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A method for retrieving char oxidation kinetic data from reacting particle trajectories in a novel test facility



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ABSTRACT

In this paper, a new method for retrieving char combustion rates is presented. The method is based on an observation that the curvature of a trajectory of a freely falling and reacting char particle in a horizontal laminar flow changes due to the change of the particles mass. An experimental facility was designed and built allowing for recording reacting particle trajectories and determining oxidation kinetics. A brief description of the experimental facility and measurement procedure is given. In this procedure, a model of a freely falling particle in a laminar horizontal flow was developed. The model comprises a set of ordinary differential equations that predict a particle trajectory for given rate constants. The trajectory predicted by the model is then fitted to the measured trajectories by changing the rate constants. The best fit corresponds to the mean rate constant. Moreover, measurement results for Janina coal char combustion in air at various temperatures are presented. The key input parameters of the model are identified by a global sensitivity analysis, and the uncertainty in the results is quantified. The method is validated by comparison with TGA results obtained from the literature. Finally, the experimental data are used to determine rate coefficients of a kinetic-diffusion surface combustion model. The presented methodology is suitable to determine the kinetic data, however its further development is required in order to improve the accuracy of the measurements and include the more complex physico-chemical processes that occur during carbon conversion.

1. Introduction

Improvement of existing combustion chambers and development of new combustion techniques requires understanding of the elementary processes occurring during fuel conversion. The understanding should be accompanied by reliable data that can be used to predict the system behavior at various conversion stages. In recent years, numerical modeling of combustion processes by means of computational fluid

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Nomenclature		t	time (s)
		Т	temperature (K) or (°C)
Nomenclature		и	horizontal velocity component (m s^{-1})
		ν	vertical velocity component (m s^{-1})
A	area (m^2); pre-exponential factor (s m^{-1})	x	horizontal spacial coordinate (m)
С	diffusion rate constant (s $K^{-0.75}$)	у	vertical spacial coordinate (m)
C_d	drag coefficient (-)		
d	diameter (m)	Greek symbols	
D	diffusion coefficient (m ² s ^{-1})		
E	activation energy (J kmols $^{-1}$)	ϕ	sphericity (–)
g	acceleration due to gravity (m s^{-2})	μ	mean (units vary); dynamic viscosity (kg m ^{-1} s ^{-1})
Gr	Grashof number (–)	ν	kinematic viscosity (m 2 s $^{-1}$)
т	mass (kg)	ρ	density (kg m ⁻³)
ṁ	mass flow rate (g s^{-1})	σ	standard deviation (units vary)
M	molecular weight (kg kmol ⁻¹)	Θ	normalized char conversion rate (s^{-1})
р	pressure (Pa)	ω	weight (–)
R	universal gas constant, $R = 8314.46 (J \text{ kmol}^{-1}\text{K}^{-1})$		
R_c	mean reaction rate constant (kg $m^{-2} s^{-1}$)	Super- and subscripts	
R_{dif}	diffusion rate (m s ^{-1})		
R_{kin}	kinetic rate (m s ^{-1})	0	initial
Re	Reynolds number (-)	р	particle
Ri	Richardson number (–)	S	slip; sphere
Sc	Schmidt number (–)	t	terminal; total
Sh	Sherwood number (-)		

dynamics (CFD) tools became an integral part of the design and optimization processes. The models used in the simulations require closure approximations, which are based on experimental data. In order to improve the predicted system behavior, the quality of the data should be high and the closure models themselves should be fast, robust and accurate. Kinetic parameters of drying, devolatilization and char gasification/combustion, together with ignition characteristics, are crucial elements of simulations of combustion processes. It should be stressed that the experimental data, from which the kinetic parameters are obtained, should be determined at relevant process conditions. Specifically the temperature, the heating rate, the thermal history, the pressure and the atmosphere are of importance [1,2]. Drop tube furnaces (DTF) are already standard devices used to retrieve such data. In recent years, many studies were devoted to characterization of solid fuels. These include ignition characteristics [3-7], kinetic parameters of devolatilization [1,2,8,9], combustion [10-13] and gasification [14–18] processes. The conditions achievable in drop tube reactors are close to or are the same as those observed in the real pulverized coal systems. The investment and operating costs of a DTF are however relatively high and the measurement procedures are time consuming. Another method that is frequently used to obtain kinetic data is the Thermogravimetric analysis (TGA). It is however restricted to low heating rates and lower temperatures (below 1000 °C) due to the inability of observing the real diffusion restrictions at high temperatures. At lower temperatures combustion and gasification rates are controlled by chemical reactions at the solid fuel particle surface. Therefore, TGA



is frequently used in combination with a DTF to determine fuel characteristics at low and high temperature limits [15,16].

In this paper, a new method of retrieving char combustion rates is presented. The method is based on the fact that the trajectory of a freely falling and reacting char particle in a horizontal laminar flow changes due to change of particle mass. An experimental facility, a laminar flow drop furnace (LFDF), was designed and built at the Institute of Thermal Technology, Gliwice, Poland that implements the idea. The experimental facility, as well as basic concepts of the new method, have already been introduced in a previous study [19,20]. In the present work, the method is presented in detail and results of determination of char combustion rate in air are described. A global sensitivity analysis (SA) and uncertainty quantification (UQ) are then conducted to determine the most influential parameters in the model and to quantify uncertainty in the retrieved particle density and mean reaction rate constants. The obtained results are then compared with TGA data adopted from the literature, which were conducted for the same coal and atmosphere. Finally, the experimental data are used to fit a kinetic-diffusion surface combustion model.

2. The experimental facility

The concept of the experimental facility [19,20] is based on an observation that the curvature of the trajectory of a freely falling particle in a horizontal flow changes due to changes of the particle's mass. This behavior can be visualized by comparing trajectories of burning

> Fig. 1. Behavior of non-reactive and reactive particle falling in laminar flow field.

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