Chemical Engineering Journal 154 (2009) 162–167

Contents lists available at ScienceDirect

Chemical Engineering Journal

journal homepage: www.elsevier.com/locate/cej

Towards a comprehensive model for liquid flow modulation in trickle bed reactors

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ARTICLE INFO

Article history:
Received 26 November 2008
Received in revised form 21 March 2009
Accepted 23 March 2009

Keywords:
Liquid flow modulation
Trickle bed reactors
Modeling at the reactor scale
Hydrodynamics

ABSTRACT

The response of an isothermal TBR to a liquid flow modulation ON–OFF strategy is examined through a model aimed at the reactor scale. The reaction is gas-limited and first order with respect to both reactants. Liquid hydrodynamic behavior is considered by means of two different approaches: the Liquid Draining Approach, based on experimental results and the ideal, Square Wave Approach. Model allows the evaluation of, among other variables, the liquid holdup, the liquid velocity and the liquid reactant conversion time variations at different axial positions within the reactor. An enhancement factor due to periodic operation is defined by computing a temporal average of the liquid reactant conversion during an invariant cycling state, referred to its corresponding steady-state conversion. For all the conditions investigated, attainable enhancements are lower when the actual draining model is assumed.

1. Introduction

Catalysts employed in Trickle Bed Reactors (TBRs) are often characterized by a high reactivity, hence internal and external mass transport rates at particle level are frequently rate limiting. If the reaction is gas-limited, the possibility of performance enhancement exists because of the competition between the phases in supplying reactants to the catalyst. Cyclic operation, an example of which is liquid flow modulation (LFM), represents a mode of running a reactor in which inlet liquid flow rates are periodically changed between two predetermined levels, while the gas phase passes continuously during the entire period. This technique can be implemented with very low investment. The system is forced to run continuously in a transient mode in which the external surface coverage of the catalyst particles varies periodically; the supply of the gaseous reactant is enhanced and improvements can be achieved.

As generalized first by Schadlich and Hofmann [1], enhancements in desired process state variables are possible under cycling if the system is non-linear. In TBRs, there are several sources of non-linear behavior: reaction kinetics, mass transfer and catalyst wetting. Thorough understanding of these reaction–transport–wetting phenomena and of their interactions is complicated and, in spite of numerous works reporting the improvements arising from periodic operation of TBRs [2,3], a cycling strategy is still not being applied commercially mainly due to the lack of an established methodology of design. Hence, rigorous experimental and modeling efforts are carried out to understand the phenomena underlying LFM before commercial implementation.

Several models have been proposed along with experimental results. Lange et al. [4] studied the hydrogenation of α-methylstyrene under liquid flow modulation. The authors developed a heterogeneous model consisting of unsteady-state mass and enthalpy balances of the reaction components within the gas, liquid and catalyst bed. The model allowed prediction of the overall TBR performance incorporating partial wetting. Stegasov et al. [5] studied the SO_2 oxidation over an activated carbon catalyst in a dynamically operated, adiabatic trickle bed. A dynamic, heterogeneous model (accounting for partial wetting effects) was used to predict the temperature profile in the bed and the acid concentration leaving the reactor. Khadilkar et al. [6] have proposed a model for describing the unsteady-state operation of a trickle bed reactor considering the multicomponent characteristics of these systems by using the Maxwell–Stefan approach to mass transfer. The catalyst scale was taken into account through the three pellet apparent rate approach; i.e., three possible external wetting conditions for a completely internally wetted slab type catalyst: (i) with both sides wetted, (ii) a half-wetted pellet, and (iii) a pellet with both sides externally dry. Liu et al. [3] investigated the unsteady-state operation of non-isothermal TBR for the hydrogena-

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doi:10.1016/j.cej.2009.03.042

tion of dicyclopentadiene in the presence of Pd/Al_2O_3 catalyst under periodic operation, and proposed a model to interpret their results. Mass and enthalpy balances were solved taking into account the approach suggested by Lange et al. [7] to calculate the dynamic liquid holdup. However, the models developed for the reactor scale generally have neglected the dynamics inside the particle. This phenomenon should not be ignored since internal diffusion dynamics can strongly influence catalytic processes for nonsteady-state operations [8–11].

