ISSN 2004-2965 Energy Proceedings, Vol. 21, 2021

International Conference on Applied Energy 2021
Nov. 29 - Dec. 5, 2021, Thailand/Virtual
Paper ID: 443

Zero-Dimensional Kinetic Model for Biomass Gasification Suitable for Both Fixed and Fluidized Bed Reactors

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ABSTRACT

A zero-dimensional (0D) kinetic model for biomass gasification is here presented for the estimation of the resulting syngas composition and chemical properties. It is based on the description of the surface reactions kinetics taking place in the char reduction area. This model is enriched by an appropriate kinetics for the prediction of the TAR moles in the synthesis gas and by an energy balance equation between reactant species and products to predict the gasification temperature. Although it has been first developed for fixed bed downdraft reactors, it has also been validated for fluid bed reactors after an appropriate calibration of the residence time. The model well reproduces the measured trends, with an overall error lower than 12%.

Keywords: Gasification, Numerical Modelling, Fixed Bed, Fluidized Bed, Kinetics.

NOMENCLATURE

Abbreviations	
0D	Zero Dimensional
ER	Equivalence Ratio
LHV	Lower Heating Value
Symbols	
y, w, z, x_i	Moles of O_2, N_2, H_2O and of i_{th} specie
α, β	Biomass H/C and the O/C ratio
λ	H_2O/CO_2 formation ratio
M_{TAR}	Moles of TAR
ν	Net Reaction Rate
K_{pi}	Equilibrium constant of i_{th} reaction
k_{ai}	Apparent rate constant of i_{th} reaction
ρ_c	Carbon Density
$d_{p,c}$	Equivalent diameter of char particle
P_x	Partial pressure
T	Gaseous temperature
C	Carbon
CO_2	Carbon Dioxide
H_2O	Water Vapor
CO	Carbon Monoxide
H_2	Hydrogen
CH_4	Methane
N_2	Nitrogen

1. INTRODUCTION

Biomass gasification is a sustainable process to produce a gaseous fuel (syngas) that can be exploited for energy purposes. It has unquestionable environmental advantages as regards the development of waste conversion systems and does not contribute to the accumulation of greenhouse gases (GHGs) in the atmosphere [1]. Moreover, the valorization of residuals for energy purposes is a viable opportunity in decentralized zones, ensuring benefits on air quality, rational use of resources, and autonomy of operation with respect to the centralized energy infrastructure [2].

The thermochemical conversion through gasification can be practiced in fixed bed gasifiers, where distinctive consequential conversion processes take place, as drying, pyrolysis, combustion and char reduction, or in fluidized bed gasifiers characterized by a bed of granular solid kept in semi-suspended condition (fluidized state) by insufflating air. Here, an excellent mixing and temperature uniformity is achieved, reducing the risk of biomass agglomeration. All conversion processes take place simultaneously, with a gas residence time in the system shorter than in fixed bed gasifiers [3].

Selection and peer-review under responsibility of the scientific committee of the 13_{th} Int. Conf. on Applied Energy (ICAE2021).

However, given the extreme sensitivity that characterizes the gasification process to several operative parameters (mostly particle size, moisture and ash content of the materials to be processed), the development of validated numerical models is an effective approach to predict the gasification yields in reduced times and costs. Within the scientific literature, 0D models are the most followed numerical approaches [4, 5], as they are characterized by high simplicity and easily achievable solutions.

Wang and Kinoshita [6] developed a zero-dimensional model of biomass gasification based on the surface reactions kinetic approach to predict the gasification yield in fluidized bed reactors. In the specific, the evolution of the overall biomass gasification process was controlled by the kinetics of the char reduction reactions, these lasts assumed slower with respect to those characterizing the pyrolysis. Therefore, the concentration of volatiles and char, classified as the only products of pyrolysis, were estimated and used as initial conditions in the char reduction region simulated by the kinetic model [6]. However, this model required the residence time, the bed temperature and the Equivalence Ratio (ER) imposed as input values. These parameters can be easily derived when considering gasification in fluidized bed reactors.

