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Influence of periodic operation on flow distribution in single phase packed beds

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ABSTRACT

A 3-D computational fluid dynamics (CFD) model is presented to understand the influence of periodic operation in single phase packed bed reactors (PBRs). Unit cell approach is adopted to represent the packed bed with spherical particles having face centered cubic (FCC) and modified simple cubic (SC) 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 velocity 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. Single phase flow in packed beds finds several applications in heat transfer and reaction processes. This study essentially demonstrates the potential benefits of periodic operation to obtain homogeneous liquid distribution in packed beds with cubic close packing, which is of paramount importance in improving overall reactor performance.

1. Introduction

A column with packed bed has been a strong foundation in various fields of chemical and petroleum industries for processes involving filtration, absorption, desorption, distillation, and catalytic reactions e.g., hydrodesulfurization, hydrodenitrogenation, cracking [1–6]. In packed bed reactor (PBR), there is flow of single- or multi-phase component(s) through interstices in between catalytic packing particles [7–9]. The mechanism of mixing and other transport processes caused by fluid-solid and fluid-fluid interactions in PBRs [10,11], are governed by flow through constricted and tortuous paths, which in turn lead to different flow patterns [12,13]. Consequently, modeling of PBRs comprising non-linear hydrodynamics coupled with varying transport phenomena is a challenging task. Development of a physically realistic model would thus require prior knowledge of the forces associated with such interactions in order to obtain a holistic understanding of the key influential parameters on hydrodynamics and other transport phenomena. Further complication arises while modeling periodically operated (unsteady or cyclic) PBRs that are used for process intensification [14,15]. 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 [16–18]. Periodic operation of PBRs has become a point of interest for many researchers owing to its significant contribution in improved rate of reaction, higher throughputs and reactor service life [18,19]. It involves periodic toggling of inlet feed between a high level (peak) and a low level (base) flow rate, which is typically termed as the *min–max* operation. When the base flow rate is set to zero, it is referred as *on–off* operation [20]. Based on the duration of pulse incursion, it can further be classified as slow mode (pulse duration in minutes) and fast mode (pulse duration in seconds) [21–24].

Majority of industrial process reactions in multiphase PBRs are classified as either liquid or gas phase limiting reactions according to which an appropriate mode of cyclic operation may be employed. Gas phase limited reactions are typically favored by partial wetting of catalyst particles to ensure a greater passage of gas to the surface of the particles [25]. Continuous operation of multiphase PBRs often leads to liquid maldistribution, thereby compromising reactor performance as a result of incomplete wetting of the catalyst surface. A remedial method for improved reaction rates can be achieved by temporally manipulating catalyst wetting, as a result of the on–off slow mode liquid induced pulsing flow [26–28]. Additionally, in case of exothermic reactions, this strategy also helps in eliminating the chances of hot spot formation by periodically removing the heat of reaction during pulse

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Nomenclature

a	ratio of wetted area to volume of the cell (m^2/m^3)
D_i	distribution index
d_P	particle diameter (m)
E_1, E_2	Ergun's constant
f	total friction factor
g	acceleration due to gravity (m/s^2)
l	length of bed (m)
ΔP	pressure drop, (Pa)
Re_p	particle Reynolds number ($\rho u d_P/\mu\epsilon$)
u	superficial velocity (m/s)
u_c	time averaged velocity for continuous operation (m/s)
Greek symbol	
ϵ	bed voidage
ρ	density (kg/m^3)
Subscripts	
p	peak
b	base

incursion periods [29]. On the contrary, liquid limited reactions require a high flow of liquid reactant at the surface of catalyst particles to ensure comprehensive wetting efficiencies, which is inevitable for solid–liquid mass transfer [25]. Although a steady state operation in pulse flow regime i.e., high gas and liquid flow rates can accomplish such scenario, shorter phase contact time adversely affects conversion efficiency in addition to excessive mechanical energy demand resulting from higher pressure drop. A fast mode of liquid induced pulsing flow can address this issue by eliminating the requirement of a higher flow rate and at the same time by maintaining a steady base flow rate of an uninterrupted liquid stream [25]. A more detailed insight on the merits and applicability of periodic flow operation in PBRs has been summarized by Atta et al. [30].

