Numerical Study on Catalytic Hydrodeoxygenation of Pyrolytic Bio-Oil Model Compound, Guaiacol, in Fluidized Bed Reactor

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Original Research

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Abstract

The bio-oil obtained by thermochemical conversion of lignocellulosic biomass consist of large fractions of oxygenated compounds which deteriorate its quality leading to low calorific value, high viscosity, high density, high moisture content, etc. Therefore, the bio-oil should be deoxygenated using hydrogen in the presence of appropriate catalyst to improve its properties. Adequate literature on pyrolysis of biomass within the framework of computational fluid dynamics is available but only a couple of papers available on hydrodeoxygenation of bio-oil obtained by pyrolysis. Thus, in this study, guaiacol has been selected as a representative model compound of phenolic fraction of bio-oil for upgrading it by catalytic hydrodeoxygenation. The reaction process has been implemented in a fluidised bed reactor in the presence of palladium catalyst, Pd/Al₂O₃ using computational fluid dynamics (CFD) based solver, ANSYS Fluent 14.5. The range of conditions considered herein are: weight-hourly space velocity (WHSV) = 1, 3 and 5 h⁻¹ ; superficial H₂-gas velocity, $u = 0.075, 0.15$ and 0.25 m/s; catalyst load = 0.06 kg and temperature, $T = 548$ K, 573 K, and 598 K. The solver has been thoroughly validated in terms of grid dependence study, time step size dependence study validating hydrodynamics and HDO results wherever possible with existing literature results. The HDO of guaiacol produces phenol as the most abundant compound along with significant amount of cyclopentanone and methanol. The formation of cyclopentanone from HDO of guaiacol is favourable at high temperature whereas low temperature conditions favour formation of methanol and phenol.

Full Text

Due to technical limitations, full-text HTML conversion of this manuscript could not be completed. However, the manuscript can be downloaded and accessed as a PDF.

Figures

Figure 1

Schematic illustration of a fluidized bed reactor used in this study.

Figure 2

Combined effects of grid, drag models and comparison of the present bed expansion ratio with the literature [33] counterparts under identical conditions.

Figure 3

Combined effects of grid size, time step and drag models on time average height of fluidized bed at superficial velocity $u = 0.38$ m/s.

Figure 4

Mass fraction of HDO products of guaiacol as a function of WHSV at different temperatures and constant H₂-gas velocity ($u=0.075$ m/s).

Figure 5

Mass fraction of HDO products of guaiacol as a function of WHSV at different temperatures and constant H₂-gas velocity (u=0.25 m/s).

Figure 6

Mass fraction of HDO products of guaiacol at T=548 K as a function of H₂-gas velocity at different WHSV.

Figure 7

Mass fraction of HDO products of guaiacol at $T=598 K$ as a function of H_2 -gas velocity at different WHSV.

Figure 8

Distribution of reactant and products of guaiacol HDO at $u=0.075 m/s$ and $T=573 K$.

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