In this sense, some models have been proposed to understand the dynamic behavior of particles under LFM. Boelhouwer [12] solved dynamic mass balances considering internal diffusion for the case of wash coated catalyst particles with an impermeable core. A time-varying liquid holdup at the column inlet was used to model the unsteady-state hydrodynamics. The catalyst was divided into two sections: one section is continuously wetted by the liquid phase while the other part is alternately exposed to the gas and liquid phases. However, mass transfer between the dry and wet zones was not considered. Reactant and product profiles were obtained during fast cycling BASE-PEAK modulation and it was found that the rate of internal diffusion largely determines the optimal cycle period. Reactor enhancement during cycling was not evaluated. Dietrich et al. [9] proposed a model for a partially wetted slab to account for the internal dynamics under liquid flow modulation. The model was solved with different strategies and the recommended one depended not only on the extent of the mass transfer limitations but also on the time dependency of the surface wetting. The authors pointed out that, when integrated into a reactor scale model, a two-dimensional particle model requires a very large number of grid points if a reasonably high spatial resolution is to be achieved and thus rapidly becomes numerically exorbitant. Therefore, they suggested a compromise between accuracy and computational effort which could involve a multiple-zone approach. Ayude et al. [11] have formulated and solved a comprehensive model, aimed at the particle scale, to describe the course of a gas liquid reaction taking place within a spherical, isothermal heterogeneous porous catalyst particle subjected to ON–OFF liquid flow modulation considering both an egg-shell and a uniform distribution of the active species. These contributions have put in evidence the paramount importance of hydrodynamics on reactor behavior even at catalyst scale during LFM operation.

In this context, several works have examined the hydrodynamics of trickle bed reactors under LFM, pursuing particularly to describe the time evolution of key parameters profiles along the reactor [13–18]. Among them, Ayude et al. [18] have carried out a systematic characterization of the liquid holdup time evolution at different axial positions within a mini-pilot scale cold mock up of a TBR operated with ON–OFF liquid flow modulation. Results indicate that liquid holdup time variations are attenuated along the bed. The transient behavior of the liquid holdup, which was found to be restricted mostly to the dry period of the cycle, was fitted to a first-order exponential decay function that accounts for variations of the gas and the liquid velocities, the cycle period, the split and the bed depth. A procedure to reconstruct the liquid holdup time variation during the dry period was also proposed.

The objective of the present contribution is to examine the response of an isothermal TBR to a slow liquid flow modulation ON–OFF strategy. For this, the particle scale model proposed by Ayude et al. [10] is extended towards the reactor scale including the previously acquired hydrodynamic information [18] or Liquid Draining Approach (LDA). Particularly, reactant conversion time variations are estimated at different axial positions within the reactor. Outcomes will be compared to a situation which assumes that the whole bed follows the ideal Square Wave Approach (SWA) for the liquid velocity and the liquid holdup.

2. Model development

In the present contribution, the model is formulated considering a reaction carried out under gas-limited, isothermal, isobaric conditions over porous spherical catalyst particles. The approach is focused on the analysis of the mass transport and accumulation effects present in LFM for a situation under nearly isothermal conditions, such as the catalytic oxidation of organic pollutants in diluted aqueous solutions [19–21]. For heavily exothermic reactions, thermal effects should be included in the model.

The trickle bed reactor has an inner diameter of 4 cm and a bed height of 70 cm. The kinetics is assumed to be first order with respect to reactants A and B, present in the gaseous and liquid phase, respectively. Catalyst particles have uniform activity distribution. The mass balances equations for both reactants in the liquid phase need to be solved simultaneously with the mass balances at the particle scale. The gas phase mass balance is not included, since pure gas reactant A, with negligible pressure drop, and a non-volatile liquid reactant B are considered.

ON–OFF liquid flow modulation is induced by a cyclic square wave of the liquid velocity at the reactor entrance. The cycle period (i.e., period) is the time that elapses between repetitions of the same input conditions and the cycle split (i.e., split) is the fraction of the period during which the liquid phase flushes the bed.

