

# Quantifying Mixing in a Multiple-feed Fluidized Bed Reactor for Catalytic Fast Pyrolysis of Lignocellulosic Biomass

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## Introduction

The objective of this work is to quantify the mixing quality within a multiple-feed fluidized bed reactor used for catalytic fast pyrolysis (CFP) of lignocellulosic biomass. The reactor under development is in experimental stages and utilizes CFP to convert biomass into gasoline-range aromatics in a single step reaction [1]. A non-standard inlet, a downward-facing, central, vertical feed tube, is used to input the cellulose deep into the reactor. The cellulose is oxygenated into vapors before entering the reactor [2], and these vapors then enter the catalyst pores wherein they are converted to aromatics. Due to the high operating temperatures (773 K) necessary for CFP, an enclosed and insulated reactor must be used, which means the hydrodynamic mixing of the catalyst, the fluidizing gas (an inert He gas), and the biomass gas stream can only be indirectly measured from the aromatic yield and other byproducts. Computational fluid dynamics (CFD) simulations using ANSYS© Fluent, version 14.0, were used to simulate the internal hydrodynamics by neglecting chemical reactions, considering only a two-phase mixture as well as inert tracer gases from each inlet. From here, the mixing of the catalyst and a given gas stream inlet was quantified using time-ensemble statistics of the mixture fraction, which is defined in terms of an inert tracer gas proceeding from the inlet of interest [3].

## Theory

### Two fluid model

The Eulerian-Eulerian two fluid model (TFM) treats both the solids and gas phase as interpenetrating continua each occupying a percent ( $\alpha_s$  and  $\alpha_g$ , respectively) of a computational cell in space [4]. By conservation of mass,  $\alpha_s + \alpha_g = 1$  within every cell. Each phase is treated as a liquid with the catalyst having a much greater density ( $\rho_s$ ) than the gas ( $\rho_g$ ). The kinetic theory of granular flow (KTGF) is used to account for the catalyst viscosity,

particle collisions, frictional stresses between particles, and the drag between the particles and the gas [5, 6, 7].

## Governing equations

The governing conservation equations of mass and momentum utilized in ANSYS Fluent are derived by Ishii [8], and these equations were rewritten for gas-solids flows by Enwald et al. [9]. The conservation equations as reproduced in van Wachem et. al [10] are shown in this work. The continuity equations for the solids and gas phases are listed below, respectively, as

$$\frac{\partial \alpha_s}{\partial t} + \nabla \cdot (\alpha_s \mathbf{v}_s) = 0 \quad (1)$$

and

$$\frac{\partial \alpha_g}{\partial t} + \nabla \cdot (\alpha_g \mathbf{v}_g) = 0; \quad (2)$$

Enwald et al.'s [9] conservation of momentum equations are shown below for the solids and gas, respectively:

$$\rho_s \alpha_s \left( \frac{\partial \mathbf{v}_s}{\partial t} + \mathbf{v}_s \cdot \nabla \mathbf{v}_s \right) = -\alpha_s \nabla P + \nabla \cdot \bar{\bar{\tau}}_s - \nabla P_s + \alpha_s \rho_s \mathbf{s} + \beta(\mathbf{v}_g - \mathbf{v}_s) \quad (3)$$

and

$$\rho_g \alpha_g \left( \frac{\partial \mathbf{v}_g}{\partial t} + \mathbf{v}_g \cdot \nabla \mathbf{v}_g \right) = -\alpha_g \nabla P + \nabla \cdot \alpha_g \bar{\bar{\tau}}_g + \alpha_g \rho_g \mathbf{g} - \beta(\mathbf{v}_g - \mathbf{v}_s) \quad (4)$$

Conservation of energy as given in the ANSYS Fluent Theory Guide [11] is given for phase  $k$  as

$$\frac{\partial}{\partial t} (\alpha_k \rho_k h_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{v}_k h_k) = \alpha_k \frac{\partial P_k}{\partial t} + \bar{\bar{\tau}}_k : \nabla \mathbf{v}_k - \nabla \cdot \mathbf{q}_k, \quad (5)$$

where  $h_k$  is the specific enthalpy of phase  $k$ . See the notation for the definition of each of the terms in these equations.

# Nomenclature

$\beta$	Interphase drag coefficient (kg/(m <sup>3</sup> ·s))
$g$	Gravity constant (m/s <sup>2</sup> )
$q_k$	Heat flux of phase $k$ (W/m <sup>2</sup> )
$v_k$	Velocity of phase $k$ (cm/s)
$\bar{\bar{\tau}}_k$	Viscous stress tensor of phase $k$ (N/m <sup>2</sup> )
$\rho_k$	Density of phase/species $k$ (kg/m <sup>3</sup> )
$\alpha_k$	Volume fraction of phase $k$ (dimensionless)
$d_s$	Particle diameter (m)
$h_k$	Specific enthalpy of phase $k$ (J/kg)
$P$	Pressure (Pa)
$P_s$	Solids pressure (Pa)
$t$	Time (s)

# References

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