Despite several potential benefits of periodic flow operation, commercial scale multiphase PBRs are refrained from the implementation of any cyclic strategy due to the nonlinear hydrodynamics, which might endanger process control safety. However, comprehensive modeling approaches and methodical experimentation might be used to obtain sound predictions [26]. However, detailed analysis solely based on experimentation may be inadequate to address the influence of all key parameters owing to the involvement of a considerable amount of time and money. Recent advances in computational fluid dynamics (CFD) based models can be effectively exploited to validate a set of comprehensive experimental data and can further be extended to gain an insight into flow field problems like channeling, distribution, and temperature variations. Flow inhomogeneities degrade the performance of a PBR dealing with reactive flow systems [31]. In multiphase PBRs, several studies have been reported for periodic operation of the liquid feed (owing to higher inertial effect) instead of gas feed to improve liquid distribution inside the bed [32,33]. The presence of a gas phase will influence the liquid distribution, but it is imperative to get a fundamental understanding of the liquid flow behavior that will be subjected to periodic operation.

Maldistribution or inhomogeneity in local liquid velocity in the bed voidage is typically quantified in terms of local liquid flow rate or velocity [34,35]. For single phase operation in packed beds, homogeneity in local fluid velocity is essential due to its direct influence on heat transfer and reaction kinetics. Karthik and Buwa [36] simulated turbulent, unsteady single phase flow (pure and multicomponent) to investigate the effect of particle shape and orientation on fluid flow, pressure drop, heat transfer and reaction efficiency. They reported that cylindrical particles led to reduced velocity variation, which had a significant impact on improved reaction rate and overall reactor performance. Nemec and Levec [9] studied single phase pressure drop with flow rates corresponding to trickle regime in a region of uniformly sized spherical and non-spherical particles. They showed that pressure drop through packed bed was the result of frictional losses, described by the linear dependence upon the flow velocity, and inertia, characterized by the quadratic dependence upon the local flow velocity. Guardo et al. [37] showed the effect of buoyancy forces over flow patterns and convective flow of a single-phase in fixed beds at supercritical condition. Flow distribution, velocity gradients and flow direction were found to influence the extraction rate and heat transfer, which accentuated with the increase in flow rate for gravity assisted flow. Freund et al. [31] analyzed single-phase reacting flows by a carrier gas using Monte Carlo method to generate random packing and Latice-Boltzmann method for transport of reacting species. They reported that for reacting flows, packing structure and local homogeneity in flow velocity had significant effect on overall reactor performance. Furthermore, high reactive zones marked by local peaks of product concentration resulted in catalyst deactivation as a consequence of hot spots formation in exothermic reactions. Jiang et al. [38] numerically predicted bed-scale gas velocity distribution based on minimization of the total rate of energy dissipation. They reported that local gas velocity distribution had significant effect on transport and reaction rates. Energy dissipation rate was found to be influenced by bed structure, local velocity distribution in radial and axial directions, and presence of internal obstacles i.e., packing particles. Papageorgiou et al. [39] studied catalyst preparation by impregnation based on the adsorption-diffusion mechanisms of single and multi-component single-phase liquid. They stated that the distribution or local flow homogeneity was crucial to control desired parameters of synthesized catalyst. Additionally, insights on spatial distribution of the velocity gradients facilitated the understanding of transport phenomena at the wall [40]. Dasgupta and Atta [41] described the benefits of min–max mode operation over continuous flow for non-Newtonian fluids in packed beds with cubic close packing. For multiphase PBRs, comparative studies between on–off and min–max operations have been carried out to understand their influence on liquid distribution and reactor performance [32,42]. Researchers have also explored the possibility to remove fines deposition inside the bed by implementing min–max operation under both slow and fast modes in multiphase operation [23,43].

Interestingly, limited research has been directed towards the development of computational modeling approaches to address the effect of operating parameters on periodic PBRs [44–47]. Additionally, none of the studies have addressed the effect of bed porosity and particle orientation on the hydrodynamic behavior of the system. We recently reported a detailed analysis of local velocity distribution for single phase Newtonian and non-Newtonian liquids in periodically operated PBRs [41]. However, that study was restricted to only min–max mode of flow operation. Moreover, there were no reports on the comparison of cyclic modulation strategies (on–off and min–max) in single phase PBRs, and on identification of the optimum operation in terms of mode and split ratio, which can establish homogeneous velocity distribution inside the bed. Accordingly, we demonstrated a comparative analysis between three splits of min–max and on–off flow operations, and described its advantages over continuous flow having superficial velocity identical to peak value of cyclic operation [48]. Although an optimized split and flow modulation strategy was identified, that study was inconclusive on the comparison of flow modulated results with their corresponding time averaged continuous flow cases, which can establish the benefit of flow modulation for a common basis. In light of the