



A comprehensive dual-scale wood torrefaction model: Application to the analysis of thermal run-away in industrial heat treatment processes



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ARTICLE INFO

Article history:

Received 8 July 2012

Received in revised form 25 March 2013

Accepted 27 March 2013

Available online 4 June 2013

Keywords:

Biomass
Mild pyrolysis
Stack
Board
Simulation
Exothermic reaction
Industrial process

ABSTRACT

A dual-scale model of the torrefaction of wood was developed and used to study industrial configurations. At the local scale, the computational code solves the coupled heat and mass transfer and the thermal degradation mechanisms of the wood components. At the global scale, the two-way coupling between the boards and the stack channels is treated as an integral component of the process. This model is used to investigate the effect of the stack configuration on the heat treatment of the boards. The simulations highlight that the exothermic reactions occurring in each single board can be accumulated along the stack. This phenomenon may result in a dramatic heterogeneity of the process and poses a serious risk of thermal runaway, which is often observed in industrial plants. The model is used to explain how thermal runaway can be lowered by increasing the airflow velocity, the sticker thickness or by gas flow reversal.

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1. Introduction

In order to prevent attack of wood by fungi or insects, several chemical substances are commonly used. However many of these are hazardous to the environment. The heat treatment of wood under inert atmosphere at temperature levels ranging from 200 °C to 300 °C (mild pyrolysis) is an alternative to the use of chemicals, as it increases the dimensional stability and durability of wood. Due to a thermal degradation of the cell wall constituents, mild pyrolysis significantly changes the material properties, which results in better durability and stability than natural wood [1–4]. However, one has to keep in mind that this is to the detriment of decreased mechanical strength, density and surface roughness [5,6]. In spite of these drawbacks, heat-treated solid wood has become popular and several production plants now exist throughout Europe [7]. These industrial plants must overcome serious problems such as thermal runaway and internal checking to obtain a relevant and homogeneous final product quality. There are several explanations for these phenomena, such as the huge variability of biological products and the dispersion of the initial moisture content and particle shape. However, the dual spatial coupling (within boards

and within the stack) in the presence of exothermic reactions is likely to be the main source of problems.

Furthermore, the growing interest in biomass as a source of renewable energy gives rise to a crucial demand in biomass pre-conditioning. For example, torrefaction is a pretreatment required in the multistep process from biomass to liquid (BtL), which includes a gasification followed by a Fisher-Tropsch synthesis [8,9]. In this case, the reduction of the mechanical resilience becomes an advantage, allowing the fibrous behavior to be lost and fine particles and powder flowability to be obtained with a reduced grinding energy [10]. In this case, the optimal treatment can be tuned according to the global mass loss due to thermal degradation [11]. However, it is very difficult to obtain this ideal treatment between and among particles, which emphasizes the need for predictive modeling tools.

Over the last few decades, numerous works have been devoted to the modeling of coupled heat and mass transfer in porous media: formulation, characterization, computational solution, and validation [12]. However, the specific domain of biomass torrefaction involves reactive transfer because chemical reactions occur together with heat and mass transfer. The thermo-activated nature of the chemical reactions together with the presence of reaction heats explains why this coupling is two-way: the reaction kinetics depend on the local value of temperature whereas the temperature field is influenced by the sink/source terms due to the reaction

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Nomenclature

C_p	specific heat ($\text{J kg}^{-1} \text{K}^{-1}$)	Sc	Schmidt number
c	molar concentration (mol m^{-3})	Sh	Sherwood number
D_{AB}	diffusion coefficient of vapour in air ($\text{m}^2 \text{s}^{-1}$)	T	temperature (K)
ΔY_k	length of the control volume in the longitudinal direction of the board (m)	x_v	molar fraction of vapor
ΔZ_k	height of the control volume in the thickness direction of the board (m)	x	airflow direction (m)
h	external heat transfer coefficient ($\text{W m}^{-2} \text{K}^{-1}$)	<i>Superscripts and Subscripts:</i>	
h_m	external mass transfer coefficient (m s^{-1})	a	air
j	mass flux exchanged between the boards and the airflow ($\text{kg s}^{-1} \text{m}^{-2}$)	b	bound
q	mass flux in channels formed by two adjacent board layers ($\text{kg s}^{-1} \text{m}^{-2}$)	end	end board face
L	characteristic length (m)	j	general index for a board layer
M_v	the molar mass of vapor (kg mol^{-1})	k	number of the CV on the board face
Nu	Nusselt number	lo	lower board face
Pr	Prandtl number	N_{cv}	total number of CVs on the board face
Re	Reynolds number	$surf$	surface
		up	upper board face
		v	vapour
		∞	external value

heat. The complete modeling of these phenomena, at the particle level or at the level of a particle set, either for a fixed or agitated bed, is complex and was addressed here using a stepwise approach.

