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Single char particle model for naphthalene reduction in a biomass gasification system

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ABSTRACT

Tar removal in biomass gasification systems is one of the key challenges to overcome for the successful commercialization of this technology. This study focused on tar conversion over the active char particle besides the simultaneous carbon conversion of the char particle. In the presented model, the char particle was assumed a sphere surrounded by a gas film in a bulk gas composition of naphthalene, nitrogen, steam, hydrogen, carbon monoxide, carbon dioxide and methane. The model treated the heterogeneous gasification reaction kinetics, external and internal mass transfer and changing particle properties during gasification. In addition, the effect of different parameters on naphthalene and carbon conversion was investigated. The investigated parameters were particle size, temperature and time on stream. The gas and solid mass balance equations besides the energy balance equation were solved in the radial direction using a set of initial and boundary conditions. The model results show that the naphthalene and carbon conversion reactions were kinetically limited at the reference conditions of 850 °C bulk gas temperature and 600 μm char particle size. Further, the model calculations show that isothermal char particle can be assumed up to a bulk temperature of about 1160 °C. The variation of the physical properties and pore structure of the char particle with carbon conversion affects the active surface area of the particle. Finally, the results of the single particle model will be extended to a fixed bed reactor model and will be validated with experiments.

1. Introduction

There is a global trend to reduce the dependence on fossil fuels by creating a diversified energy portfolio. This portfolio includes a certain share of renewable energies that varies according to the available renewable sources. Biomass is considered one of these promising renewable energy sources because of its abundance as it provides 14% of the global energy consumption [1], and its potential to reduce global CO_2 emissions [2]. There are many technologies available to utilize the energy content in biomass. Among these technologies, biomass

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Table 1 – Reference values of the model parameters.

Parameter	Symbol	Value
Pressure	P (Pa)	$1.01 \cdot 10^5$
Tar	$C_{10}H_8$	Naphthalene
Bulk temperature	T (°C)	850
Gas residence (space) time	τ (s)	0.3
Superficial gas velocity	u_o (m·s^{-1})	0.08
Char particle size	d_p (μm)	600
Standard gas composition	CO	13%
(volume fraction)	CO_2	11%
	H_2O	11%
	H_2	6%
	CH_4	4%
	$C_{10}H_8$	0.2%
	N_2	Balance

gasification is considered one of the preferable options due to its higher efficiency in power production than the combustion technology. In addition, it can be used in the production of chemicals and fuels. Nevertheless, this technology faces certain technical obstacles that need to be resolved in order to be successfully commercialized. Tar removal is considered the most challenging technical obstacle.

Tars is defined as a generic term comprising all organic compounds present in the producer gas excluding gaseous hydrocarbons (C1–C6) and benzene [3]. Tar can be removed by various methods among which hot gas cleaning is considered the most economical one. This method applies a catalyst under a temperature that essentially matches that of the gasifier [4]. There has been extensive research in literature on catalysts for tar removal. However, there is a limited research that focuses on biomass char despite its promising potential as a catalyst for tar removal.

Because of the growing interest in biomass gasification, several models have been developed in order to explain and optimize the gasification process. In addition, models for tar reduction over different catalysts have been proposed. However, limited modeling has been done on tar reduction over biomass char as a catalyst downstream the biomass gasifier. Several char particle gasification models are available in literature. Most of these models are concerned with the rate of gasification of a single particle [3,4] and the evolution of the particle pore structure during gasification [5]. Raza et al. [5]. developed a simplified particle model to simulate the gasification of char particle in the gasifier. They used the carbon dioxide as the gasification agent that reacts with the char. Wang et al. [6]. developed a generalized model for the prediction of single char particle gasification dynamics, accounting for a chemical reaction with multicomponent mass and heat transfer, structure evolution and peripheral fragmentation. The importance of the model presented in this paper is the focus on tar conversion over active char besides the simultaneous carbon conversion in the char particle.

In a previous work done by Abu El-Rub et al. [7,8], biomass char showed high activity for tar removal under fixed bed conditions. It was found that the pore structure and mineral content of the char particle are the key elements for the char activity. In order to get a better understanding for the effect heat and mass transfer on tar reduction with char, a single char particle model was developed. The model was developed for naphthalene reduction using a porous char particle in an environment of N_2, H_2O, H_2, CO, CO_2 and CH_4. The investigated parameters were particle size, temperature, and time on stream. The results of the single char particle model presented in this paper will be further extended to a fixed bed reactor model that will be validated with experiments.

2. Model development

In this model, the char particle was considered as a sphere surrounded by a gas film in a bulk producer gas with a constant composition. The model treats the intrinsic gasification reaction kinetics, external and internal mass transfer, and changing particle properties during gasification. The model reference conditions are given in Table 1.

2.1. Assumption

The following assumptions were incorporated in the model:

1. The char particle is spherically symmetric. This allows a simplified one-dimensional solution to the species conservation equations.
2. The char particle has a constant external diameter. This assumption approximates the findings presented in a previous work conducted by Abu El-Rub et al. [9]. It was found that the char conversion reaction does not proceed uniformly in the char particle and is not a shrinking particle reaction. Hence, the reaction with the char is somewhere in between.
3. The tar is represented by naphthalene as a model tar component. This assumption is justified by the comparison made in a previous work [9] between naphthalene and real tar conversion over char. It shows that naphthalene is a good representative for real tar.

Table 2 – Modeled tar and char gasification reactions.

Reaction	Rate of reaction (kJ·mol^{-3}·s^{-1})	Reference
$C_{10}H_8 + 10H_2O \rightarrow 10CO + H_2$	$-r_1 = \eta \cdot 10^{-4} e^{-61,000/(RT)} C_n \cdot a$	[7]
$C + H_2O \rightarrow CO + H_2$	$-r_2 = \eta \cdot 2.62 \cdot 10^8 e^{\left(-\frac{237,000}{RT}\right)} \cdot (C_{H_2O}\ RT)^{0.57} \cdot a \cdot \frac{w_c \rho_c}{M_c}$	[10,11]
$C + CO_2 \rightarrow 2CO$	$-r_3 = \eta \cdot 3.1 \cdot 10^6 e^{\left(-\frac{215,000}{RT}\right)} \cdot (C_{CO_2}\ RT)^{0.38} \cdot a \cdot \frac{w_c \rho_c}{M_c}$	[10,11]
$C + 2H_2 \rightarrow CH_4$	$-r_4 = \eta \cdot 9.14 \cdot 10^{-10} e^{\left(-\frac{149,050}{RT}\right)} \cdot (C_{H_2} RT) \cdot S_o \cdot a \cdot w_c \cdot \rho_c$	[12]
$H_2O + CO \cdot H_2 + CO_2$	$r_5 = 2.78 \cdot 10^3 \cdot e^{\left(-\frac{12,5060}{RT}\right)} C_{H_2O} C_{CO} - 1.05 \cdot 10^5 \cdot e^{\left(-\frac{-45,466}{RT}\right)} C_{H_2} C_{CO_2}$	[13]