The catalyst pellets may exhibit external partial wetting, according to its dependency with the liquid velocity. Total internal wetting is considered during the whole cycle. To represent the liquid hydrodynamic behavior, for the sake of comparison, two approaches have been employed.

On one hand, the experimental evidence observed by Ayude et al. [18] has been taken into account to solve the equations; this approach will be called "Liquid Draining Approach" (LDA). In this case, the model assumes that, once the liquid flow rate is cut off, the liquid drains and the liquid holdup diminishes progressively up to the static liquid holdup, if the dry time is long enough. Liquid velocity decreases with the liquid holdup and, consequently, the wetting efficiency also decrease. When the liquid flow is switched ON, the liquid velocity for the wet cycle is almost immediately re-established; therefore, the liquid holdup is considered constant during the ON cycle.

In the second approach, called "Square Wave Approach" (SWA), the liquid holdup is assumed to follow a square wave drainage model; i.e., instantaneously drops to the static holdup during the OFF cycle and returns to a given predetermined value during the ON cycle.

Based on these assumptions, the following mass balance equations are proposed:

mass balances inside the particles

$$\varepsilon_P \frac{\partial C_A}{\partial t} = D_A \left(\frac{\partial^2 C_A}{\partial r^2} + \frac{2}{r}\frac{\partial C_A}{\partial r} + \frac{\cot\theta}{r^2}\frac{\partial C_A}{\partial \theta} + \frac{1}{r^2}\frac{\partial^2 C_A}{\partial \theta^2} \right) - kC_A C_B \tag{1a}$$

$$\varepsilon_P \frac{\partial C_B}{\partial t} = D_B \left(\frac{\partial^2 C_B}{\partial r^2} + \frac{2}{r}\frac{\partial C_B}{\partial r} + \frac{\cot\theta}{r^2}\frac{\partial C_B}{\partial \theta} + \frac{1}{r^2}\frac{\partial^2 C_B}{\partial \theta^2} \right) - bkC_A C_B \tag{1b}$$

Symmetry in the angle Φ is considered. The wetting efficiency, f, is introduced into the model with respect to a critical value of the angle, θ_f, as $2f = 1 - \cos(\theta_f)$ [8]. The relationship assumes that the wetting efficiency represents the fraction of the sphere area covered by liquid and corresponds to the area of the spherical cup.

Then, boundary conditions postulated for the whole cycle are

$$r = 0, \quad \frac{\partial}{\partial r} C_i = \text{finite}, \quad \text{if } 0 \le \theta < \frac{\pi}{2} \text{ and } \frac{\pi}{2} < \theta \le \pi, \quad i = \text{A, B} \tag{2a}$$

$$\frac{\partial}{\partial r} C_i = 0, \quad \text{if } \theta = \frac{\pi}{2}, \quad i = \text{A, B} \tag{2b}$$

$$r = R, \quad -\frac{\partial}{\partial r} C_\text{A} = \frac{k s_\text{A}}{D_\text{A}} (C_\text{A}^\text{L} - C_\text{A}), \quad \text{if } \theta \le \theta_f \qquad -\frac{\partial}{\partial r} C_\text{B} = \frac{k s_\text{B}}{D_\text{B}} (C_\text{B}^\text{L} - C_\text{B}), \quad \text{if } \theta \le \theta_f \tag{2c}$$

$$C_\text{A} = C_\text{A}^*, \quad \frac{\partial}{\partial r} C_\text{B} = 0, \quad \text{if } \theta > \theta_f \tag{2d}$$

$$\frac{\partial}{\partial \theta} C_i = 0, \quad i = \text{A, B}, \quad \theta = 0 \text{ or } \theta = \pi \tag{2e}$$

mass balances outside the particles

The mass balance equations for the liquid phase in the liquid external film are given as

$$\varepsilon_\text{l} \frac{\partial}{\partial t} C_\text{A}^\text{L} = -\frac{\partial}{\partial z} (u_\text{l} C_\text{A}^\text{L}) + k_\text{gl} a_\text{B} (C_\text{A}^* - C_\text{A}^\text{L}) - f k_\text{sA} a p (C_\text{A}^\text{L} - C_\text{A}) \tag{3a}$$

$$\varepsilon_\text{l} \frac{\partial}{\partial t} C_\text{B}^\text{L} = -\frac{\partial}{\partial z} (u_\text{l} C_\text{B}^\text{L}) - f k_\text{sB} a p (C_\text{B}^\text{L} - C_\text{B}) \tag{3b}$$

