$ , and  $T_{82}$  are temperatures of the gasification agents steam, air and pure  $O_2$ .

The  $H_{f,F}^0$  is the heat of the formation for feedstock, estimated as described in eq. (28):

$$H_{f,F}^0 = LHV_F + h_{f,3}^0 + 0.5 \cdot \alpha \cdot h_{f,4}^0 \quad (28)$$

where  $LHV_F$  is the low heating value for feedstock estimated with equation by Channivala and Parikh [10], and  $h_{f,3}^0$  and  $h_{f,4}^0$  are heats of formation at standard pressure for CO and  $H_2O$  in the gaseous phase.

Equation (29) presents the equation for calculation of the enthalpy of the producer gas, where  $h_{f,j}^0$  are standard heats of formation for gaseous species:

$$H_R = v_2'' h_{f,2}^0 + v_3'' h_{f,3}^0 + v_4'' h_{f,4}^0 + v_5'' h_{f,5}^0 + \sum_{j=1}^7 \int_{T_0}^T v_j'' c_{p,j} dT \quad (29)$$

Equation (30) presents the equation for calculation of CGE, where LHV is for d.b. producer gas and  $V$  is d.b. producer gas yield:

$$CGE = \frac{LHV \cdot V}{LHV_F} \quad (30)$$

### Numerical formulation of the model

For solving the system of equations, numerical methods have been implemented, including the Newton Raphson for a system of non-linear equations according to eqs. (31) and (32).

$$\begin{bmatrix} \frac{\partial f_1(k)}{\partial \psi_2} & \frac{\partial f_1(k)}{\partial \psi_5} & \frac{\partial f_1(k)}{\partial v_7''} \\ \frac{\partial f_2(k)}{\partial \psi_2} & \frac{\partial f_2(k)}{\partial \psi_5} & \frac{\partial f_2(k)}{\partial v_7''} \\ \frac{\partial f_3(k)}{\partial \psi_2} & \frac{\partial f_3(k)}{\partial \psi_5} & \frac{\partial f_3(k)}{\partial v_7''} \end{bmatrix} \begin{bmatrix} \Delta\psi_2 \\ \Delta\psi_5 \\ \Delta v_7 \end{bmatrix} = \begin{bmatrix} f_1(k) \\ f_2(k) \\ f_3(k) \end{bmatrix} \quad (31)$$

$$\begin{aligned} \psi_2(k+1) &= \psi_2(k) + \Delta\psi_2 \\ \psi_5(k+1) &= \psi_5(k) + \Delta\psi_5 \\ v_7(k+1) &= v_7(k) + \Delta v_7 \end{aligned} \quad (32)$$

For better convergence, an initial guess has been set according to eqs. (33)-(35):

$$\psi_2(0) = \frac{0.5}{0.5\gamma + 3.7619 v_7'' + 1} \quad (33)$$

$$\psi_5(0) = 0 \quad (34)$$

$$v_7''(0) = 0 \quad (35)$$

### Overall assessment layout

Five scenarios have been established for testing the applicability of the simplified equilibrium model. Gasification of two waste materials have been observed: MSW and RDF.

*Scenario I* is set to compare the un-calibrated model predictions and experimental results for allothermal MSW gasification with and without catalytic support by Zhao *et al.* [11]. Experimental gasification has been performed by the fixed bed downdraft gasifier with air as the gasification agent. As allothermal conditions are not documented, gasification is predicted as autothermal.

*Scenario II* is modified *Scenario I*. Gasification is predicted as allothermal by non-calibrated model.

In *Scenario III* the model is separately calibrated to alothermic gasification with and without catalytic support and predictions are compared to the same experimental results as in *Scenario I* and *Scenario II*.

*Scenario IV* examines the non-calibrated model prediction by experimental data results for allothermal RDF gasification with stronger and weaker catalytic support by Arena *et al.* [12]. Experimental gasification has been employed by using the fluidized bed gasifier with preheated air as the gasification agent.

