Modeling Gas Effects in a Bubbling Fluidized Bed Reactor for Biomass Pyrolysis

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Contents

Abstract

Fast pyrolysis of biomass in a fluidized bed reactor is typically conducted in a nitrogen gas environment. Recycling product gas can improve the economics of operating such a system by reducing reliance on pure process streams.

1 Introduction

Fast pyrolysis is a versatile method for thermochemical conversion of solid biomass into liquid bio-oil which can be used for bio-fuel and high-value chemical production. Bio-oil is commonly generated in bubbling fluidized bed and circulating fluidized bed reactor systems in which biomass particles rapidly devolatilize in the absence of oxygen into mixtures of light gases, condensable

bio-oil vapors, and solid char [2, 3, 7]. Since biomass pyrolysis normally occurs in a non-oxidizing environment, the fluidization gas (carrier gas) is often pure nitrogen [7]. To maximize bio-oil yields, the reactor typically operates at temperatures near 500°C and must maintain particle residence times up to 10 seconds and gas residence times less than 2 seconds [3]. Deviations from these conditions can result in significant production and quality penalties, therefore optimal reactor design and control become crucial to achieving commercially viable bio-oil production.

To improve the economic possibilities of biomass fast pyrolysis systems, char can be burned for process heat while recycled pyrolysis gas can assist with fluidization [2, 5]. The major generated components of pyrolysis gas are CO, CO_2, CH_4, H_2, and other light hydrocarbons [1, 11]. Several experiments investigated the effects of these gases on reactor conditions and pyrolysis yields [5, 8, 11] but modeling the effects of the different gases was not discussed.

There are several models available that investigate the hydrodynamics and conversion of biomass at fast pyrolysis conditions in fluidized bed reactors [9, 6]. As is typical for biomass pyrolysis, these models assume the fluidization gas is pure nitrogen. The authors are not aware of any published models in the biomass pyrolysis literature that account for the effects of fluidization or carrier gas other than nitrogen.

This paper uses engineering correlations, reduced-order modeling techniques, and CFD simulations to investigate the effects of gas mixtures in a fluidized bed biomass pyrolysis reactor. The scope of this study is to evaluate different gas mixtures and there effects on the hydrodynamics and biomass conversion in fluidized bed reactors operating at fast pyrolysis conditions.

2 Experimental apparatus

The NREL 2FBR system thermochemically converts biomass particles at fast pyrolysis conditions. The system is comprised of a bubbling fluidized bed reactor for fast pyrolysis of woody biomass particles. This reactor is referred to as the "pyrolyzer" in this work. An overview of the system is shown in Figure 1. Dimensions and typical operating conditions of the pyrolyzer are given in Figure 2. More information about the NREL pyrolysis system is available elsewhere [4, 10].
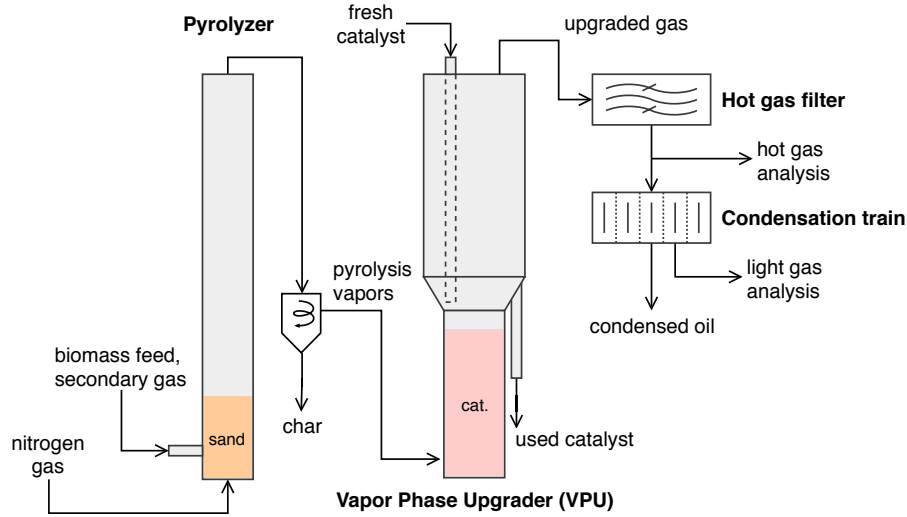
Figure 1: Overview of the NREL 2FBR system. Biomass fast pyrolysis occurs in the pyrolyzer (left) and gaseous products are catalytically upgraded in the vapor phase upgrader (right).
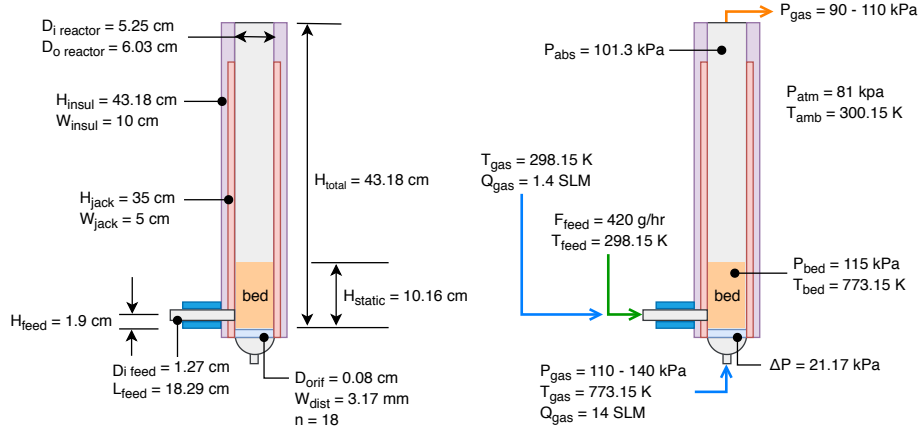

