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Simplification of devolatilization models for thermally-thick particles: Differences between wood logs and pellets



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HIGHLIGHTS

• Detailed particle model clarified the importance of several physical phenomena.

• Major difference between wood logs and pellets was isotropy of particles.

• Wood logs and pellets required different simplification strategies.

• Analytical solution of the shrinking core model and sub-models were proposed.

• The model with proposed simplification strategies agreed well with experimental data.

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ABSTRACT

Many phenomena affects devolatilization of relatively large wood particles, e.g. wood pellets and logs, including mass and heat transfer, chemical reactions and physical transformation such as shrinkage. Many studies investigated the importance of these phenomena through detailed mathematical models at particle scale, but the models need to be simplified at a certain degree to be implemented into large-scale simulation for gasifiers and boilers. This paper first presents how each physical and chemical parameter should be modelled for wood logs (low density and anisotropic) and wood pellets (high density and isotropic) through parametric studies with a detailed particle simulation. They required different sub-models for effective thermal conductivity and heat of reactions due to the difference in isotropy of particles between pellets and logs. Then, we demonstrated that a constitutive equation, i.e. analytical solution of the shrinking core model, is sufficient to express devolatilization rate of thermally-thick particles at the temperature of 1173 K with proper sub-models of physical and chemical parameters. The constitutive equation agreed better with experimental data of wood log than wood pellets, mainly because of the error caused during the consideration of the effect of convective cooling of char layer on thermal conductivity. Both detailed and simplified particle models were validated with the experimental data in an isothermal macro thermogravimeter allowing devolatilization of large particles. © 2015 Elsevier B.V. All rights reserved.

1. Introduction

Thermochemical conversion of biomass such as combustion and gasification has attracted a lot of attention as a promising technology for an alternative to fossil fuel based technologies. Numerical simulation is a powerful tool for optimization of reactor designs and operational conditions. However, it is a big challenge to develop simulation models that are sufficiently accurate and computationally efficient because it is necessary to treat highly complicated multi-scale, multi-phase and multi-physics problems [1]. One of such complexities appears when relatively large biomass particles such as wood chips, logs, pellets, and briquettes are used as fuel. Heat conduction inside the particles affects apparent devolatilization rate of such particles, so-called thermally thick particles. Hence, it is essential to address particle-scale mass and heat transfer when describing the fuel conversion of thermallythick particles in the reactors.

Some recent studies have implemented particle-scale mass and heat transfer models into reactor-scale simulation models of biomass gasification and combustion either with representative particle model [2–4]or discrete particle model [5]. These models solve particle-scale mass and heat transfer equations numerically in parallel with reactor-scale equations, leading high computational load. For example, introduction of *n* particles with *N* grid points into reactor-scale simulation with *M* grids would yield total number of grids as $(N + 1) \times M$ for RPM and $n \times N + M$ for DPM. It is still