A novel and improved version of this kinetic model is here presented where the syngas composition, heating value and the temperature characterizing the biomass gasification process are estimated *a priori* through an iterative procedure, thus leading to a more general formulation suitable to be applied to both fixed bed and fluidized bed reactors, after a proper calibration of the residence time.

2. MATERIALS AND METHODS

The general equation assumed for biomass gasification is:

$$CH_\alpha O_\beta + y\cdot O_2 + z\cdot N_2 + w\cdot H_2O = x_1\cdot C + x_2\cdot H_2 + x_3\cdot CO + x_4\cdot H_2O + x_5\cdot CO_2 + x_6\cdot \mathrm{CH}_4 + x_7\cdot N_2 + x_8\cdot \mathrm{TAR} \qquad (1)$$

where $CH_\alpha O_\beta$ is the chemical representation of biomass, while y, z, w and x_i are the moles of the various components. The subscripts α and β respectively express the biomass hydrogen-to-carbon and the oxygen-to-carbon ratio accordingly with the ultimate analysis of the processed feedstock.

The moles of the reactants species resulting from pyrolysis and entering the char reduction zone can be estimated through the following equations:

$$x_2 = 0;\ x_3 = 0;\ x_7 = z; \qquad (2 - 4)$$

$$x_1 + x_5 + x_6 + 6\cdot x_8 = 1; \qquad (5)$$

$$2\cdot x_4 + 4\cdot x_6 + 6\cdot x_8 = \alpha + 2\cdot w; \qquad (6)$$

$$x_4 + 2\cdot x_5 = 2\cdot y + \beta + w; \qquad (7)$$

$$x_4 = \lambda\cdot x_5 + w; \qquad (8)$$

where λ denotes the water vapor/carbon dioxide formation ratio, assumed equal to the unity in this study [6]. The moles of TAR are estimated through the following temperature-dependent relationship [7]:

$$x_8 = 0.036\cdot \mathrm{e}(-0.003\cdot \mathrm{T})/\mathrm{M_{TAR}}; \qquad (9)$$

where M_{TAR} is the molecular weight of the benzene molecule while T represent the mixture temperature expressed in Kelvin. The set of equations (2 – 9) is solved through the Newton – Rhapson algorithm.

The modelled reactions characterizing the char reduction zone are the following:

R1: $C+CO_2 \leftrightarrow 2CO$ (*Boudouard Reaction*)

R2: $C+H_2O\leftrightarrow H_2+CO$ (*Water-gas Reaction*)

R3: $C+2H_2\leftrightarrow CH_4$ (*Methanation Reaction*)

R4: $H_2O+CH_4\leftrightarrow CO+3H_2$ (*Steam Reforming*)

where each net reaction rate is estimated as:

$$R1\colon \nu_1 = -\mathrm{k}_{a1}\frac{x_5-\frac{x_3^2}{P_x K_{p1}}}{\sum\left(K_j+\frac{1}{p}\right)x_j}\left(\frac{x_{1,0}}{x_1}\right)^{1/3}\frac{x_1}{\rho_C d_{p,c}}; \qquad (10)$$

$$\mathrm{R2}\colon \nu_2 = -\mathrm{k}_{a2}\frac{x_4-\frac{x_2 x_3}{P_x K_{p2}}}{\sum\left(K_j+\frac{1}{p}\right)x_j}\left(\frac{x_{1,0}}{x_1}\right)^{1/3}\frac{x_1}{\rho_C d_{p,c}}; \qquad (11)$$

$$\mathrm{R3}\colon \nu_3 = -\mathrm{k}_{a3}\frac{x_2^2-\frac{x_6 P_x}{K_{p3}}}{P_x\sum\left(K_j+\frac{1}{p}\right)x_j}\left(\frac{x_{1,0}}{x_1}\right)^{1/3}\frac{x_1}{\rho_C d_{p,c}}; \qquad (12)$$

$$R4 : \nu_4 = -\mathrm{k}_{a4}\frac{x_4 x_6-\frac{x_2^2 x_3}{{P_x}^2 K_{p4}}}{P_x\sum\left(K_j+\frac{1}{p}\right)x_j}\left(\frac{x_{1,0}}{x_1}\right)^{1/3}\frac{x_1}{\rho_C d_{p,c}}; \qquad (13)$$