Figure 2: Dimensions and typical fast pyrolysis operating conditions of the NREL 2FBR pyrolyzer.

3 Modeling approach

Engineering correlations, reduced-order models, and CFD modeling techniques were used to investigate the effects of recycled gas on the operation of a fluidized-bed biomass pyrolysis reactor. The following sections discuss approaches imple-

mented in this work for calculating gas properties and the associated effects on fluidization conditions and pyrolysis yields.

3.1 Gas properties

Density (kg/m^3) of an individual gas is calculated from the ideal gas law

$$\rho_{gas} = \frac{P\,M}{R\,T} \tag{1}$$

where P is pressure (Pa), M is molecular weight (g/mol), R is the gas constant [(m^3 Pa) / (K mol)], and T is temperature (K). Gas viscosity (μP) is given as

$$\mu_{gas} = A + B\,T + C\,T^2 + D\,T^3 \tag{2}$$

where coefficients A, B, C, and D are obtained for a given gas from tables in Yaws' Handbook and T is gas temperature (K). Thermal conductivity (k) of the gas is given as

$$k_{gas} = A + B\,T + C\,T^2 + D\,T^3 \tag{3}$$

where coefficients A, B, C, and D are also from the Yaws' Handbook and T is again the gas temperature (K).

For a gas mixture, density is calculated as a weighted average of the individual gas densities. The viscosity of a gas mixture can be calculated from a variety of correlations.

3.2 Fluidization correlations

Here.

3.3 CFD simulation

Here.

3.4 Pyrolysis kinetics

The Di Blasi kinetic scheme was implemented to predict the conversion of the biomass into gas, tar, and char products. Figure 3 gives an overview of the Di Blasi scheme and its reaction mechanisms. Reactions 1–3 are the primary conversion of the biomass while reactions 4–5 are secondary reactions that reduce tar yield at long residence times.
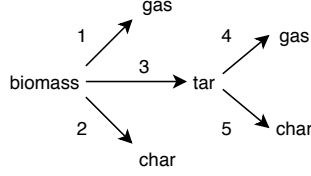
Figure 3: Diagram of the Di Blasi pyrolysis kinetics for conversion of biomass to gas, tar, and char products.

3.5 Parameters

Parameters for the reduced-order model and CFD simulations are provided in Table 1. Biomass particle parameters and properties are representative of loblolly pine. Bed particle parameters are for typical sand material. Operating conditions and reactor dimensions are based on the previously discussed NREL 2FBR fluidized bed pyrolysis unit.

Table 1: Biomass, bed, and reactor modeling parameters. Particle diameters represent the Sauter-mean diameter.

