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Analysis of single phase Newtonian and non-Newtonian velocity distribution in periodic packed beds

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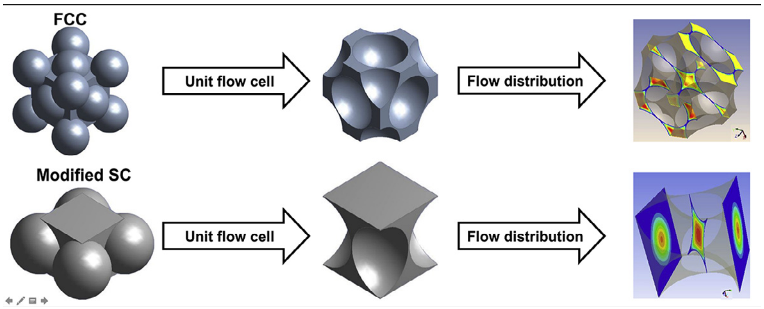
HIGHLIGHTS

- 3-D CFD model is presented to simulate periodic operation in packed bed reactors.
- Velocity distributions are studied for two different packing arrangements.
- Flow maldistribution during fast mode of min–max periodic operation is assessed.
- Analyzed a distribution index to understand the effect of periodic operation on velocity distribution.

GRAPHICAL ABSTRACT



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ABSTRACT

A three dimensional computational fluid dynamics (CFD) model based on unit cell concept is presented to analyze the hydrodynamics of periodic operation in packed bed reactors (PBRs). Flow profiles, mass flux distribution, and pressure drop results are studied for various split ratios with Newtonian and non-Newtonian power law liquids. Two different structured packing arrangements are considered to understand the effect of particle orientation on the flow maldistribution during fast mode of min–max periodic operation. For a fixed operating condition, better radial liquid distribution is observed for periodic operation with higher split ratio in face centered cubic (FCC) geometry, however, at lower split ratio, well irrigation of the bed is obtained for modified simple cubic (SC) geometry. For both the geometries, shear thinning liquid imparts least maldistribution. Comparison of periodic operation results against continuous flow advocate benefits of the former in terms of liquid distribution in the bed irrespective of splits. This fundamental study essentially sets the foundation of modeling multiphase flow modulation in periodic PBRs.

1. Introduction

Packed bed reactor (PBR) is one of the classical reactor configurations that has wide spread application in several chemical and biochemical process industries, as well as, in petroleum refinery industries for absorption, distillation, stripping, separation processes, and catalytic reactions [1–5]. Hydrodynamics of PBRs are mostly involved with one or multiple fluid phases flowing through tortuous paths formed by catalyst packing arrangements [6–8]. Interactions between phases at different length scales are eventually dictated by flow regimes in PBR [9,10]. This 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 [11,12]. Several researches have shown the efficacy

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Nomenclature

c_0	density concentration (kg/m^3)
d_p	particle diameter (m)
D_i	distribution index
f^*	friction factor for power law fluids
g	gravitational acceleration (m/s^2)
k	consistency index (Pa · s^n)
l	length of bed (m)
n	flow behavior index
$\triangle P$	pressure drop (Pa)
Re_p^*	modified particle Reynolds number
u_c	time averaged velocity for continuous operation (m/s)
v	superficial velocity (m/s)

Greek symbols

ϵ	bed voidage
μ_{eff}	effective viscosity (kg/m · s)
ρ	density (kg/m^3)
σ	surface tension (N/m)

of flow modulation at the inlet in obtaining better performance of the PBR efficiency, mainly in terms of reaction conversion rate [13,14].

In multiphase cyclic or periodic operation, a fluid phase at the inlet is periodically toggled between a low-level (base) and a high-level (peak) to contact with another fluid stream which flows continuously through the bed [15]. This operation is typically known as the *min–max* flow operation, and when the base velocity is set to *zero*, it is termed as *on–off* flow operation [15]. It is noteworthy to mention that the flow regime during both peak and base liquid flow rates correspond to trickle-flow regime, i.e. low gas and liquid mass flux. Based on the duration of pulse incursion, periodic operation can be further classified in two different modes, namely, slow mode (pulse duration in minutes) [16], and fast mode (pulse duration in seconds) [17,18]. The slow mode operation is also typically characterized by a considerable fluctuation in pressure drop throughout the bed, whereas insignificant change is observed during the fast mode operation [18,19].