where ν_i is the net reaction rate, K_{pi} is the equilibrium constant, k_{ai} is the apparent rate constant for each reaction calculated through the Arrhenius equation [6], $x_{1,0}$ is the initial molar number of atomic carbon, ρ_c is the density of carbon, $d_{p,c}$ is the equivalent diameter of char particles and P_x is the partial pressure. The Arrhenius equations used for the estimation of the k_{ai} constants [6], as well as the initial TAR moles, are calculated by imposing a first guess temperature value. Therefore, the following differential equations are solved through the 4_{th} order Runge-Kutta algorithm to achieve the species molar fractions in the char reduction zone at the end of the imposed residence time:

$$C: \frac{dx_1}{dt} = \nu_1 + \nu_2 + \nu_3; \tag{14}$$

$$H2: \frac{dx_2}{dt} = -\nu_2 + 2\nu_3 - 3\nu_4; \tag{15}$$

$$CO: \frac{dx_3}{dt} = -2\nu_1 - \nu_2 - \nu_4; \tag{16}$$

$$H2O: \frac{dx_4}{dt} = \nu_2 + \nu_4; \tag{17}$$

$$CO2: \frac{dx_5}{dt} = \nu_1; \tag{18}$$

$$CH4: \frac{dx_6}{dt} = -\nu_3 + \nu_4; \tag{19}$$

$$N2: \frac{dx_7}{dt} = 0. \tag{20}$$

Once the previous algebraic–differential set of equations is solved, the temperature value is updated by solving the enthalpy balance equation between reactants (sum of the formation enthalpy of water vapor in the biomass and the gasifying agent, of the biomass organic and inorganic matter and of the gasifying agent species) and products (sum of the formation and specific enthalpies of each product species, these lasts integrated between a reference temperature of 25 °C and the initial guess value). The convergence is reached when an estimated error ε between the guessed and estimated temperature value is assumed equal to 0.001. The flowchart shown in Figure 1 summarizes the proposed iterative procedure.

3. RESULTS

The developed model is first applied to simulate the syngas yield deriving from the gasification of pine sawdust in a fluidized bed at different ER [8]. The residence time is imposed according to the data deriving from the studied experimental facility. Figure 2 reports the comparison between the experimental and numerical species volume fractions on dry-ash free (daf) basis, as a function of the ER. The agreement is considered satisfactory, as the model well reproduces the measured trends, with an overall error of the 9%. Moreover, Figures 3.a,b,c respectively show the evolution of the estimated gaseous temperature, TAR fraction, and syngas Lower Heating Value (LHV) with the ER. The achieved trends agree with previous studies of the literature [9], confirming how operative conditions closer to pure combustion increase the gaseous temperature, reducing the syngas energy content. The proposed model is then applied to simulate the gasification process of poplar wood in a downdraft fixed bed reactor at an ER of 0.36. The residence time has been increased 4 times with respect to the previous operative condition. Figure 4 reports the comparison between the experimental and numerical species volume fractions on dry-ash free (daf) basis, of the measured and estimated gaseous temperature and of the syngas LHV. All the results are considered in a satisfactory agreement with the made measurements, with an overall error below 12%.

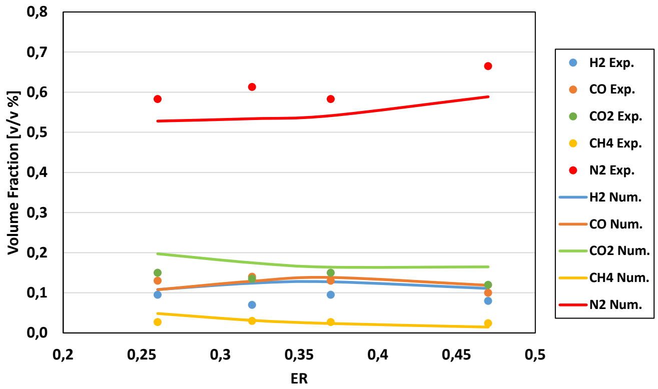

Fig. 2. Comparison of the experimental – numerical species volume fractions on daf basis as a function of the ER in a fluidized