To compare results, the relationship between the liquid velocity for steady-state operation ($u_\text{l,ss}$) and during the ON cycle of periodic operation ($u_\text{l,w}$) is taken into account as

$$u_\text{l,w} = u_\text{l,ss} (1.\,\text{s}^{-1}) \tag{4}$$

During the OFF cycle, the liquid velocity is evaluated considering that:

$$\frac{\partial u_\text{l}}{\partial z} = -\frac{\partial \varepsilon_\text{l}}{\partial t} \tag{5}$$

The increase in liquid holdup during the wet cycle is considered instantaneous for both hydrodynamic approaches (LDA and SWA).

For the LDA, the liquid holdup time profile subsequent to the liquid flow interruption is given by Ayude et al. [18]:

$$\varepsilon_\text{l} = (\varepsilon_\text{l,ON} - \varepsilon_\text{l,static}) e^{(-t/\chi)}$$
$$\frac{\partial \varepsilon_\text{l}}{\partial t} = -\frac{(\varepsilon_\text{l,ON} - \varepsilon_\text{l,static})}{\chi} e^{(-t/\chi)} \tag{6}$$
$$\chi = e^{6.3} \left(\frac{z}{L}\right)^{0.49} \left(\frac{P u_\text{l,ss}}{L}\right)^{0.39} s^{0.18} Re_\text{l,ss}^{-0.92} Re_\text{g}^{-0.21}$$

For the SWA, the liquid holdup time profile subsequent to the liquid flow interruption is given by a square wave.

Once the superficial liquid velocity is assessed, mass transfer coefficients can be evaluated following Goto and Smith [22] as

$$k_\text{gl} = k_\text{gl,ss} \left(\frac{u_\text{l}}{u_\text{l,ss}}\right)^{0.41} \tag{7a}$$

$$k_{s_i} = k_{s_i,\text{ss}} \left(\frac{u_\text{l}}{u_\text{l,ss}}\right)^{0.56}, \quad i = \text{A, B} \tag{7b}$$

From the hydrodynamic experiments carried out with liquid flow modulation, it has been evidenced that, when the liquid flow is interrupted, liquid velocity decreases progressively as the drainage proceeds. Then, mass transfer coefficients also decrease and for $Re < 1$, they are assumed to be constant, following Kehinde et al. [23], who stated that, at low Reynolds numbers, mass transfer coefficients tend to a limiting value.

Table 1
Operating conditions used in simulations.

Catalyst	Pt/γ–Al_2O_3
Particle diameter	3.1 mm
Bed diameter	0.04 m
Bed length	0.7 m
Temperature	70 °C
Oxygen pressure	1 atm
$bC_\text{A}^*/C_\text{B0}$	1/34
Thiele modulus	6.5
Cycle period	120–1200 s
Split	0.05–0.9
Mean superficial liquid velocity	0.15 cm/s
Superficial gas velocity	3.3 cm/s

Correspondingly, as the liquid velocity decreases, the wetting efficiency also decreases. The wetting efficiency, f, is evaluated following the correlation proposed by Herskowitz [24]:

$$f = f_\text{ss} + 0.0739 \ln \left(\frac{u_\text{l}}{u_\text{l,ss}}\right) \tag{8}$$

An enhancement factor due to periodic operation is defined by computing a temporal average of the liquid reactant conversion during an invariant cycling state, referred to its conversion under steady-state operation (X_ss) with a mean liquid velocity $u_\text{l,ss}$:

$$\xi = \frac{X_\text{mean}}{X_\text{ss}} \tag{9a}$$

$$\text{where } X_\text{mean} = \left[\frac{\int u_\text{l} X dt}{\int u_\text{l} dt}\right]_\text{invariant cycle} \tag{9b}$$

2.1. Model parameters

The operating conditions employed for the calculations are shown in Table 1. The setting is the one used by Muzen et al. [19]. Liquid velocities employed have been considered in order to match conditions explored by Ayude et al. [18], for which the hydrodynamics under periodic operation has been characterized.

