Energy xxx (2014) 1–7

Contents lists available at ScienceDirect

Energy

journal homepage: www.elsevier.com/locate/energy

Volatile species release during torrefaction of biomass and its macromolecular constituents: Part 2 – Modeling study

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ARTICLE INFO

Article history:
Received 20 September 2013
Received in revised form
4 April 2014
Accepted 3 May 2014
Available online xxx

Keywords:
Biomass
Cellulose
Hemicelluloses
Lignin
Model
Torrefaction

ABSTRACT

Based on the torrefaction experiments carried out on beechwood and on its macromolecular constituents – cellulose, lignin and xylan – in part 1 of this paper, a simple torrefaction model was developed to predict both solid and the eight main volatile species yields versus temperature, residence time and biomass macromolecular composition. This model consisted in the superposition of kinetic "sub-models" describing the torrefaction of each constituent. The interactions observed in part 1 between constituents were then taken into account by means of an empirical factor related to cellulose decomposition rate. The model reproduced quite well the experiments and enabled to show the influence of each constituent on torrefaction yields.

1. Introduction

The general context of the study is detailed in part 1 of this two-paper series. The reader is invited to consult the experimental part (part 1) before considering the following modeling part (part 2) to better understand the study.

As mentioned in part 1, at the moment, torrefaction mechanisms are still poorly understood [1]. There are only few kinetic models dedicated to biomass torrefaction [2–4]. These models are mainly inspired from pyrolysis models, for which an abundant literature is available, as reviewed by Di Blasi [5]. Pyrolysis and torrefaction models both describe biomass thermal degradation, but in different ranges of temperature, *i.e.* the range of temperature in pyrolysis is higher than that associated to torrefaction – typically higher than 300 °C. Hence, the reactions and mechanisms involved are expected to be – at least partly – different and the substantial work done to develop pyrolysis models cannot be directly applied to torrefaction conditions.

As solid is the main product of torrefaction, the objective of torrefaction models is generally the description of solid mass loss versus time and temperature. Only Bates and Ghoniem have recently developed a model able to predict the composition of volatiles [3]. As highlighted by the authors, their model suffers from the lack of experimental data for validation, with only one study available about volatile species emission during torrefaction [6]. Moreover, although it has been shown that both solid yield and volatile species yields were highly influenced by the biomass type [6–8], the torrefaction models mentioned above generally do not describe the influence of biomass type. As most pyrolysis models,they consider biomass as a global solid and are thus feedstock-specific. Only Rousset et al. [2] have developed a model which could be applied to various biomasses. Their approach was based on an approach previously developed in pyrolysis by Koufopanos et al. [9]. This approach consists in considering the summative contribution of the biomass macromolecular constituents, which are known to react differently under the effect of heat [10]. Unfortunately, this model was limited to the description of solid mass loss versus time. Moreover, the model physical meaning was disputable, since its parameters were not derived from experiments on constituents.

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http://dx.doi.org/10.1016/j.energy.2014.05.023
0360-5442/

Nomenclature

A	initial solid, –
A_1	intermediate solid produced by reaction 1, –
A_2	torrefied solid produced by reaction 2, –
c_s	variation of mass percent of constituent s, wmf%
Ea	activation energy, J.mol^{-1}
F	function describing the difference between model and experimental yields, wmf%
k	kinetic parameter, s^{-1}
k_0	preexponential factor, s^{-1}
$K_{1or\ 2}$	sum of kinetic parameters associated to step 1 or 2, s^{-1}
R	universal gas constant, J.mol^{-1}.K^{-1}
T	temperature, K
t_N	interaction factor, –
V_1	volatile species produced by step 1, –
V_2	volatile species produced by step 2, –
V_x	complementary species, –
Y_A	Yield of remaining initial solid, wmf%
$Y_{A1\ or\ A2}$	yield of solid produced by step 1 or step 2, wmf%
Y_S	total yield of solid, wmf%
Y_V	total yield of volatiles, wmf%
$Y_{V1\ or\ V2}$	yield of volatiles produced by step 1 or step 2, wmf%
$Y_{sum\ i}$	total yield of species i, wmf%
$\alpha_{iV1\ or\ V2}$	parameter describing the production of species i in step 1 or 2, –
ω_j	initial mass fraction of constituent j, wmf%
w%	mass percent
wmf%	moisture-free mass percent

