



# Thermochemical equilibrium modeling of a biomass downdraft gasifier: Constrained and unconstrained non-stoichiometric models



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## ABSTRACT

The objective of this work is to develop a non-stoichiometric equilibrium model to study parameter effects in the gasification process of a feedstock in downdraft gasifiers. The non-stoichiometric equilibrium model is also known as the Gibbs free energy minimization method. Four models were developed and tested. First a pure non-stoichiometric equilibrium model called M1 was developed; then the methane content was constrained by correlating experimental data and generating the model M2. A kinetic constraint that determines the apparent gasification rate was considered for model M3 and finally the two aforementioned constraints were implemented together in model M4. Models M2 and M4 showed to be the more accurate among the four developed models with mean RMS (root mean square error) values of 1.25 each.

Also the gasification of Brazilian *Pinus elliottii* in a downdraft gasifier with air as gasification agent was studied. The input parameters considered were: (a) equivalence ratio (0.28–0.35); (b) moisture content (5–20%); (c) gasification time (30–120 min) and carbon conversion efficiency (80–100%).

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## 1. Introduction

The capability of using different types of solid or liquid fuels and even agricultural residues or byproducts to obtain synthesis gas has led to the study of downdraft gasifiers today. In many engineering applications, equilibrium calculations are useful to predict the outcome of the system being studied. Thus, equilibrium is the first approach used to predict the outcome of the gasification process in downdraft gasifiers.

The thermochemical equilibrium approach can be applied, to any reacting system, by using either the stoichiometric or non-stoichiometric method. The stoichiometric method involves the use of equilibrium constants. In order to define these constants, a number of chemical reactions must be chosen. The stoichiometric coefficients of the chosen reactions are then used to calculate the equilibrium constants. For this reason, this method is often called the stoichiometric equilibrium method. The non-stoichiometric equilibrium method involves the minimization of the Gibbs free energy of the system. No specific chemical reaction, other than the assumed global reaction, is required. This method can be used to

perform calculations either when the system undergoes chemical reactions and when it does not. This method is called non-stoichiometric because of the absence of any particular chemical reaction.

The comparison of the aforementioned equilibrium methods has been carried out in earlier works. One of the first reports proposing Gibbs energy minimization method as a better approach was presented by Zeleznik and Gordon [1]. The authors state that to calculate the flame temperature for the combustion of a hydrocarbon in air, using the stoichiometric method, 20 or more chemical reactions may need to be considered. The non-stoichiometric method based on the minimization of the Gibbs free energy of the system is more suitable for large systems since it does not depend on a large number of reactions.

In previous work the authors have addressed the thermochemical equilibrium modeling of downdraft gasifiers by using the stoichiometric method [2] and introducing modifications to the equilibrium constants in order to improve the accuracy of the resulting model, which was better than that of a pure equilibrium model.

In the present work the non-stoichiometric equilibrium modeling of downdraft biomass gasifiers is addressed and also

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**Nomenclature**

$a_{ij}$	number of moles of element “ $i$ ” which is present in species “ $j$ ”
$(b_i)_R$	number of moles of element “ $i$ ” in the reactants
$C_p$	specific heat at constant pressure
ER	gasification equivalence ratio
HHV	high heating value, MJ/kg for biomass and MJ/N m <sup>3</sup> for syngas
$\bar{G}_{f,i}^0$	specific Gibbs free energy of formation on a molar basis at standard pressure (kJ/mol)
$\bar{h}$	specific total enthalpy on a molar basis, kJ/mol
$\frac{\Delta \bar{h}}{T}$	specific sensible enthalpy on a molar basis, kJ/mol
$\bar{h}_{f,-298}^0$	specific standard enthalpy of formation on a molar basis, kJ/mol
LHV	low heating value, MJ/N m <sup>3</sup>
MC	moisture content, %
$M_i$	molecular weight of species “ $i$ ”, g/mol
$m_0$	initial mass (kg)
$m_f$	final mass (kg)
$n_i$	mol number of species “ $i$ ”
$n_{Tot}$	total mole number of synthesis gas
$p$	pressure, kPa
$p_0$	standard pressure, kPa
$P_{CH_4}$	methane percentage in dry basis (%)
$r_b$	apparent gasification rate for the Boudouard reaction (s <sup>-1</sup> )
$r_w$	apparent gasification rate for the steam gasification reaction (s <sup>-1</sup> )
$R$	universal constant of ideal gases, kJ/mol K
$T$	temperature, °C for results presented and K for calculations
$V$	volume, m <sup>3</sup>
$x_j$	mol number of species “ $j$ ” with respect to carbon content in feedstock