*Scenario V* examines the calibrated model prediction by the same experimental data results for allothermal RDF gasification with stronger catalytic support compared to *Scenario IV*.

But, at first, the model was compared to published equilibrium model for autothermal gasification of biomass feedstock presented by Jarungthammacote and Dutta [13]. The model was calibrated to the same gasification experimental results as compared model, then calibration coefficients and predicted results have been compared with both models.

### The feed material

Three kinds of feedstock have been selected to perform this study: MSW and RDF materials for model assessment scenarios and rubber wood for comparison with referenced model.

The MSW feedstock has been selected to perform model assessment for the *Scenarios I-III*. Fraction composition of material is presented in tab. 4 ultimate composition on d.b. is presented in tab. 5 and MC of material is 40.1 wt.% on as received base (*a.r.*) as obtained by Zhao *et al.* [11].

Waste composition of RDF1 and RDF2 feedstock's published by Arena *et al.* [12] is selected for the simulation *Scenario IV* and *Scenario V*. These RDF materials originates from MSW and household packaging waste with low MC content. Ultimate analysis these materials is presented in tab. 5 on d.b. MC of RDF1 is 1.3 wt.% and of RDF2 is 2.0 wt.% on *a.r.* base reported.

**Table 4. Fraction composition of MSW [wt.%]**

Feedstock	Paper	Plastics	Wood	Kitchen garbage	Textile	Rubber
MSW	23.0	20.4	9.2	42.2	4.0	1.2

**Table 5. Ultimate analysis of MSW [wt.%]**

Feedstock	Ultimate analysis [wt. %]					
	C	H	O	N	S	Ash
MSW	55.6	9.7	28.3	0.9	0.2	4.3
RDF1	85.0	13.8	0.0	0.0	0.0	1.2
RDF2	68.1	10.2	14.3	0.0	0.1	7.3
Rubber wood	50.6	6.5	42.0	0.2	0.0	0.7

Rubber wood as feedstock has been selected to validate both – this model and referenced model versus experimental results. Ultimate analysis of this feedstock is presented in tab. 5 on the basis of dry ash free (d.a.f) material., MC of material is 13.8 wt.% on *a.r.* base as reported by Jayah *et al.* [7].

### Assessment of modeled predictions

The model developed for this study was tested by comparing the prediction results with published experimental data from other researchers.

The error in this comparison for the producer gas composition is estimated by the root mean square (RMS), defined as shown in eq. (36):

$$RMS_{comp} = \sqrt{\frac{\sum_1^N (Exp. - Mod.)^2}{D}} \quad (36)$$

where *Exp* is the value from the experimental results, *Mod* – the predicted value from the model, and *D* – the number of data.

## Results

### Model validation with wood fuel

The producer gas composition system analysis for wood feedstock [7] has yielded that gasification is conducted above the CBP, so solid carbon is not considered in the prediction. Tables 6 and 7 present validation data for 7 runs: run R1 is experimental for a downdraft fixed bed

**Table 6. The ER [-] and gasification temperature [°C], d.b. producer gas composition [vol.%], LHV [MJNm<sup>-3</sup>] and gas yield on as received base feedstock [Nm<sup>3</sup>kg<sup>-1</sup>]**

Run	ER [-]	T [°C]	H <sub>2</sub> [vol.%]	CO [vol.%]	CO <sub>2</sub> [vol.%]	CH <sub>4</sub> [vol.%]	LHV [MJNm <sup>-3</sup> ]	V [Nm <sup>3</sup> kg <sup>-1</sup> ]	RMS <sub>comp.</sub> [vol.%]
R1	0.36	827	17.0	18.4	10.6	1.3	4.23	2.56	-
R2	0.44	827	18.0	17.9	11.8	0.1	3.57	2.66	0.9359
R3	0.36	827	21.0	22.7	9.4	0.2	4.53	2.94	3.8247
R4	0.42	827	17.9	19.5	10.9	0.1	3.76	3.12	0.9757
R5	0.42	827	16.8	17.9	12.1	1.1	3.72	2.56	0.7668
R6	0.34	827	19.5	22.9	9.8	1.6	4.83	2.78	3.7277
R7	0.40	827	16.4	19.5	11.2	1.3	3.98	2.96	0.7925
R8	0.36	827	18.9	21.5	10.4	1.3	4.51	2.86	2.6944



lab-scale gasifier as presented in the reference [7], runs R2 and R5 are reference non-calibrated and calibrated models' predictions by Jarungthammacote and Dutta [13], while runs R3, R4 are non-calibrated and R6, R7, R8 calibrated predictions of this model.