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Nomenclature

Α	Pre-exponential factor, s ⁻¹	3	emissivity, –	
Bi	Biotnumber, –	λ	thermal conductivity, W m ⁻¹ K ⁻¹	
Ср	specific heat, J kg ⁻¹ K ⁻¹	μ	viscosity, Pa s	
D	particle diameter, m	ξ	bridge factor, –	
$D_{\rm eff}$	effective mass diffusivity, $m^2 s^{-1}$	ρ	density, kg m ⁻³	
$d_{\rm por}$	pore diameter, m	σ	Stefan-Boltzmann constant, W m^{-2} K ⁻⁴	
Ē	activation energy, J mol ⁻¹	Φ	permeability, m ²	
h	specific enthalpy, $I \text{ kg}^{-1}$	ϕ	void fraction, –	
$h_{\rm off}$	effective heat transfer coefficient. W $m^{-2} K^{-1}$	ŵ	rate of reaction, kg m ^{-3} s ^{-1}	
Δh°	heat of reaction. I kg ⁻¹			
k	rate constant. s ⁻¹	Subscrip	ht	
L	length of cylindrical particle, m	Jubscrip	accumulation	
m	mass of the sample, g	a		
Nu	Nusselt number. –	ave	char	
Р	pressure Pa	C	conduction	
P(L/D)	shape correlation factor. –	C	convection	
Pr	Prandtl number –	dov	develatilization	
0	rate of heat flow or accumulation W	uev	anvironment	
R	narticle radius m	e	effortive value	
Rc	ideal gas constant LK^{-1} mol ⁻¹	en f	final	
Re	Revnolds number _	l Guite	IIIIdi 	
r	radial position m	finite		
r.	position of reaction front m	G	gds	
r dev T	temperature K	I ·	inert gas	
1 +	time c	1	specie i	
	time, s rescuelesity m s ⁻¹	J	reaction j	
U V	gas velocity, ill s volume m^3	max	at maximum rate of reaction	
V MZ	volume of control volume, m	por	pore	
VV	molecular mass, kg mol	S	surface	
X	conversion, –	SCM	special value for the shrinking core model	
X	residual mass, –	Т	tar	
Y	volume fraction, –	W	wood	
		0	initial	
Greek letters				
α	thermal diffusivity, $m^2 s^{-1}$			
β	heating rate, K s ^{-1}			

unknown how complex the particle-scale models should be to express fuel conversion sufficiently. Some studies showed that it is important to consider not only intra-particle mass and heat transfer but also gas flow surrounding the particle [6,7], particle shrinkage [8,9], particle shape [10], and internal microstructure [11]. On the other hand, some studies demonstrated that the detailed particle model such as internal mass transport phenomena [12] or temperature dependent physical properties [13] are unnecessary to acquire the accurate predictions. In fact, some studies have shown that simple particle models agreed with the experimental data sufficiently well by considering only conduction and devolatilization reactions [14,15].

Simultaneous numerical solution of particle-scale and reactorscale models is a time consuming process [16]. Therefore, some studies have tried to decrease the computational load by using some simplification such as applying shrinking core model, SCM (i.e. assumption of infinitely thin reaction zone or sharp interface) [17–22]. The shrinking core model assumes that the devolatilization of biomass particle proceeds as the propagation of infinitely thin reaction front from the surface to the centre of particles. Experimental studies have supported this assumption by showing the propagation of reaction front over the time [23,24]. Such simplifications have demonstrated the improved computational performance. However, a comparison study of various multi-scale models for a packed-bed catalytic reactor [25] showed that the most effective way to decrease the execution time of multi-scale simulation without the loss of accuracy is to derive constitutive equations for particle-scale. Constitutive equations are usually derived either by finding analytical solution of the differential equation or by expressing the independently solved numerical solution with polynomial functions.

The objective of this paper is to demonstrate the methods to simplify the model for fuel conversion of thermally thick particles during devolatilization, especially the suitability of the constitutive equation of the shrinking core model (SCM). We modified the SCM from the previous study for coal particles [24] to be suitable for wood particles. We also investigated the simplification strategies of physical and chemical parameters with detailed particle models to avoid parameter fitting in the constitutive equation. Wood pellets and wood logs were used to consider the differences in physical nature of particles, i.e. density and isotropy.

2. Experimental

2.1. Sample

Cylindrical-shaped wood logs of Cercidiphyllum japonicum (Katsura tree) and wood pellets (90 wt.% pine and 10 wt.% spruce, Bioenergi i Luleå AB) were used. The particle diameters of wood logs were 9.5 and 14.5 mm with various length-to-diameter (L/D) ratios. Particle diameters of wood pellets were 6 and 8 mm with the L/D ratios of 1–4. The mean apparent density of wood logs was around 500 kg m⁻³ and that of wood pellets was around 1100 kg m⁻³. The sample was dried in an oven at 368 K for more than 8 h prior to the

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