Generally, a mode of operation is adopted based on the type of reaction systems, i.e., either gas or liquid phase limited reactions. For gas-limited reactions, partial wetting of catalyst particles is desirable to eliminate the liquid mass transfer resistance and to ensure high mass flux of gaseous reactant at the catalyst surface [20]. However, in steady state operation, partial wetting of catalyst surface results in liquid maldistribution which strongly affects reactor performance. In this scenario, on–off slow mode liquid induced pulsing flow results in temporal variations of the catalyst wetting efficiency and helps in achieving improved conversion efficiencies [21–23]. The heat of reaction is also removed during the pulse incursion that helps in minimizing hot-spot formation [24]. However, for liquid-limited reactions, complete catalyst wetting and maximum particle–liquid mass transfer are warranted for the best result [20]. Under steady state, this scenario can be achieved by operating the bed in pulse flow regime, i.e., high liquid and gas mass flux operation, which in turn demands excess mechanical energy and can lead to lesser conversion due to shorter contact time between phases. Contextually, min–max fast mode of liquid-induced pulsing flow can considerably decrease the requirement of higher liquid flow rates [20]. Furthermore, there exists a continuous stream of liquid phase during the base velocity period. A relatively slow mode operation may substantially reduce the chance of hot-spot formation without operating the bed in pulse flow regime. Atta et al. [15] have summarized the advantages, present state and challenges of these periodic operation in packed beds.

Effect of catalyst particle shape, size, and porous nature on the pulse characteristics was studied by Trivizadakis et al. [25]. They reported different liquid holdup traces based on the particle shape. Experimentally, Ayude et al. [26] analyzed liquid holdup modulation for different superficial velocities, bed depth and cycling parameters. Ayude et al. [27] investigated the effect of flow rates, splits and cyclic periods in on–off operation on oxidation of methanol. They showed a significant improvement in catalyst activity of about 30% for larger split (shorter off duration) at constant modulation periods. This study also portrayed the fast mode of liquid feed modulation to be beneficial with respect to reaction rate. Tukač et al. [28] carried out comparative studies between min–max operation and continuous flow with various splits and found an increase in reaction rate by 30% for optimal periodic conditions. Although, the pressure drop values were higher for min–max operation as compared to steady state, however, the same was lower for shorter splits. Hamidipour et al. [18] attempted to reduce fine deposition in the bed by applying various modes of min–max flow operation. It was observed that neither the slow mode nor the fast mode was able to minimize the problem. However, a new strategy, semi fast mode (minutes lasting pulse and seconds lasting base) was proposed to effectively reduce the issue and to prolong the reactor life. Similarly, few studies have also addressed the effect of other operating conditions, like pressure and temperature, on the periodic operation efficiency [17,29,30]. Borremans et al. [31] conducted a comparative study on the effect of periodic flow on liquid distribution. It was observed that both on–off and min–max cyclic flow operations resulted in better liquid distribution than steady state only at low mean liquid flow rates. The distribution improved further as the base was set to zero i.e. on–off flow. They also observed that for a very limited number of conditions steady state operation actually resulted in a better liquid distribution than the periodic flow. Liu et al. [32] employed a non-invasive visualization technique to endorse the argument that periodic flow improved liquid distribution under a slow mode on–off operation.

Despite the proven advantages, implementation of periodic flow operation in commercial PBRs is still far from reality, mainly due to process control safety. Although, the design and scale up of steady state PBR for commercial purposes is well established, the design concept of periodic PBR needs more attention, even heuristically, to understand the influence of all key parameters. However, comprehensive investigation solely based on experiments is not only cumbersome but also sometimes expensive. With enhanced capabilities of CFD methods, computational studies can not only complement various aspects of a physical phenomena but also can help in understanding certain aspects that are generally not attainable by experiments. Surprisingly, limited researches have attempted to develop CFD based models for unsteady PBRs to understand the influence of operating parameters [33–36]. Moreover, none of these studies have addressed the effect of packing arrangements on flow distribution during periodic operation. Additionally, hydrodynamics of periodic PBRs, fed with non-Newtonian liquid, has rarely been addressed.

In a single phase PBR study, Freund et al. [37] mentioned that local inhomogeneities could significantly affect overall reactor