As the gasification temperature has been maintained at the level of experimental run R1, the ER value for all runs of this model comply better with the experiment than the reference model. The ER of R7 – the best prediction by this model is slightly over predicted (within 11%) which is acceptable when taking into account real circumstances (uptight gasifier, introduction of air with feedstock stream) as reported by del Alamo *et al.* [14]. As in the reference model, gasifier heat losses were not presented, although this model has considered it for runs R4, R7 with 5% and R8 with 1.5% of feedstock LHV – that is why, in this cases, the predicted producer gas LHV was slightly lower but for the calibrated model is suited well with the experimental results. For reference, this non-calibrated model CH<sub>4</sub> prediction is under estimated, and originated from a model which has not considered chemical kinetics. The RMS for producer gas composition was low, similar to referenced model and improved by model calibration. The prediction results for runs R6-R8 showed that by calibrating model by means of CH<sub>4</sub> and CO content as gasification temperature is maintained constant, ER, heat loss of gasification reactor or both have to be adjusted – calibrating has impact on energy balance calculation. Hence when experimental results are known and heat loss of gasification reactor or heat supplied for allothermal gasification are unknown, they could be predicted by the model calibration. Also for every new heat loss or heat supplied values new calibration coefficients are needed.

**Table 7. Gasification process heat loss [MJkg<sup>-1</sup>], model calibration coefficients, RMS producer gas composition error [vol.%]**

Run	$Q_{diss}$ [MJkg <sup>-1</sup> ]	$t_4$ [-]	$t_2$ [-]	$RMS_{comp.}$ [vol.%]
R2	0.00	1.0	1.0	0.9359
R3	0.00	1.0	1.0	3.8247
R4	0.98	1.0	1.0	0.9757
R5	0.00	0.91	11.28	0.7668
R6	0.00	0.91	11.28	3.7277
R7	0.98	0.98	13.50	0.7925
R8	0.31	0.98	10.00	2.6944

### Model simulation with MSW – Scenarios I-III

Tables 8 and 9 presents gasification data for *Scenario I-III*. Predicted results have been compared to experimental results by Zhao *et al.* [11]. The experiment has been set on laboratory scale downdraft fixed bed gasifier to examine influence of hot slug from refining processes of iron

**Table 8. The ER [-], gasification temperature [°C], d.b. producer gas composition [vol.%], LHV [MJNm<sup>-3</sup>] and gas yield on d.b. [Nm<sup>3</sup>kg<sup>-1</sup>],**

Run	ER [-]	T [°C]	H <sub>2</sub> [vol.%]	CO [vol.%]	CO <sub>2</sub> [vol.%]	CH <sub>4</sub> [vol.%]	LHV [MJNm <sup>-3</sup> ]	V [Nm <sup>3</sup> kg <sup>-1</sup> ]
R9	0.31	800	14.8	17.5	19.0	0.5	3.98	2.00
R10	0.31	800	15.8	27.5	11.0	2.3	5.99	1.62
R11	0.43	800	22.8	12.8	11.3	0.2	4.15	2.73
R12	0.31	800	30.9	17.2	9.5	0.4	4.48	2.27
R13	0.31	800	30.1	18.0	8.8	0.5	4.48	2.24
R14	0.31	800	19.9	29.0	0.2	2.2	4.44	1.96
R15	0.31	900	12.2	24.0	12.8	0.5	4.52	2.27
R16	0.31	900	27.5	31.0	5.8	3.0	7.95	1.66
R17	0.48	900	19.7	13.0	10.6	0.1	3.79	2.79
R18	0.31	900	30.5	19.0	8.2	0.2	4.48	2.25
R19	0.31	900	28.3	21.3	6.3	0.5	4.47	2.29
R20	0.31	900	20.3	25.6	2.8	2.9	4.38	1.96