**Chemical symbols**

A	ash
C	carbon
CO	carbon monoxide
CO <sub>2</sub>	carbon dioxide
CH <sub>4</sub>	methane
H	hydrogen (monatomic)
H <sub>2</sub>	hydrogen (diatomic)
H <sub>2</sub> O	water
H <sub>2</sub> S	hydrogen sulfide
O	oxygen (monoatomic)
O <sub>2</sub>	oxygen (diatomic)
N	nitrogen (monoatomic)
N <sub>2</sub>	nitrogen (diatomic)
S	sulfur
SiO <sub>2</sub>	silica

**Greek symbols**

$\gamma$	nitrogen to oxygen ratio in the gasification agent, mol-N <sub>2</sub> /mol-O <sub>2</sub>
$\lambda_j$	Lagrange multiplier of element $j$

**Superscripts**

g	gaseous state
l	liquid state
s	solid state

**Subscripts**

CC	carbon conversion
P	products
R	reactants
t	total
UC	unconverted carbon

some constraints were added in order to produce more accurate results. Until now most of the published papers, which deal with non-stoichiometric modeling applied to gasification, mainly introduce a gasification efficiency, this modification was included in models M1 and M2. However model M2 also includes a constraint regarding the CH<sub>4</sub> (methane) content which was determined by correlating published experimental data. Model M3 includes a kinetic constraint regarding the apparent gasification rate of biomass; this constraint permits the introduction of time as a variable and also permits the approximate determination of the gasification efficiency. The introduction of this kinetic constraint to the equilibrium modeling of biomass gasification constitutes the major contribution of the present work. Model M4 includes the two aforementioned constraints, namely, the CH<sub>4</sub> content constraint and the apparent gasification rate constraint.

**2. Downdraft gasifiers**

Gasification is a process for converting carbonaceous materials to a combustible or synthetic gas; gasifiers generally operate in sub-stoichiometric conditions [3]. Within this process, four sub-processes can be identified [4]:

(a) a drying process in which feedstock that contains water is heated in order to vaporize its water content;

(b) a thermal decomposition or pyrolysis process in which there is no participation of oxygen. The feedstock is converted into char, and it changes its chemical composition without adding hydrogen;

(c) a gasification process in which a combustible or synthetic gas is obtained as a result of several chemical reactions involving carbon, steam, hydrogen, carbon dioxide, and other substances; and

(d) a combustion process in which gases, vapors and char undergo combustion in order to supply the energy required for the other sub-processes.

There are not clear delimitations between the aforementioned processes; all of them can occur at the same time in a specific particle [5].

Downdraft or countercurrent gasifiers obtain their name from the flux characteristics of the feedstock and the gasification agent. The feedstock enters at the top of the apparatus, while the gasification agent enters into a lower section of the gasifier. Products of pyrolysis and combustion flow downward. The hot gas then moves downward over the remaining hot char, where gasification takes place [4]. The minimum temperatures required to gasify the most refractory part of almost any biomass are about 800–900 °C [6]. According to Reed and Das [7], two kinds of downdraft gasifiers can be identified: Downdraft Imbert gasifiers and Stratified Downdraft

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