Parameter	Description	Value
$d_{p, bed}$	diameter of bed particle	235 μm
ϕ_{bed}	sphericity of bed particle	0.0
$d_{p, bio}$	diameter of biomass particle	135 μm
ϕ_{bio}	sphericity of biomass particle	0.0
ρ_{bio}	density of biomass particle	540 kg/m^3
$h_{reactor}$	reactor height	43.18 cm
h_{static}	static bed height	10.16 cm
tk	reactor temperature	773 K

4 Results and discussion

Molecular weight, viscosity, density, and thermal conductivity of the individual gases investigated in this paper are shown in Figure 4. The gas properties were calculated at a pressure of 101,325 Pa and a temperature of 773.15 K (500°C). The lightest gas in terms of molecular weight and density is hydrogen while the heaviest gas is carbon dioxide. Viscosity for all the gases except hydrogen ranged from 300–350 μP. Thermal conductivity for all the gases is near 0.05 W/(m K) except for hydrogen which is approximately 0.35 W/(m K).
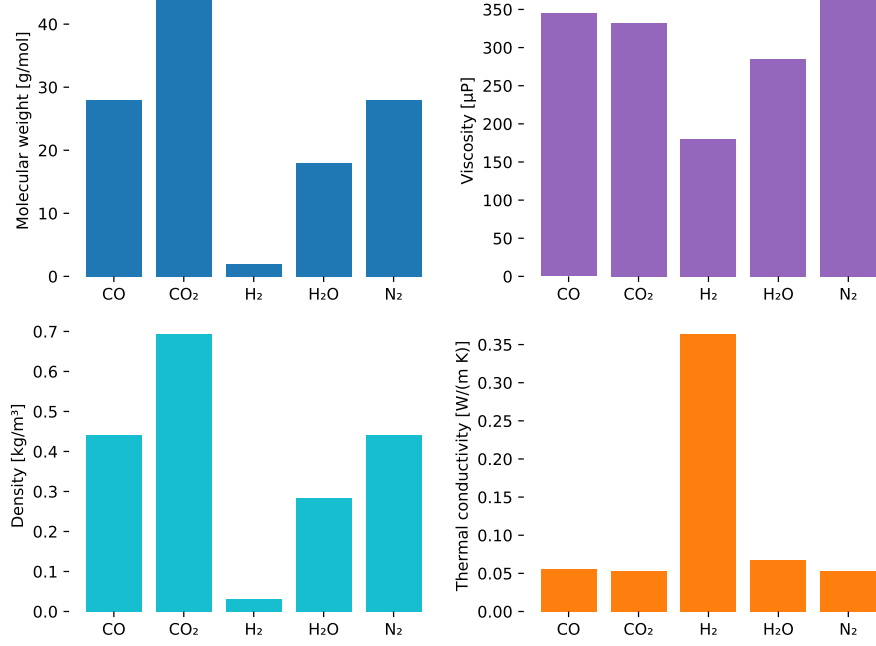
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Figure 4: Comparison of molecular weight, viscosity, density, and thermal conductivity for individual gases at 101,325 Pa and 773.15 K.

Properties for molecular weight, viscosity, and density for the gas mixtures investigated in this paper are shown in Figure 5. Similar to the individual gas properties, the mixture properties were calculated at 101,325 Pa and 773.15 K (500°C). The fraction of each gas in the mixture is given by the values shown at the top of each column in the figure. For example, the hydrogen and nitrogen mixture is comprised of 80% hydrogen and 20% nitrogen which is labeled as $0.8 + 0.2$. As expected, the carbon dioxide mixture is the heaviest in terms of molecular weight and density.
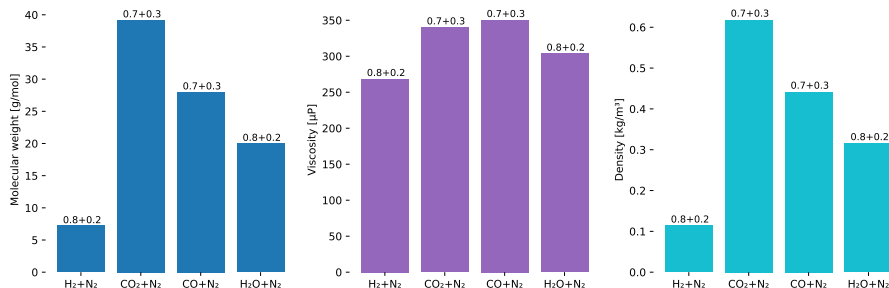
Figure 5: Comparison of gas mixture properties for molecular weight, viscosity, and density at 101,325 Pa and 773.15 K. Fraction of each gas component is shown at the top of each column.

5 Conclusion

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6 Source code

Python models used to generate results for this article are available on the CCPC GitHub at `https://github.com/ccpcode` in the X repository. Functionality provided by the Chemics package was used for gas properties and various fluidization calculations. See the Chemics documentation at `https://chemics.github.io` for more information.

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