steel on gasification of MSW. This experimental results showed that this hot slug consisting of 42.5 wt.% CaO, 11.3 wt.% Al<sub>2</sub>O<sub>3</sub>, 8.3 wt.% MgO, 35.4 wt.% SiO<sub>2</sub>, 1.2 wt.% Fe, and 0.7 wt.% S, had catalytic effect on MSW gasification. For all experimental runs gasification agent is preheated air. In case of experimental runs R10 and R16 before examining its composition producer gas is passing over hot slag at gasification temperature 800 °C and 900 °C, while for runs R9 and R15 producer gas of the same gasification temperatures is not in contact with hot slag. The experimental runs R10 and R16 are regarded as allothermal gasification with and experimental runs R9 and R15 without catalytic support.

**Table 9. Gasification process heat loss [MJkg<sup>-1</sup>], model calibration coefficients, RMS producer gas composition error [vol.%]**

Run	$Q_{\text{sup}}$ [MJkg <sup>-1</sup> ]	$t_4$ [-]	$t_2$ [-]	$RMS_{\text{comp}/1}$ [%]	$RMS_{\text{comp}/2}$ [%]
R11	0	1.0	1.0	8.4834	5.7890
R12	1.810	1.0	1.0	8.2695	8.8091
R13	1.810	1.35	0.82	–	8.5993
R14	1.810	15.00	0.01	5.7236	–
R17	0	1.0	1.0	14.0535	6.6251
R18	2.025	1.0	1.0	7.1409	9.5047
R19	2.025	3.50	0.55	–	8.4423
R20	2.025	45.00	0.10	8.2037	–

Prediction runs R11 and R17 by non-calibrated model for autothermal gasification are set for *Scenario I*. To achieve the same gasification temperature as by experimental runs ER is adjusted. Runs R12 and R18 are non-calibrated model predictions for *Scenario II*. The ER is kept at same level as experimental runs. Targeted gasification temperature of experimental runs has been adjusted by the variation of the heat supplied to the system. Runs R13, R14, R19, and R20 are predictions by calibrated model for *Scenario III*. For all this prediction runs ER and supplied heat to the system are kept at level as established in *Scenario II*. Model calibration by means of CH<sub>4</sub> and CO content has been made to approach catalytic supported gasification for R14 and R20 and to approach gasification without catalytic support for R13 and R19. The  $RMS_{\text{comp}/1}$  is estimated for comparison to catalytic supported gasification experimental values.

#### **Model simulation with RDF – Scenarios IV and V**

Table 10 presents data for RDF gasification for *Scenario IV* and *Scenario V*. The experiment has been set by bubbling fluidized bed gasifier as reported by Arena *et al.* [12] for two different RDF materials. Gasification agent air has been preheated at 600 °C. Influence of the bed material olivine, a nesosilicate of iron and magnesium, on gasification process has been originally studied and catalytic effect for gasification of material RDF1 has been confirmed but is less influential for RDF2. This has been explained by active role of magnesium and inhibited effect of iron for RDF2 gasification experiment [12]. Thus, experimental run R21 for RDF1 is regarded as allothermal gasification with support of catalytic effect. No solid carbon presence in producer gas is reported for this experimental run. Experimental run R26 for RDF2 is regarded as allothermal gasification without catalytic support. Beside higher hydrocarbons presence of 99 g/Nm<sup>3</sup> solid carbon in producer gas on d.b. is reported. For *Scenario IV* experimental runs R21 and R26 are compared respectively with this non-calibrated model's prediction runs R22 and R27.

