



## Full Length Article

# Biomass modelling: Estimating thermodynamic properties from the elemental composition



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## HIGHLIGHTS

- Accuracy of heating value correlations on a consistent database of biomass samples.
- Complete and coherent lignocellulosic biomass model for numerical simulations.
- Enthalpy and Gibbs free energy as linear correlations of the elemental composition.
- Exergy in terms of thermodynamic properties and composition of the environment.

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## ABSTRACT

In the context of modelling biomass conversion processes, the accurate representation of biomass, which is a complex and highly variable material, is of crucial importance. This study provides a rather simple and flexible way to represent biomass, especially suited in the context of thermochemical conversion processes. The procedure to represent the *enthalpy of formation*, the *Gibbs free energy* and the *exergy* of biomass in terms of its elemental composition (C, H, O, N, S) and moisture content is outlined.

The correlations relating the heating value to the elemental composition of biomass are evaluated through a database of over one hundred raw and pretreated biomass samples. Results show that such correlations can predict the higher heating value (HHV) within an accuracy of 1.93% and 2.38%. One of the correlations is then applied to represent the *enthalpy of formation* of biomass as a linear function of the elemental composition.

The procedure is extended to estimate the *Gibbs free energy of formation* and subsequently the *exergy* of biomass, which are expressed as linear functions of the elemental composition. The method proposed for the estimate of exergy allows taking directly into account the composition of the reference environment. Results show that the method proposed in this study agrees within 1% accuracy with the widely used correlation proposed by Szargut et al. (1988). The values obtained for *Exergy*, over the range of compositions of the samples considered, vary in general between 105% and 115% of the lower heating value (LHV) and 103% and 107% of the higher heating value obtained using the literature correlation by Boie (1953).

On the basis of these correlations, this study provides the thermodynamic properties of C, H, O, N, S and *bound water* ‘pseudo-compounds’ that can be used in the thermodynamic properties evaluation packages used in flowsheeting software and in numerical simulations for a coherent description of biomass as a function of its composition.

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## 1. Introduction

The first challenge in the thermochemical modelling of biomass conversion systems is to model biomass itself, the raw material. Biomass is not a standard compound and its chemical, elemental composition, as well as its thermal properties vary significantly.

Different solutions are adopted or suggested, for example, to model biomass in flowsheeting software. In an example bioethanol production unit, modelled in ProSim Plus<sup>®</sup> [1], biomass is represented as a mixture of its chemical constituents by adapting the properties of glucose, such as the chemical formula, the heat of formation and the molecular weight, to represent cellulose, hemicellulose and lignin. Aspen Plus<sup>®</sup> allows the implementation of organic substances as non-conventional solid compounds through the definition of attributes in terms of ultimate (i.e. elemental

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## Nomenclature

### Acronyms

ar	as received basis
daf	dry ash free basis
db	dry basis
EMC	equilibrium moisture content
fsp	fiber saturation point
HHV	higher heating value
hw	hard wood
LHV	lower heating value
MAE	mean absolute error
MBE	mean bias error
MC	moisture content
RMSE	root mean square error
SI	supplementary information
SRC	short rotation coppice
SRF	short rotation forestry
sw	soft wood

### Roman letters

BOO	biomass on a dry basis, 0% moisture (–)
$B_{ch}^{\circ}$	standard chemical exergy ( $\text{kJ mol}^{-1}$ )
BX	biomass on a wet basis, X% moisture (–)

$c_{p,dry}$	heat capacity, dry basis ( $\text{kJ kg}_{BOO}^{-1} \text{K}^{-1}$ )
$c_{p,wet}$	heat capacity, wet basis ( $\text{kJ kg}_{tot}^{-1} \text{K}^{-1}$ )
$G^{\circ}$	standard Gibbs free energy ( $\text{kJ mol}^{-1}$ )
$H^{\circ}$	standard enthalpy ( $\text{kJ mol}^{-1}$ )
HHV	higher heating value ( $\text{kJ kg}_{BOO}^{-1}$ or $\text{kJ mol}^{-1}$ )
$K_B$	constant by Battley (–)
LHV	lower heating value ( $\text{kJ kg}_{BOO}^{-1}$ or $\text{kJ mol}^{-1}$ )
$M_m$	molar mass ( $\text{g mol}^{-1}$ )
$M_b$	moisture content referring to <i>bound</i> water ( $\text{kg}_{H_2O} \text{kg}_{BOO}^{-1}$ )
$M_{fsp}$	moisture content after evaporation of <i>free</i> water ( $\text{kg}_{H_2O} \text{kg}_{BOO}^{-1}$ )
MC	moisture content ( $\text{kg}_{H_2O} \text{kg}_{BOO}^{-1}$ )
$R$	ideal gas constant ( $\text{J mol}^{-1} \text{K}^{-1}$ )
$S^{\circ}$	standard entropy ( $\text{kJ mol}^{-1} \text{K}^{-1}$ )
$T$	temperature (K or °C)
TOO	Torrefied biomass, 0% moisture (–)