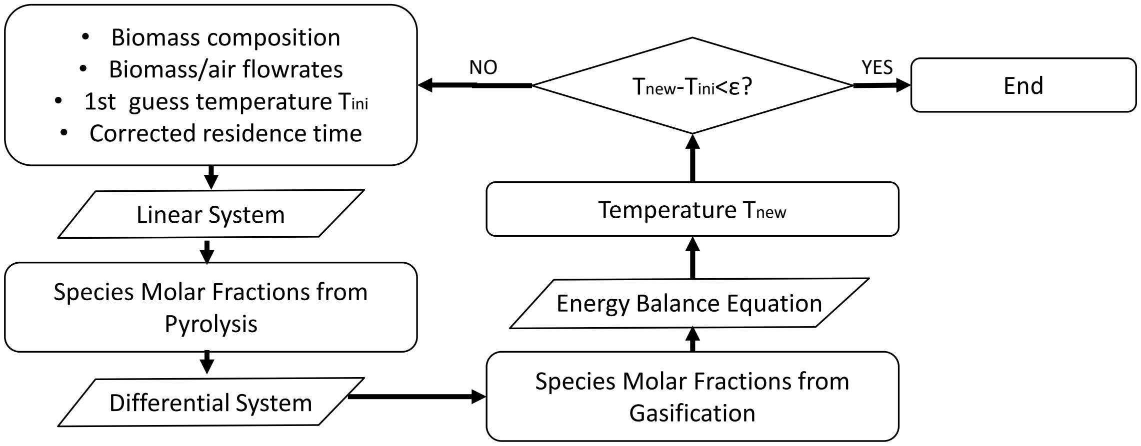

Fig. 1. Flowchart of the implemented iterative procedure.

4. CONCLUSIONS

A 0D kinetic model for biomass gasification is here presented, to predict the syngas yield and heating value and gasification temperature characterizing the gasification process of woody biomasses in both fluidized and fixed bed reactors. The model is based on the description of the kinetics of the surface reactions that take place in the char reduction zone. Novel aspect is related to an appropriate kinetics for the prediction of the TAR moles which has been added, along with an energy balance equation between reactant species and products, for the *a priori* forecast of the gasification temperature in the reactor. Although it has been developed for fixed bed downdraft reactors, it has also been validated for fluidized bed reactors, after appropriate calibration of the residence time. The presented model shows a good agreement in both the considered conditions, as the evolution of the main parameters well respect the trends depicted from literature, with an overall error remaining below the 12%. Future works will be focused on employing the here presented methodology for the estimation of non-woody biomasses.

