



## Torrefaction modelling for lignocellulosic biomass conversion processes

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### ABSTRACT

The objective of this study is to develop a model for the description of torrefaction. The model is conceived in the context of process modelling and therefore it aims at providing coherent mass and energy balances of solid and gaseous products, rather than a physical description of the process. The rationale underlying the proposed model stems from the representation of torrefaction and its products on a C–H–O ternary diagram and its focus is the description of the solid product in terms of yield, composition and heating value. The heating value of the gaseous products is determined by considering water, carbon dioxide and acetic acid as the major volatile products and closing the mass balance. It is possible to extend the number of species considered in the torrefaction gases if experimental data regarding the volatile products are available. The proposed model is simple, of easy implementation and calibration, of fast resolution and its results have been validated against experimental data. This work represents the basis for a future evaluation and optimisation of torrefaction as a pretreatment step in the thermo-chemical conversion of biomass.

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### 1. Introduction

Torrefaction is a thermo-chemical process generally carried out in the 200–300 °C temperature range, at low heating rates (<50 °C/min), and relatively long reaction times (about 1 h) [1]. It may be used as a pre-treatment technology to upgrade lignocellulosic biomass to a higher quality fuel, for its subsequent conversion into heat or other energy carriers, such as electricity and biofuels.

During torrefaction biomass is completely dried and its hygroscopic nature is at least partly lost (only 1 to 6%<sub>wt</sub> moisture may be regained) [1] and microbial activity is reduced [2]. The torrefied solid, compared to raw biomass, exhibits better grindability [3,4] and better transport properties for injection (in a boiler or gasifier, for example). Energy content of torrefied biomass is higher while ignition times are shorter [5]. These features make torrefied

biomass similar to coal and therefore suitable for co-firing and gasification, with minimal efficiency loss even in existing equipment designed for coal [6]. Furthermore because of the improved storage properties and the higher energy density, transportation costs may be reduced with the production of high quality pellets [6].

This study presents a simple torrefaction model to estimate the solid and gaseous yields, and their corresponding heating values. The results of the model are compared to experimental values obtained in previous studies at CEA Grenoble (Commissariat à l'énergie atomique et aux énergies alternatives) and the literature. The model is implemented in a flow sheeting software (Vali by Belsim [7]), in order to estimate the complete mass and energy balances of a torrefaction unit. This includes the combustion of the off-gases used to provide at least part of the heating requirement of the process.

Torrefaction has a high potential of becoming a leading pre-treatment technology for the efficient exploitation of biomass for energy purposes. It has gained increasing attention from both industry and research institutions in terms of a deeper understanding of the fundamental reaction mechanisms and the engineering of novel reactor designs.

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### Acronyms

AWL	anhydric weight loss
LHV	lower heating value
HHV	higher heating value
FTIR	Fourier transform infrared spectroscopy

### List of symbols

B00	biomass, 0% moisture
$c_p$	heat capacity, $\text{kJ kg}^{-1} \text{K}^{-1}$
$E_A$	activation energy, $\text{J mol}^{-1}$
$\Phi$	humidity, $\text{kg}_{\text{H}_2\text{O}} \cdot \text{kg}_{\text{tot}}^{-1}$
$\Delta_f H^\circ$	standard enthalpy of formation, $\text{kJ/mol}$
$k$	reaction rate, $\text{s}^{-1}$
$\dot{m}$	mass flow, $\text{kg s}^{-1}$
$T$	Temperature, $^\circ\text{C}$ or $\text{K}$
T00	torrefied biomass, 0% moisture

## 2. Review of torrefaction

The products of torrefaction are a brown/dark coloured solid, permanent gases and condensable species as summarized in Fig. 1 by Bergman [1].

The solid product displays decreasing hydrogen to carbon (H/C) and oxygen to carbon (O/C) elemental ratios that tend towards those of coal with increasing severity of torrefaction (the severity of torrefaction is the degree of conversion and increases with temperature and reaction time). Torrefaction products may be classified differently according to different authors. Here, as a reference, the definition given by Bergman [1] is adopted, as displayed in Fig. 1. According to Bergman *permanent* gases are  $\text{H}_2$ ,  $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{CH}_4$  (compounds with a boiling point below  $-33^\circ\text{C}$ ) and light aromatics such as benzene and toluene. The *condensable* products include three subgroups: water, lipids and organics. Water is a product of thermal decomposition and evaporation of residual moisture. Lipids and organics, usually referred to as *extractable* species, are present in the original biomass and are partly released during torrefaction [8]. Organics may be also produced during devolatilisation and carbonisation [1]. The solid yield, the type and amount of gases produced strongly depend on the operating conditions and also the initial biomass type [1,9]. A review of the numerous *condensable* and permanent gases identified during torrefaction is provided by Tumuluru et al. [9].