Parameters values for the mean liquid velocity are evaluated from correlations listed in Table 2.

2.2. Model resolution

All continuous equations were replaced by their finite difference approximations. Nonsteady-state mass balances for the gas and liquid reactants within the spherical particles are solved by the alternating direction implicit method. Simultaneously, mass balances for the bulk liquid are solved using explicit finite differences. Convergence of results was tested for different discretization steps. Steps of 0.03 s, 0.016 (dimensionless) and 0.10 radians were finally selected, for time, radial and angular direction, respectively; since no changes in outcomes were observed below these values.

It was verified that initial conditions at the beginning of the operation were irrelevant since the analysis is focused on the invariant state attained under liquid flow modulation. Initial conditions for

Table 2
Correlations used to estimate the parameters at the mean liquid velocity.

Parameter	Correlation
$k_\text{gl} a_\text{B}$	Goto and Smith [22]
$k_\text{sA} a p$	Goto and Smith [22]
f	Herskowitz [24]
ε_l	Ayude et al. [18]
ε_s	Sáez and Carbonell [25]

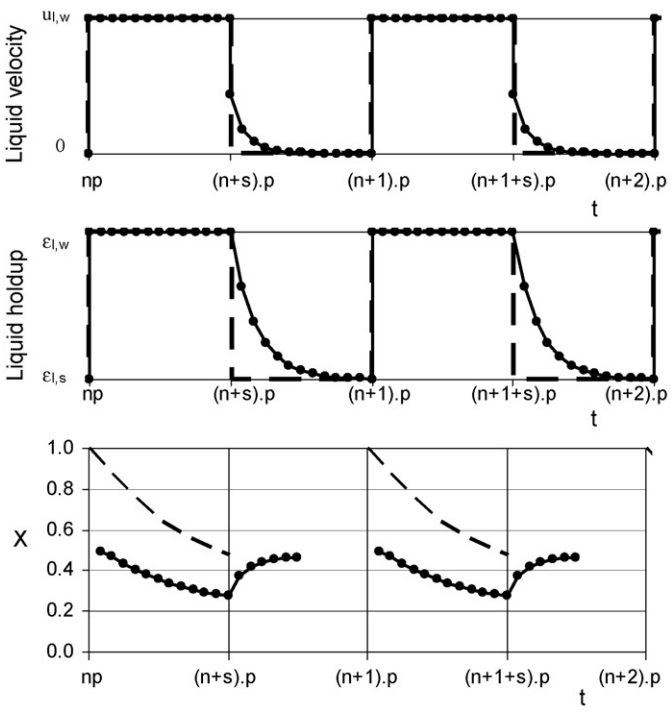

Fig. 1. Comparison between the LDA (–●–) and the SWA (– –) outputs at the TBR outlet. (a) Liquid velocity profiles; (b) liquid holdup profiles; (c) liquid reactant conversion profiles. Operating conditions: $u_{l,ss}$ = 0.15 cm/s, u_g = 3.3 cm/s, P = 1200 s; s = 0.5.

each cycle are given by the set of values calculated at the end of the previous cycle, at each position in the pellet and the whole reactor. The number of cycles needed to achieve the invariant cycling state certainly depends on the initial reactant concentrations, the cycling parameters, and the hydrodynamic approach assumed.

Reactants radial and angular profiles within the catalyst, as well as axial variation in the reactor can be evaluated with the model for any moment during the cycle.