For *Scenario V* predictions R23, R24, and R25 by calibrated model are performed to be compared to allothermal gasification with catalytic support of experimental run R21. For R23

and R24 same calibration coefficients have been employed as for R14 (similar gasification temperature) – 15.00 for CH<sub>4</sub> and 0.01 for CO but heat loss is for R23 not regarded and for R24 heat loss value is set at 1.85 MJ/kg to get same gasification temperature as in experimental run. For R25 run new calibration coefficients have been employed –7.50 for CH<sub>4</sub> and 1.00 for CO and heat loss 1.00 MJ/kg.

**Table 10. The ER [-], gasification temperature [°C], d.b. producer gas composition [vol.%], LHV [MJ/Nm<sup>3</sup>], producer gas yield [Nm<sup>3</sup>/kg], RMS [vol. %]**

Run	ER [-]	T [°C]	H <sub>2</sub> [vol. %]	CO [vol. %]	CO <sub>2</sub> [vol. %]	CH <sub>4</sub> [vol. %]	C <sub>n</sub> H <sub>m</sub> [vol. %]	LHV [MJNm <sup>-3</sup> ]	V [Nm <sup>3</sup> kg <sup>-1</sup> ]	RMS <sub>comp</sub> [vol. %]
R21	0.28	816	27.1	20.1	1.7	2.1	0.5	6.50	5.65	–
R22	0.28	818	28.4	29.2	0.2	0.4	–	7.06	5.72	4.7395
R23	0.28	936	26.6	26.6	0.2	1.8	–	7.10	5.64	3.1300
R24	0.28	816	22.9	26.3	0.2	3.5	–	7.15	5.37	3.2275
R25	0.28	818	25.8	28.0	0.1	2.1	–	7.11	5.53	3.8114
R26	0.22	869	6.8	3.7	11.1	7.3	4.8	6.80	2.65	–
R27	0.28	800	13.8	18.2	7.6	0.4	–	3.46	3.27	7.9775

## Analysis

### Model simulation with MSW – Scenario I-III

Model prediction data for gasification without catalytic support is regarded as autothermal (*Scenario I*) shows that ER is high over predicted (within 55% of experimental value). The d.b. producer gas LHV prediction is improved (moderate over prediction within 13%) if allothermal gasification conditions are considered (*Scenario II* and *Scenario III*). The same trend is showed for d.b. producer gas yield (moderate over prediction within 12%) and CGE (moderate over prediction within 26%). Thus, for this parameters calibration of the model is not needed, but allothermal gasification is to consider.

Analysis of model prediction data for catalytic supported gasification regarded as autothermal (*Scenario I*) has again showed high over predicted ER (within 55%). The d.b. producer gas LHV prediction is better for allothermal gasification conditions (*Scenario II* and *Scenario III*) if compared to *Scenario I*, but is high underestimated for both of these scenarios (within 45%) compared to experimental values. When model is calibrated (*Scenario III*) producer gas yield prediction is improved (prediction covered within 2%) but it makes no considerable improvement of CGE prediction which is still high under predicted (within 35%). Despite more effort needed to find new calibration coefficients, *Scenario III* should be recommended.

Comparison of producer gas composition RMS for gasification without catalytic effect showed that model calibration (*Scenario III*) has little impact on producer gas composition prediction improvement (within 8.8 vol.% before and 8.6 vol.% after calibration). For catalytic supported gasification this effect is showed more significant (within 14.1 vol.% before and 8.2 vol.% after calibration).

The H<sub>2</sub> is very high over predicted for all scenarios and both gasification types. Similarly, CO is high under predicted for *Scenario II* (within 37%), but for *Scenario III* the predictions are moderate (within 20%). The CH<sub>4</sub> prediction is for catalytic supported gasification strong under predicted and model calibration – *Scenario III* is recommended. Hence by model calibration CO (within 20%) and CH<sub>4</sub> predictions are better but this is not true for H<sub>2</sub> and composition RMS.

