

Abstract

Packed bed reactor (PBR) is one of the classical reactor configurations that has widespread applications in several chemical and biochemical process industries, as well as, in petroleum refinery industries. Hydrodynamics of PBRs is mostly involved with one or multiple fluid phases flowing through tortuous paths formed by catalyst packing arrangements. Familiarized with the steady state hydrodynamics over the past two decades, researchers have explored the efficacy of unsteady state PBRs in sustainable operation and prolonged reactor life. This work aims to systematically investigate the influence of periodic/cyclic flow operation with single-phase Newtonian and non-Newtonian fluids in PBRs with structured packing arrangements. Thereafter, two-phase gas liquid flow coupled with chemical reaction studies are carried out to understand benefits of cyclic flow over steady state operation. Firstly, a 3D computational fluid dynamics (CFD) model is developed to understand the influence of periodic operation in single-phase PBRs. Unit cell approach is adopted to represent the packed bed with spherical particles having face centered cubic (FCC) and modified simple cubic (MSC) packing arrangements. Three different *on-off* and *min-max* flow splits are analyzed and compared for single-phase liquid flow operation. Comparison of results reveals the benefit of periodic mode in terms of homogeneous flow distribution than that of the continuous mode operation. The effect is more pronounced at higher split ratios for FCC, and vice versa for modified SC arrangement. Moreover, *on-off* operation in both packing orientations exhibited a relatively better flow homogeneity as compared to *min-max* mode. Liquid distribution analysis indicates the improvement in flow homogeneity at the expense of a higher pressure drop in periodic operation. The model is further extended to study the influence of power law index (n) for non-Newtonian fluids. Flow homogeneity was found to deteriorate for higher n values accompanied by an increase in pressure drop with respect to Newtonian cases. Nonetheless, the effect of packing arrangement on hydrodynamics showed the same trend as in the case of Newtonian fluid.

Later, a 2D axis-symmetric CFD model of a hydrotreating PBR operating in trickle flow regime is developed to delineate the efficacy of flow modulation in HDS and HDN reaction systems following Langmuir-Hinshelwood and power law rate kinetics, respectively. Fast and slow modes of *on-off* and *min-max* flow modulations with different split ratios are compared with time averaged continuous operation for reaction conversion. *On-off* and *min-max* flows resulted in significant improvement in conversion as compared to time averaged steady state operation, which was more pronounced for *on-off* flow. All cases of *on-off* and *min-max* flows for slow mode proved beneficial than time averaged continuous operation with respect to maximum improvement in conversion. However, this was accompanied by significantly higher undulations in overall pressure drop, in addition to conversion decreasing drastically during peak flow periods. Nevertheless, fast mode of *on-off* and *min-max* operations at low split ratio resulted in improved conversions with lower undulations in overall pressure drop. Non-linear hydrodynamics combined with multiscale transport processes engenders the modeling of PBR a challenging task, particularly in addressing the scale up issues for its commercial application. Complexity in modeling of PBRs further increases while incorporating unsteady state (cyclic or periodic) operation of the bed for process intensification. Although computational studies cannot completely diminish the necessity of exhaustive and at times expensive experimental investigation, CFD models can certainly complement with various aspects of physical phenomena that are not attainable by experiments. The findings of this work are expected to not only provide a comprehensive modeling approach for single and two phase hydrodynamics and reactions in periodically operated PBRs, but also to explore the viability of cyclic flow operation as a process intensification technique.

Keywords: Computational fluid dynamics; Process intensification; Periodic operation; Packed bed reactors; Non-Newtonian liquid; Two-phase flow