3. Results and discussion

Model allows the evaluation of, among other variables, the liquid holdup, the liquid velocity and the liquid reactant conversion profiles at any point of the reactor and for any moment of the ON–OFF operation. Fig. 1 presents theoretical outcomes (obtained at quasi-steady-state in the dynamic liquid at the end of the column) considering the two different drainage behaviors during the OFF cycle: Ideal or Square Wave Approach (SWA) and the measured outcomes (LDA) obtained by Ayude et al. [18] at a cycle period of 1200 s and a split of 0.5. For both draining situations, the hydrodynamic patterns during the ON cycle are the same, as shown in Fig. 1a and b. When the SWA is assumed, the liquid drainage is immediately completed (see Fig. 1a, dashed line), consequently the external liquid holdup decays instantly towards the static holdup, as seen in Fig. 1b (dashed line). External mass transfer resistances decreases sharply for reactive A and reaction proceeds between the flowing gas and the liquid retained inside the pores of the pellet. The other approach considers that, during the OFF cycle, the liquid velocity and the liquid holdup decrease progressively with time (as seen in Fig. 1a and b). Then, mass transport coefficients within the liquid film also decrease. Nevertheless, since the gas–solid contact area is larger than during the ON period due to a decrease in the wetting efficiency, an increase in conversions is observed arising from the higher exposure of the particle to the gas phase. When the drainage is complete ($u_l \approx 0$), and therefore, the static holdup is attained, no liquid is leaving from the TBR (Fig. 1a, both approaches).

Fig. 1c presents the conversion profiles evaluated in the dynamic liquid at the end of the TBR for SWA and LDA. When the liquid flow is restored, a high conversion is initially observed. Then, liquid reactant conversion decays approaching the pseudo steady-state value; that is, the condition that would be achieved if the reactor is operated under steady-state at the liquid velocity of the ON

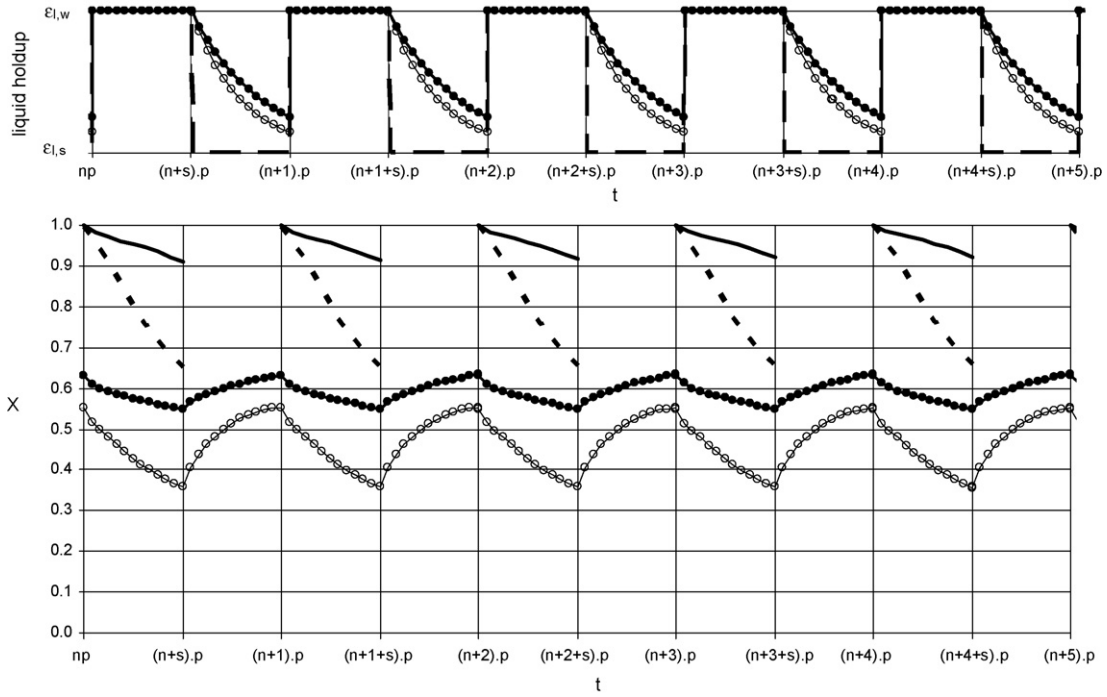

Fig. 2. Comparison between the LDA at the TBR middle (–○–) and outlet (–●–) and the SWA outputs at the TBR middle (– –) and outlet (—). (a) Liquid holdup profiles; (b) liquid reactant conversion profiles. Operating conditions: $u_{l,ss}$ = 0.15 cm/s, u_g = 3.3 cm/s, P = 120 s; s = 0.5.