### **Model simulation with RDF - Scenario IV and Scenario V**

For the catalytic supported allothermal gasification of *Scenario IV*  $H_2$  prediction is close to experimental value (over predicted within +5%), the CO is moderately over predicted (within 22%), but  $CH_4$  is significantly under predicted. The LHV prediction value is slightly overestimated (within 9%), the producer gas yield prediction is covered by the experimental run (within 1%) and the CGE prediction is slightly overestimated (within 10%). Thus, catalytic supported RDF allothermal gasification by bubbling fluidized bed gasifier is well covered by non-calibrated model.

If allothermal gasification of *Scenario IV* is weakly catalytic supported,  $H_2$  and CO prediction are strongly overestimated, while  $CH_4$  is also strong underestimated. Beside tar there are higher hydrocarbons present in higher amount in the experimental run for RDF<sub>2</sub> but they are not included into this prediction model. This experimental composition has attributed to missing catalytic effect of iron. Magnesium and iron activate endothermic decomposition reactions of hydrocarbon fragments produced by thermal cracking reactions which are first precursors of tar formation. Magnesium catalytically enhances dehydrogenation and isomerization reactions of fragments which are running in olivine bed while iron catalytically assists the dehydrogenation and carbonization reactions running on iron fines entrained in producer gas flow. If iron catalytic activity is missing the tar formation is not inhibited and unsaturated hydrocarbons with two or three carbon atoms are still formed by remaining catalytic activity of magnesium. For RDF<sub>2</sub> feedstock iron fines are not leaving olivine bed material as reported by Arena *et al.* [12].

The value of 86 g/Nm<sup>3</sup> for solid carbon is slightly under predicted (within 13%). The difference lies in lower content of predicted other hydrocarbon gas species. The LHV prediction is underestimated (within 50%) again because of the presence of higher hydrocarbon species in experimental producer gas. The producer gas yield prediction is overestimated (within 23%) and CGE prediction is underestimated (within 38%). Predicted ER is higher and gasification temperature is underestimated. Hence for weakly catalytic supported RDF allothermal gasification by bubbling fluidized bed gasifier non-calibrated model is good tool for solid carbon prediction, but less for producer gas yield and CGE. Analysis for *Scenario V* showed that the best calibration was R25. Despite the fact that RMS for R23 was best, existing calibration coefficients were used (from *Scenario III*) but gasification temperature prediction was worse. There was no improvement for predictions of  $H_2$ , CO, LHV or producer gas yield except for CGE, which was now covered by experimental value (within 2%) and new exact value for  $CH_4$ . On other hand new calibration coefficients are needed. Hence for catalytic supported RDF allothermal gasification by bubbling fluidized bed gasifier hence calibration of the model makes no sense.

### **Conclusions**

This simplified equilibrium model is set for determining producer gas composition, LHV and gas yield prediction for MSW and RDF gasification reactors working at autothermal and also at allothermal conditions. The model is independent from individual gasification reactor geometry as it is of a zero-dimensional approach. The gasification temperature range is set from 800 °C to 1600 °C as at that values the gasification reactions are fast enough to be regarded as completed. Solid carbon and only simple gas species with no higher hydrocarbon gases in the producer gas prediction are included. This model is aimed to be used near to atmospheric pressure as predicted gas species are regarded as ideal gases and mostly MSW and RDF full scale gasification reactors are of fixed bed or fluidized bed type working around this pressure.

Gasification of MSW without catalytic support by fixed bed downdraft gasifier is well covered by non-calibrated model and no calibration is needed. For MSW catalytic supported gasification calibration of the model is of benefit. Catalytic supported RDF allothermal

gasification by bubbling fluidized bed gasifier is well covered by non-calibrated model. There was no improvement for predictions of  $H_2$ , CO, LHV or producer gas yield except for CGE, but new calibration coefficients were needed for catalytic supported RDF allothermal gasification by bubbling fluidized bed gasifier calibration of the model makes no sense. For weakly supported RDF allothermal gasification by bubbling fluidized bed gasifier non-calibrated model is good tool for solid carbon prediction, but less for producer gas yield and CGE prediction.

