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Sensitivity analysis applied to independent parallel reaction model for pyrolysis of bagasse

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ABSTRACT

The independent parallel reaction model (IPR model) is applied in this work to study the slow dynamic pyrolysis of sugarcane bagasse, based on a thermogravimetric analysis of three ranges of particle diameters. The kinetic parameters and mass fraction of each principal pseudo-component of biomass (hemicellulose, cellulose and lignin) are estimated using the Differential Evolution Algorithm. A comparison of the estimated mass fractions and Arrhenius parameters against experimental values reported in the literature shows good agreement. The influence of various kinetic parameters of the model is also analyzed by means of sensitivity studies using derivative methods based on the DASPK 3.0 code. The results of the relative parametric sensitivity indicate that activation energies affect bagasse conversion more strongly than other parameters, followed by the pre-exponential factors of Arrhenius equation and mass fractions. The sensitivity of the IPR kinetic model to the orders of reaction is very slight.

Keywords: Biomass; Differential Evolution; Kinetic model; DASPK code

1. Introduction

Sugarcane bagasse is a lignocellulosic by-product of sugarcane processing to manufacture raw sugar and ethanol. Today, bagasse is often discarded or burned in power plants. Since raw bagasse produces low heat of combustion, its consumption as a primary fuel can be considered wasteful from the standpoint of energy. The transformation of bagasse into a secondary source of energy would significantly increase the total energy yield.

Knowledge of kinetic parameters is essential for the design and optimization of the pyrolysis process. The literature contains several kinetic models, e.g., the single reaction model (Senneca, 2007; Radmanesh et al., 2006; Gonzáles et al., 2003), the consecutive reaction (CR) model (Gonzáles et al., 2003; Mui et al., 2008; Gronli et al., 1999), and the independent parallel reaction (IPR) model (Manyà et al., 2003; Müller-Hagedorn and Bockhorn, 2007; Gómez, 2006). Although widely used, the single reaction model is extremely simplified and may be unsuitable for describing the last stages of the pyrolysis process. In the consecutive reaction model (CR model), each peak in the DTG (differential thermogravimetric analysis) curve corresponds to the individual and sequential decomposition of the pseudo-components, giving the impression that no interactions occur between them. The inaccurate assumption of the CR model, in which the decomposition of one subcomponent only begins after the degradation of another ends, may lead to unrealistic model parameters. In the independent parallel reaction (IPR) kinetic model, the pseudo-components are degraded individually in the same temperature range, ensuring a possibly simultaneous decomposition. Therefore, the rate of weight loss is calculated considering the individual reaction rates and their respective mass fraction.

In context-aware parameter estimation, optimization methods based on natural phenomena and structural approaches have been developed to overcome the problems of classical optimization methods. Differential Evolution (DE) is one of the most promising methods (Storn et al., 2005).

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