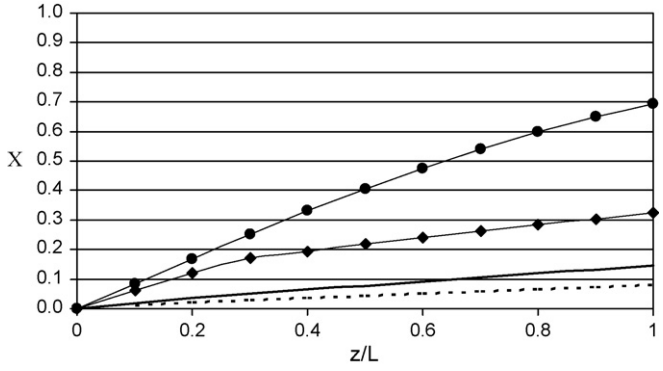

Fig. 3. Mean liquid reactant conversion attained at the invariant state as a function of the bed length for the LDA (–♦–) and the SWA (–●–). (—) Steady-state operation at the mean liquid velocity. (– –) Steady-state operation at $u_{l,w}$. Operating conditions: $u_{l,ss}$ = 0.15 cm/s, u_g = 3.3 cm/s, P = 900 s, s = 0.66.

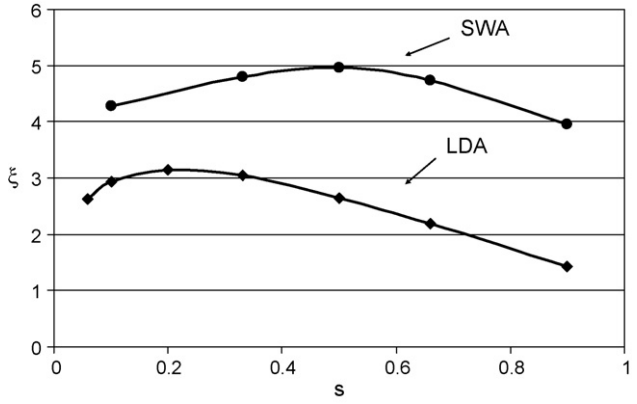

Fig. 4. Comparison among the enhancement vs. s curves obtained for the LDA and the SWA outputs. Operating conditions: $u_{l,ss}$ = 0.15 cm/s, u_g = 3.3 cm/s, P = 900 s.

period. When the liquid flow is cut off, liquid reactant conversion in the dynamic liquid increases, and its value is evaluated provided there is liquid actually draining out of the reactor. The conversions attained immediately after the liquid flow is restarted are always the maxima achieved during the period, evidencing that reaction continues inside the pores of the pellet, even with no liquid flow and that the product formed during the OFF cycle leaves the reactor when the liquid phase is introduced, allowing replenishment of the liquid reactant.

Liquid holdup and conversion profiles obtained for a shorter cycling period and symmetrical split are illustrated in Fig. 2 for different bed lengths (middle and outlet). When the cycle period decreases, the liquid holdup during the dry cycle may not reach the static holdup (Fig. 2a) at any length of the bed when the LDA model is assumed. The liquid velocity profiles (not shown) indicate that the liquid drainage is faster in the upper zone. Consequently, the holdup profiles are steeper in the top section of the bed (as shown in Fig. 2). Independently of the cycling conditions investigated, for LDA, the square wave shape assumed for the liquid at the column entrance is significantly distorted along the column and the amplitude of the liquid flow waves decays along the bed [18]. On the other hand, with these cycling conditions, reactant conversions are higher due to the larger availability of liquid reactant within the catalyst. For the LDA approach it is evident that variations in reactant conversion induced by the modulation are attenuated along the column (Fig. 2b).