This simplified equilibrium model is useful tool to optimize process working parameters and adopt them to the actual waste composition, expected producer gas quality by further application (for chemicals or energy recovery applications), solid carbon elimination. It helps to analyze trends of gasification process influencing parameters, to identify allothermal or autothermal nature of gasification, to predict supply energy needed for allothermal gasification as also to identify presence of catalytic effects in gasification process. This model has also possibility to be adapted to individual gasification reactor by including its heat loss and calibrating producer gas composition to the  $CH_4$  and CO fraction value of experimental runs at desired gasification temperature and external supplied energy in case of allothermal gasification.

As gasification also takes pressurized for other feedstock materials further work should include assessment of the model for higher gasification pressures, also for some waste materials capable to be delivered as fine particles feedstock. Investigation could include modification and assessment of this model if the gas species are regarded on real gases law It would be useful to assess model also for some other gasification reactor types, especially those which implement allothermal gasification. As allothermal gasification calibration coefficients are depended on gasification temperature and external supplied energy, work on gasification reactor type calibration coefficient maps could be also of benefit. While this model has possibility to predict gasification where beside air as gasification agent also steam or pure oxygen is included, further work could include also assessment of that model for that combinations.

## Nomenclature

$CGE$	– cold gas efficiency [–]	$Q_{diss}$	– heat dissipation (loss) of the reactor [MJ kg <sup>-1</sup> ]
$ERE$	– equivalence ratio [–]	$Q_{sup}$	– heat supplied to the system [MJ kg <sup>-1</sup> ]
$\Delta G_r^\circ$	– total Gibbs energy for partial chemical reaction at standard pressure [MJ kmol <sup>-1</sup> ]	$R_m$	– universal gas constant [kJ kmol <sup>-1</sup> K <sup>-1</sup> ]
$g_f^\circ$	– specific Gibbs energy at standard pressure [MJ kmol <sup>-1</sup> ]	$S/F$	– water steam / fuel ratio [kg/kg]
$h_f^\circ$	– specific heat of formation at standard pressure [MJ kmol <sup>-1</sup> ]	$T$	– temperature [K]
$H_{f,F}^\circ$	– heat of the formation for fuel [MJ kmol <sup>-1</sup> ]	$t_r$	– equilibrium constant of partial chemical reaction calibration coefficient [–]
$c_p$	– specific heat [kJ kmol <sup>-1</sup> K <sup>-1</sup> ]	$V$	– volume of recovered dry producer gas [Nm <sup>3</sup> kg <sup>-1</sup> ]
$f$	– function of balance [–]	<i>Greek symbols</i>	
$H_p$	– enthalpy of products [MJ kmol <sup>-1</sup> ]	$\alpha$	– hydrogen content of feedstock [–]
$H_r$	– enthalpy of reactants [MJ kmol <sup>-1</sup> ]	$\beta$	– oxygen content of feedstock [–]
$K_r$	– equilibrium constant of partial chemical reaction [–]	$\gamma$	– nitrogen content of feedstock [–]
$LHV_{dry}$	– low heating value of dry producer gas [MJ Nm <sup>-3</sup> ]	$\nu$	– stoichiometric coefficient [kmol]
$LHV_f$	– low heating value of feedstock [MJ kmol <sup>-1</sup> ]	$\Psi$	– mole fraction [–]
$LHV$	– low heating value [MJ kg <sup>-1</sup> ]	<i>Subscripts</i>	
$HHV$	– high heating value [MJ kg <sup>-1</sup> ]	$i$	– index
$MC$	– moisture content [wt.%]	$J$	– index of component
$O/F$	– pure oxygen / fuel ratio [kg/kg]	$r$	– index of partial chemical reaction
$p$	– pressure [bar]	“	– product
$p_0$	– standard pressure [bar]	<i>Superscripts</i>	
		‘	– reactant

*Acronyms*

$C_{(s)}$	– solid carbon	d.b.	– dry base
CBP	– carbon boundary point	ER	– equivalence ratio
$CH_aO_bN_c$	– hydrocarbon fuel, composed of carbon, hydrogen, oxygen and nitrogen	MSW	– municipal solid waste
d.a.f.	– dry ash free	RDF	– refuse derived fuel

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