### Greek letters

$\Phi$	humidity ( $\text{kg}_{H_2O} \text{kg}_{tot}^{-1}$ )
$\sigma$	standard deviation (–)

composition) and proximate (i.e. fixed carbon, volatile matter and ash content) analysis. The heating value, the heat of formation and the heat capacity are then calculated by selecting the relevant literature correlations, generally developed for coal, in the General Coal Enthalpy Model (HCOALGEN property model [2]). The attributes can be changed through the use of subroutines to represent changes in composition during conversion, for example during coal devolatilisation. Rösensch and Wagner [3] analysed the application of the empiric correlations used in AspenPlus® to model wood and straw. They showed that the heating value correlations, developed for coal, generally underestimate the values for biomass and they indicated which correlations can predict the heating values of average wood and wheat straw samples within their standard deviation.

The objective of this study is to propose an accurate and consistent definition of biomass, especially relevant for the simulation of thermochemical conversion processes. The goal is to develop a generic representation of the thermodynamic properties of biomass that allows to easily update process performances as a function of the type of biomass, which is considered on the basis of its elemental composition. The model developed is general and may be used in any numerical simulation but in this study it is applied to represent biomass in the flowsheeting software Vali® by Belsim [4]. Therefore the methodology presented refers rigorously to thermodynamics but the formalism refers sometimes to this software. Thermodynamic properties packages offered in flowsheeting software, such as Vali®, allow in fact the definition of new pseudo-compounds, that is, user-defined compounds used to model substances that are not present in the internal database for which thermodynamic properties need to be defined. In this study, special attention is given to the coherence of the heating value calculated from the thermochemical properties of the pseudo-compounds. The heating value represents the energy content of biomass and is one of the most important properties for the design and simulation of biomass thermochemical conversion systems [5].

The steps leading to the representation of biomass are presented in detail. First of all a 'biomass database', obtained in the context of previous work, is used to extract information regarding the elemental composition and heating value of many representative

lignocellulosic biomass samples. This information is used as a basis for comparing several correlations available in the literature relating the elemental composition to the heating value in the range of compositions of biomass types considered in this study. The systematic comparison of the correlations and corresponding errors allows one to identify the correlation best fitting the experimental data. Finally, given a correlation, the approach and the fundamental assumptions used to model biomass are presented. The properties considered are the heating value with the corresponding *enthalpy of formation*, the heat capacity, the heat of adsorption of the moisture content. Furthermore the modelling approach is extended to the *entropy*, the *Gibbs free energy* and the *exergy* of biomass. In particular, the exergy model presented allows the explicit definition of the exergy of biomass based on its thermodynamic properties and the properties of the reference environment.

## 2. The definition of biomass

From a legal standpoint biomass is "the biodegradable fraction of products, waste and residues from biological origin from agriculture (including vegetal and animal substances), forestry and related industries including fisheries and aquaculture, as well as the biodegradable fraction of industrial and municipal waste" [6]. Biomass therefore includes a large variety of materials. In this study biomass refers only to lignocellulosic materials from forestry and agricultural products, namely wood and straw of different types. Biomass is generally defined by considering its chemical/structural (i.e. cellulose, hemicellulose, lignin and extractives), proximate and ultimate analysis. The ultimate analysis and the heating value are especially important for the definition of biomass in a thermochemical model, as they provide the basis for the atomic and energy balance of a conversion process.

In terms of ultimate analysis, biomass is mainly composed of C, H, and O, which define, for the most part, its heating value. It also contains small quantities of N, S, Cl. These six elements make up the organic phase of biomass. The inorganic phase contains Si, Al, Ti, Fe, Ca, Mg, Na, K, S, P, and other minor elements which are

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