Most studies performed using a thermo-balance could be considered at the micro-particle level, a spatial size small enough for the time constant of the kinetic reactions to be larger than all time constants related to the heat and mass transfer inside the particles. This configuration is easy to obtain at low heating rates, but is more delicate to define at very large heating rates, such as those encountered in flash pyrolysis [13].

The literature available at the micro-particle level is much more abundant; see for example [14–17]. From the literature data, it becomes clear that multistage mechanisms are required for the model parameters to be valid over a certain range of temperature and/or heating rate values. In spite of the numerous papers devoted to this subject, one has to emphasize that most of the works, primarily based on the analyses of experimental data, are performed at linearly increasing temperature, with heating rates of some degrees per minute. This protocol prevents the slow reaction occurring at mild temperature levels to be accurately described.

At the macro-particle level, the primary variables (temperature, moisture content, degradation levels, internal pressure...) evolve in time and space. The variable fields must therefore be computed as the process evolves. This is the perfect scale at which reactive heat and mass transfers are to be accounted for. All models published in this field are more or less comprehensive, each one having its strengths and weaknesses. For research involving biomass pyrolysis, the strong point often lies in the reaction mechanisms and the volatiles production. This implies that the overpressure due to volatiles production and the induced gas velocities are usually taken into account [13,18–21]. Some of this research considers the change of physical properties and shrinkage from native wood to char. However, in most models, less attention is paid to moisture migration: either the particle is supposed to be fully dried before the process commences, or water evaporation is governed by a simplified expression. This is certainly due to the high temperature levels encountered during rapid pyrolysis, which causes the particle to dry very fast. A more recent work [22] proposed a comprehensive model able to account for most of the phenomena involved at the level of a macro-particle. For example, their model perfectly predicts the plateau at the boiling point of water when dealing with humid particles.

However, to our knowledge, none of these works focused their attention on the overshoot in temperature due to exothermic reactions. This phenomenon is very important in the domain of mild pyrolysis, where the temperature level is low (typically in the range 200–300 °C), but the residence time is very long (up to several hours). In such conditions, the effect of some tens of degrees might have a dramatic impact on the heterogeneity of the heat treatment. Based on our extensive knowledge in the field drying, we proposed a comprehensive model of heat and mass transfer able to deal with any MC field inside the product, including liquid water [23]. As a result of this feature, our model is perfectly able to produce the two pressure peaks measured during the heat treatment of a thick board: the first one being due to water evaporation and the second one due to volatiles production. In addition, by using both endothermic and exothermic reactions in the selected kinetics model, we were able to simulate the temperature overshoot observed in experimental data. Using this model, we proved that the presence of water delays the heat treatment phase and produces a more sudden temperature increase, which exacerbates the temperature overshoot. Notice that such an overshoot seems to be visible in the experimental data presented in [22] for a 44% moist wood log.

At the upper scale of a set of particles, either fixed or agitated, the published modeling work is rare. Di Blasi [24] modeled wood gasification in a 1-D fixed bed of particles. This model, which includes a drying zone and a pyrolysis zone, is able to capture the evolution of variables such as the solid and gas temperatures, molar fractions and reaction rates. Note that, as constant internal fields are assumed within each particle, this model is a single scale model.

Compared to this short literature review, the present work proposes a full dual-scale model, whereby each particle is accounted for at the upper scale. This gives rise to a full two-way coupling between the upper model (gas flow) and the particle level (macroscopic formulation). The kinetics model is supplied at each node of each particle model. Furthermore, the present work uses multistage mechanisms selected from different literature sources for each component of lignocellulosic components: cellulose, hemicelluloses and lignins [25]. Even though most literature data were obtained over a large range of temperature levels, the macroscopic model was adequately validated for mild pyrolysis [23]. The local model solves the set of equation in 2D, allowing for the effect of

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