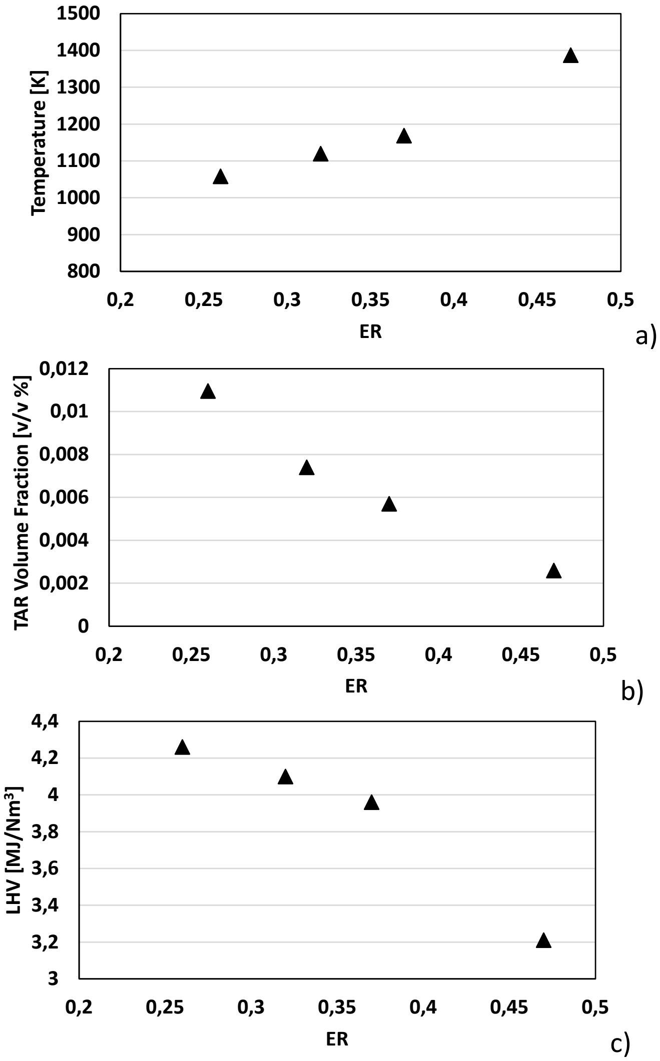

Fig. 3. Numerical gaseous temperature, b) numerical TAR volume fraction, c) numerical syngas LHV as a function of the ER in a fluidized bed.

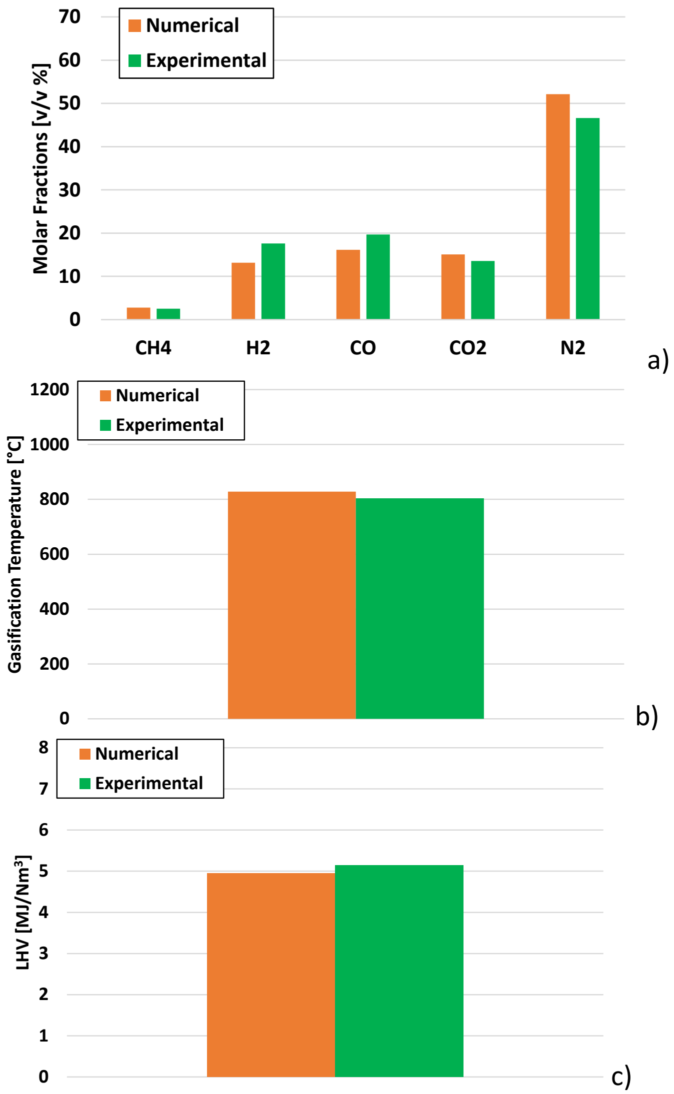

Fig. 4. Comparison of the a) experimental – numerical species volume fractions on daf basis, b) gaseous temperature, c) syngas LHV as a function of the ER in a fixed bed reactor.

ACKNOWLEDGEMENT

The research is a part of the project "PANACEA – Polygeneration from residual biomasses in urban wastewater treatment plants", funded by Ricerca di Sistema Elettrico Nazionale of the Italian Ministry of Economic Development, under Grant CCSEB_00236

“Fondo per la Ricerca di Sistema Elettrico” D.M. 30/06/2014.

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