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Comparison of numerical efficiency of the thermal and the kinetic rate drying model applied to a thermally thick wood particle

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Abstract

In this work, the drying and devolatilization of a thermally thick wood particle were modeled. The work was validated against experiments and good agreement was found. The work compared the numerical efficiency and accuracy of the thermal drying model and the kinetic rate drying model. The thermal drying model was used with a fixed boiling temperature (373 K). The kinetic data for the kinetic rate drying model was taken from an earlier work by Di Blasi [1] and additionally one set of kinetic data that was also tested, was assumed by the authors, with the main purpose of reducing the stiffness of the evaporation equation. The numerical efficiency was compared by comparing the CPU times associated with the different drying models. It was found that the thermal drying model is the most efficient drying model at both high and low moisture contents. Soft drying kinetics resulted in intermediate CPU times, while very stiff kinetics yielded the lowest numerical efficiency. No trend was observed regarding how CPU times of the different drying models behave with respect to increasing or decreasing moisture contents.

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Keywords: drying, devolatilization, mesh-based model, one-dimensional, accuracy, numerical efficiency, thermally thick, wood

1. Introduction

Due to its superiority with respect to CO_2 emissions, emitting zero net CO_2, biomass is often preferred over fossil fuels [2]. Therefore, research within the field of modeling of thermochemical degradation of biomass has been

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intensified over the last years. By obtaining a deeper understanding of drying, devolatilization as well as char conversion of biomass, one can optimize current combustion units, with the objective of operating those units at even lower emissions. This is not only strengthening the advantages of biomass over fossil fuels but is also inevitably required since emission limits for biomass combustion units become stricter [3]. A numerically efficient simulation tool is crucial when it comes to using numerical simulations for design and development of new combustion units. Those tools will be of significant importance in the future, since they are cheap and less time-consuming compared to experimental tests [4], which makes them the preferential optimization and design route of furnace manufacturers. It may be surprising that, despite its physically simple nature, drying is found to be a computationally intensive stage of the thermal conversion. A computationally fast model for drying is therefore a chief feature of an efficient thermal conversion model.

In this work, a one-dimensional simulation tool for drying and devolatilization of thermally thick cylindrical wet wood particles was developed, with the main purpose of obtaining a deeper understanding on how these two stages can be accurately modeled in a numerically efficient manner. The model was mesh-based and validated against experiments by Lu et al. [5]. Different drying models were investigated with the main purpose of discussing numerical efficiency and model accuracy. In this work, the thermal drying model and the kinetic rate drying model were compared. The authors also aimed to identify a set of kinetic drying data for the kinetic rate model that was supposed to reduce the stiffness of the evaporation reaction, while meanwhile yielding acceptable accuracy and improved numerical efficiency.

2. Model

The IDA solver included in SUNDIALS (SUite of Nonlinear and DIfferential/ALgebraic Equation Solvers) [6] was used to solve the governing equations in a fully implicit manner. More details on the governing equations can be found elsewhere [5]. The only main differences between the model by Lu et al. [5] and the model used in the current paper were that re-condensation of liquid free water was neglected in the current work and furthermore, that liquid free water movement in the current work was described by convection with the velocity derived from Darcy's law, as suggested by Grønli [7], with the permeability being $\kappa_l = 10^{-20}$ m^2. Shrinkage was modeled with the three-parameter model of Di Blasi [8] with the shrinkage parameters being $\alpha = 1, \beta = 0.75, \gamma = 1$. The integration method was the backward-differentiation formula, with the order varying between 1 and 5. This integration method was a suitable choice as it can solve very stiff equations [6]. The number of grid points in the 1D mesh was chosen such that the modeling results were grid-independent. The tolerance of the solver was set to 1×10^{-3}.

The kinetic rate drying model describes evaporation with an Arrhenius expression [9]. The kinetic rate drying model in this model was always coupled to modeling liquid water transportation by diffusion, which equals a bound water assumption. The thermal drying model assumes drying to occur at a fixed boiling temperature, most commonly 373 K, and no further temperature increase is allowed before the entire moisture content of a cell volume has been evaporated. This results in a step-function which is known to cause numerical instabilities [9]. The thermal drying model in this model was always coupled to modeling liquid water transportation by convection, which equals a liquid free water assumption.

The main input data used in the simulations are listed in Table 1, where c_P is the specific heat capacity, Δh_{evap} is the latent heat of evaporation, $\Delta h_{devol,1}$ is the heat of reaction of primary devolatilization, $\Delta h_{devol,2}$ is the heat of reaction of secondary reactions, D is the effective diffusion coefficient of the gases, D_b is the diffusion coefficient of the bound water and λ is the thermal conductivity. The permeability of the solid phase is κ_{solid}. Subscripts *w, c* and *g* refer to wood, char and gas phase, respectively.

Table 1. List of applied properties and the assigned values.

Property	Unit	Value	Reference
$c_{P,w}$	J/(kgK)	1500 + T	[9]
$c_{P,c}$	J/(kgK)	$420 + 2.09T + 6.85 \times 10^{-4} T^2$	[9]