In part 1 of this paper, an original set of experimental data was supplied about solid mass loss and volatiles production during torrefaction of beechwood, of its macromolecular constituents, *i.e.* cellulose, xylan and lignin, and of their mixtures. These data showed the ability of the additive law applied on constituents to describe torrefaction up to 250 °C and the existence of interactions between constituents at temperatures of 280 °C and 300 °C, maybe due to the ramification of cellulose fragments by lignin and xylan radicals produced at the beginning of torrefaction.

Based on the existing work in literature and on part 1 of this paper, the objective of part 2 is to derive from the experimental results a simple model able to predict both solid yield and the main volatile species yields during torrefaction versus temperature, residence time and biomass macromolecular composition through the use of a corrected additive law on biomass constituents.

First, the model principle will be described. The parameters determination will then be detailed. To end, the model performances will be discussed as well as the influence of biomass macromolecular composition on the results.

2. Model development

2.1. Preambue

The model assumptions rely on the large set of experimental results obtained in part 1. The model has therefore some physical basis and it may also be a useful tool to better understand the torrefaction processes. However, it does not claim to be an extensive phenomenological description of biomass torrefaction. Indeed, this semi-empirical model mainly aims at being a simple tool that may be integrated in reactor models for further process design.

2.2. Model description

The general principle of the model is described in the scheme of Fig. 1. The input data are the contents in biomass constituents, *i.e.* cellulose, lignin and hemicelluloses. Hemicelluloses are represented by two constituents: xylan and acetyl groups. This choice enables to describe the production of acetic acid by the hydrolysis

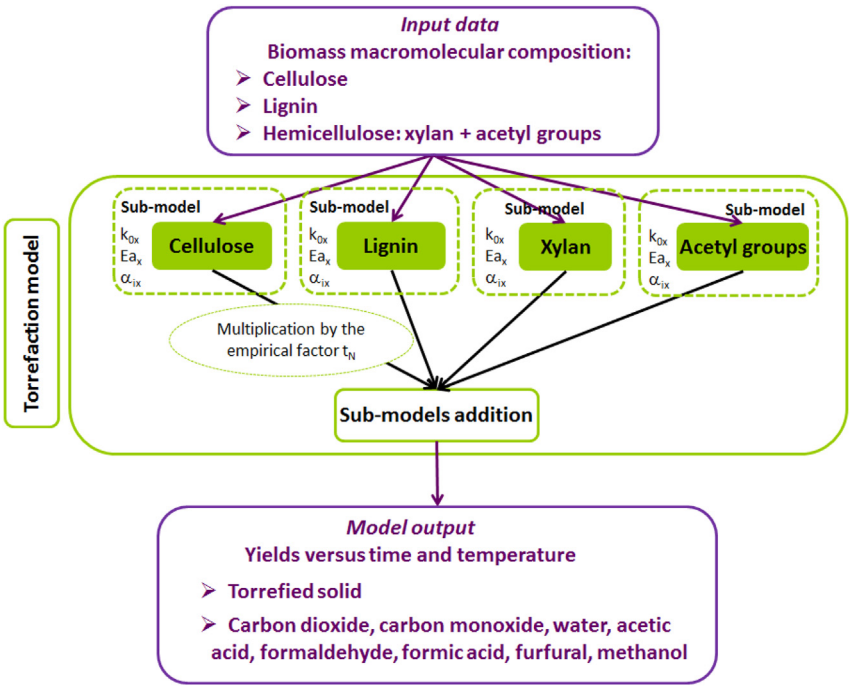

Fig. 1. Principle of the model.

Please cite this article in press as: Nocquet T, et al., Volatile species release during torrefaction of biomass and its macromolecular constituents: Part 2 – Modeling study, Energy (2014), http://dx.doi.org/10.1016/j.energy.2014.05.023