Fig. 3 presents the mean cycling conversion (Eq. (9b)) for different bed lengths obtained at the invariant state for the LDA and the SWA. Lines represent theoretical results for the steady-state operation. In any case, ON–OFF liquid mean conversions are higher than those attained at steady-state. As the bed length increases, the ON–OFF wave is attenuated according to the LDA and differences in conversion between both approaches increase. These outcomes put in evidenced that the reactor performance predicted by the SWA is considerably better than the one calculated by the LDA. Indeed, a significantly larger reactor length would be needed to accomplish the conversions predicted with the SWA if the actual hydrodynamic behavior is considered.

Split influence on the estimated enhancement considering both draining behaviors is shown in Fig. 4. The enhancement depends on the hydrodynamics and on the relative duration of the dry and wet cycles referred to the reactor residence time. The SWA gives the higher enhancements at any split, presenting a maximum at split 0.5. Attainable enhancements decrease when the LDA is considered, and the maximum enhancement appears at lower split values. This shift arises from the higher liquid retention formulated through the LDA during the dry period, leading to higher wetting efficiencies compared to the SWA; thus, reducing the gaseous reactant access to the catalyst. From Figs. 3 and 4, it arises that, when the reaction is gas-limited as in this case, reactor performance under periodic operation is always beneficial.

4. Conclusions

An ON–OFF liquid flow modulation strategy may be considered a Process Intensification technique for the case of gas-limited reactions taking place in TBRs. In this modality, the reactor is always operated in a transitory mode in which the external surface exposure of the catalyst varies periodically; the deliver of the gaseous reactant is improved and enhancements can be achieved. However, the magnitude of the improvements depends, among other variables, on mass transfer and hydrodynamic conditions. To further explore this concept we developed a model aimed at the reactor scale that allows the evaluation of the liquid holdup, velocity and reactant conversion profiles along the reactor at any moment during the ON–OFF operation. Hydrodynamic behavior is considered by means of two different approaches: a Liquid Draining Approach (LDA), based on experimental results and the ideal Square Wave Approach (SWA). With the LDA, independently of the cycling strategy imposed, the square wave liquid holdup and velocity assumed at the column entrance is significantly distorted along the column. Mean liquid reactant conversions predicted by both approaches are similar at the top of the reactor but, as length is increased, the conversions predicted with the SWA are considerable higher than those predicted considering the LDA. An enhancement factor due to periodic operation is used to compare results obtained at different conditions. Idealistically higher enhancements are attained when the SWA is assumed. The outcomes presented in this contribution highlight the importance of developing a feasible hydrodynamic model based on experimental observations to be able to predict accurately the reactor performance.

Notation

ap	specific external area of catalyst particles (1 m^{-1})
b	stochiometric coefficient
C	concentration (mol/m^3)
D	effective diffusivity (m^2/s)
f	wetting efficiency (dimensionless)
k	kinetic constant (m^3/mol s)
ks	liquid–solid mass transfer coefficient (m/s)
$k_{gl}a_B$	gas–liquid volumetric mass transfer coefficient (1 s^{-1})
L	reactor length (m)
P	cycle period (s)
r	radial coordinate within the particle (m)

R	particle radius (m)
Re	Reynolds number
s	split
t	time (s)
u	superficial velocity (m/s)
X	conversion (dimensionless)
z	axial coordinate in the bed (m)

Greek letters

ε	phase hold-up ($m^3/m^3_{reactor}$)
ε_p	particle porosity/void fraction (dimensionless)
θ	angular coordinate within the particle
θ_f	critical angular coordinate defined by the wetting efficiency
ξ	cycling enhancement, defined in Eq. (9).
Φ	azimuthal coordinate within the particle
χ	parameter defined in Eq. (6)

Superscripts and subscripts

*	saturation value
0	initial value
A	reactant in the gas phase
B	non-volatile reactant in the liquid phase
g	gas
l	liquid
L	referred to the concentration within the liquid film
OFF	dry cycle
ON	wet cycle
p	particle
ss	steady-state
static	referred to the static holdup
w	wet

Acknowledgements

Financial support from CONICET, UBA, UNMdP, UNLP and ANPCyT are gratefully acknowledged.

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