CFD-assisted Process Intensification for biomass fast pyrolysis in Gas-Solid Vortex Reactor technology

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Biomass fast pyrolysis is considered an alternative route to replace fossil fuels as primary source of energy and chemicals [1]. Fast pyrolysis of biomass can yield up to 75% (w/w) bio-oil (of the fed biomass), provided the applied reactor technology can simultaneously satisfy the several demands, the most pressing ones being: high heat flux to biomass particles, reduced contact time between generated bio-oil vapors and char particles, and rapid removal and condensation of these vapors. Gas-Solid Vortex Reactors (GSVR) are a new generation of multiphase reactors in which a rotating fluidized bed is realized via gas injection at high tangential velocities ($\sim 60-120~{\rm m~s^{-1}}$). Centrifugal instead of the gravitational force counteracts the drag force on the bed of particles, resulting in relatively denser beds and higher gas-solid slip velocities ($5-6~{\rm m~s^{-1}}$) as compared to conventional fluidized bed reactors. Due to the overall higher gas velocities ($20-40~{\rm m~s^{-1}}$ for particulate flows), the residence time of the gas phase in a GSVR is lower, thus reducing undesired gas-phase secondary reactions in the pyrolysis product mixture. Considering all these advantages, a GSVR becomes a suitable candidate to perform fast pyrolysis of lignocellulosic biomass.

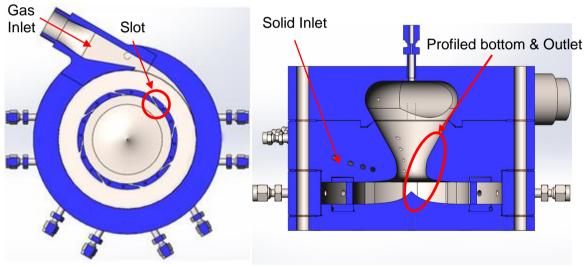


Fig. 1: Top and side view of the reactive GSVR indicating salient design features.

At the Laboratory for Chemical Technology (LCT), experimental and numerical research on the GSVU(nit) and GSVR(eactor) technology has demonstrated its suitability for Process Intensification [2] [3]. Experimental research was non-reactive only. The next step in this research is an experimental study in the reactive setup, currently operational at the LCT. This is a setup specifically designed to study heat-intensive processes such as biomass fast pyrolysis, oxidative coupling of methane, etc. To the best of our knowledge this is the first setup of its kind [4]. The GSVR design, as indicated in Fig. 1 consists of two concentric cylinders in which the fluidization gas is distributed around the annulus and enters the reactor chamber via eight rectangular 1 mm wide inlet slots positioned at a 10° angle with respect to the tangent of the

cylinder. The axial length of the reactor is 15 mm and the internal diameter of the reactor chamber is 80 mm. Biomass is fed into the reactor next to the gas inlet slots, through a circular conduit of 10 mm diameter positioned at an 18° angle with respect to the horizontal plane.

Cold flow experiments have already been performed on this setup, using compressed air as the fluidizing medium and various solid types to study the hydrodynamics of this reactor. Fig. 2 shows the formation of a densely packed, rotating bed of mono-dispersed Aluminum particles (dp = 0.5 mm), rotating counter-clockwise inside this GSVR during a cold-flow experiment. The average bed porosity is observed to be 0.4 - 0.6, indicating a relatively packed bed (with a thickness up to 7 mm) as compared to the bed porosity in a conventional fluidized bed reactor. The bed is found to be rotating with an average azimuthal velocity of 1-4 m s⁻¹. A Particle Image Velocimeter (PIV) is used to accurately measure the rotational velocity of solid bed.

Fig. 3 highlights the formation of a densely packed bed of solid particles as calculated by a Eulerian-Eulerian CFD simulations of a pie-shaped volume (1/8th of the entire reactor, consisting of one gas inlet slot) of the experimental setup.



Fig. 2: Densely packed Aluminum bed in a GSVR as captured using PIV.

2D CFD (Computational Fluid Dynamics) simulations of a GSVR for biomass fast pyrolysis using a lumped kinetic model have already been performed, predicting bio-oil yields as high as 70%. (w/w) with gas to particle heat transfer coefficients as high as ~500 – 800 W m⁻² K⁻¹ were predicted [5]. However, these 2D simulations do not take into account the end-wall effects which are expected to substantially influence the reactor hydrodynamics and hence the bio-oil yields in the GSVR. In order to predict a more detailed product composition and thus accurately quantify Process Intensifications in a GSVR, 3D reactive simulations need to be performed by coupling the hydrodynamic model with a *detailed* reaction model.

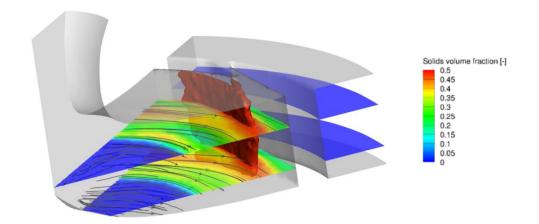


Fig. 3: Time-averaged solids volume fraction across two axial planes, iso-surfaces of solids volume fraction and streamlines indicating flow of the gas phase.

3D reactive simulations have already been performed at the LCT using a *lumped* reaction model used by Ashcraft et al. [5] and for simulation conditions enlisted in Table 1.

Reactor geometry	Pie-shaped, containing 1 gas injection slot
Simulation type	Eulerian-Eulerian; FLUENT v15
Nitrogen inlet temp (K)	842
Nitrogen inlet flow (kg hr ⁻¹)	18
Biomass feed rate (kg hr ⁻¹)	2.4
Biomass feed temp (K)	298
Time step (s)	10 ⁻⁴
Turbulence model	k-ε RNG
Primary phase	Gas Mixture (N ₂ , pyrolysis gas, bio-oil vapors)
Secondary phase – I (Granular)	Biomass
Secondary phase – II (Granular)	Char
Interphase interactions	Drag: Gidaspow correlation [6]
	Heat transfer: Gunn correlation [7]

Table 1: CFD simulation conditions in the GSVR

These simulations resulted in a high bio-oil yield (w/w) of 68% (char and pyrolysis-gas yields are (w/w) 21 and 11% respectively) showing promising prospects to carry out fast pyrolysis reactions in GSVRs. During these simulations, it was observed that the char formed tends to accumulate near the reactor exhaust zone, making it more likely to get entrained along with the gas leaving through the central outlet. The latter will additionally result in a reduced contact between bio-oil vapors and char, thus reducing the secondary reactions that lower the bio-oil yield.

Ranzi et al. [8] proposed a kinetic model for thermal degradation of biomass constituents (cellulose, hemicellulose and lignins) into a detailed product matrix via solid de-volatilization, gasphase secondary reactions and char gasification. This model is considered suitable to be implemented in 3D reactive CFD simulations, because of its comprehensive nature towards various product species. Additionally, the simplifying assumption of biomass being spherical particles

has been assessed in the present work as cylindrical shaped particles is considered a more accurate approximation.

The obtained product yields when using the detailed Ranzi model [8] and accounting for the non-sphericity of the particles will allow to further evaluate the GSVR performance.

Acknowledgements

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