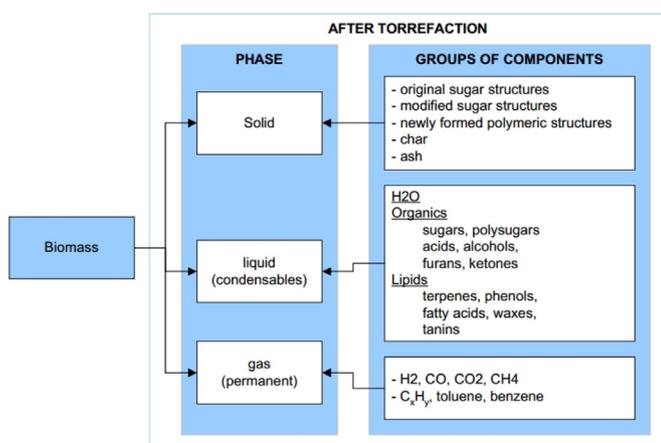


Fig. 1. Products of torrefaction, after Bergman [1].

Very few models proposed in the literature for the process modelling of torrefaction take into account the solid and gaseous yields, and their composition as a function of the operating conditions. Models used in techno-economic evaluations are generally relative to a single operating point (in terms of biomass composition, AWL (anhydric weight loss), and temperature) and therefore are represented by a single equation. Hall [10] fit a quadratic regression to relate the AWL occurring during torrefaction and temperature, while they consider constant fractions of volatiles based on experimental results. The model proposed by Medic et al. [11] also uses quadratic regressions to relate the AWL and the energy yield to temperature and moisture content. The models based on empirical correlations, obtained under specific experimental conditions, do not describe the composition of the torrefied solid and evolution of the torrefaction gases during torrefaction. An interesting and complete model describing the solid and gaseous yields as a function of temperature and residence time is proposed by Bates and Ghoniem [12], which is calibrated on the volatiles produced by torrefaction of willow and experimentally measured by Prins et al. [13,14]. These models are generally independent from the torrefaction process design, as they do not take into account the reactor technology, and heat and mass transfer mechanisms at the reactor scale.

Torrefaction reactors are generally classified into two broad categories based on the heat transfer mechanism: direct and indirect heating. For directly heated reactors biomass is in direct contact with the heating media which may be hot gas, hot solids, superheated steam (microwave reactors also fall in this category). For indirectly heated torrefiers biomass is heated across the reactor walls. Different types of torrefaction reactors are reviewed by Dhungana et al. [6] and by Chew and Doshi [15].

## 3. Torrefaction on a ternary diagram

Ternary diagrams are often used in the literature to represent organic chemical processes. Cairns and Tevebaugh [16] introduced the use of C–H–O ternary diagrams to represent carbon deposition boundaries for fuel cell applications. Prins et al. [17] used ternary diagrams to analyse the efficiency of gasification of wood and torrefied wood while Ptasincki et al. [18] used them to compare the gasification of different biofuels and coal. More recently Tay et al. [19] used ternary diagrams to develop a graphical targeting tool for the optimisation of gasification as a function of downstream process requirements, in the context of syngas based integrated biorefineries. Chen et al. [20] used ternary diagrams to describe the solid and gas products composition versus operating conditions during pyrolysis. In the present study the representation of biomass and torrefaction products on a carbon–hydrogen–oxygen (C–H–O) ternary diagram underlies the rationale for the proposed torrefaction model.

The data obtained by Nocquet [8,21,22] are used here for representation purposes as they provide both the solid and gaseous yields obtained during torrefaction. The study was carried out using the lab-scale reactor TORNADE, developed at CEA Grenoble and described in detail in Refs. [8,21,22]. Samples of 100–200 mg of beech wood are torrefied, under  $\text{N}_2$  flow, at torrefaction temperatures ranging from  $220^\circ\text{C}$  to  $300^\circ\text{C}$  in the isothermal zone of a furnace. The gaseous products are measured on-line by FTIR (Fourier transform infrared spectroscopy) at  $150^\circ\text{C}$  to avoid condensation. Condensable species are collected in two cooling baths: the first one containing freezing ice (wall temperature of  $0^\circ\text{C}$ ) and the second one containing frozen carbon dioxide mixed with isopropanol (wall temperature of  $-70^\circ\text{C}$ ). The eight main species measured were: water, formaldehyde, acetic acid, and carbon dioxide with smaller amounts of carbon monoxide, methanol, formic acid and furfural. These eight measured species combined account together for over 70% of the total volatiles

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