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Two-fluid model for counter-current dumped packing-containing columns

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1. Introduction

Gas–liquid counter-current packed columns are among the most ubiquitous contacting devices in separation processes. Nowadays, they are widely used in such diverse fields as distillation, scrubbing, and stripping. Due to lower power consumption and liquid inventory, they are also increasingly evoked as cheaper replacement alternatives to existing tray column operations (Yin, Sun, Afacan, Nandakumar, & Chuang, 2000) but also as potent candidates in catalytic distillation and petroleum refining operations (Malone & Doherty, 2000; Duduković, Larachi, & Mills, 1999). Furthermore, since packed column operation is cheap, it is of great interest for pollution abatement (Strigle, 1994).

The permanent market demands in the pursuit of cost-effective units is continually imposing the need to providing well-designed and highly efficient packings. This trend is created by the need to respond to industrial economic requirements (e.g., high mass transfer capacities, low pressure drops) and, at the same time, to comply to stringent discharge regulations.

To respond to these needs, numerous attempts continue to be made to model the hydrodynamics and the mass transfer of packed columns. These attempts range from the well-trodden (semi)empirical approaches (Stichlmair, Bravo, & Fair, 1989; Piché, Larachi, & Grandjean, 2001), to the macroscopic phenomenological models (Stichlmair et al., 1989; Billet & Schultes, 1991, 1999; Maćkowiak, 1991), and very recently to the multi-dimensional *computational fluid dynamics* modeling (Yin et al., 2000; Sun, Yin, Afacan, Nandakumar, & Chuang, 2001). Even though all of these approaches have more or less achieved success, phenomenological models still constitute the right balance of compromise between sophistication and robustness. They represent the best trade off between empiricism and cumbersome computational codes, so that their popularity will persist for industrial design.

The objective of this work is to develop a fully predictive two-fluid mechanistic model for gas–liquid counter-current random packings wherein the inter-relationship between the irrigated pressure drop, the total liquid holdup and the packing fractional wetted area is for the first time *quantitatively* highlighted. Without requiring any adjusting parameter, it further allows the *simultaneous* prediction of these three flow variables in the pre-loading zone, region of practical significance (Billet, 1989). The approach is designed to approximate the actual two-phase flow topography in random packings using two inclined and interconnected slits consisting of a dry slit solely fed by gas, and gas–liquid slit fed by liquid and remaining gas. Model validation has been performed using literature data relative to the packing wetted area, pressure drop and liquid holdup obtained under various operational contexts.

2. Conceptual model of packing-scale gas–liquid topography in the pre-loading zone

Below the loading point and for sufficiently low fluid throughputs, the liquid holdup, the gas and solid wall *shearing* actions cannot sustain full wetting of all the *individual* packing elements in the packed tower. *Packing-scale* partial wetting is a local phenomenon and should not be confounded with the large-scale liquid mal-distribution which is known to be a serious cause for deterioration of separation efficiency. The latter is indeed triggered by distributor imperfections, and can be reduced using well-designed distribution devices and strategies. The former, on the contrary, can always take place when the prevailing liquid film is not able to ensure full coverage of every packing element in the tower. Moreover, because of the statistical nature of the bed geometry and the non-stationary character of the flowing

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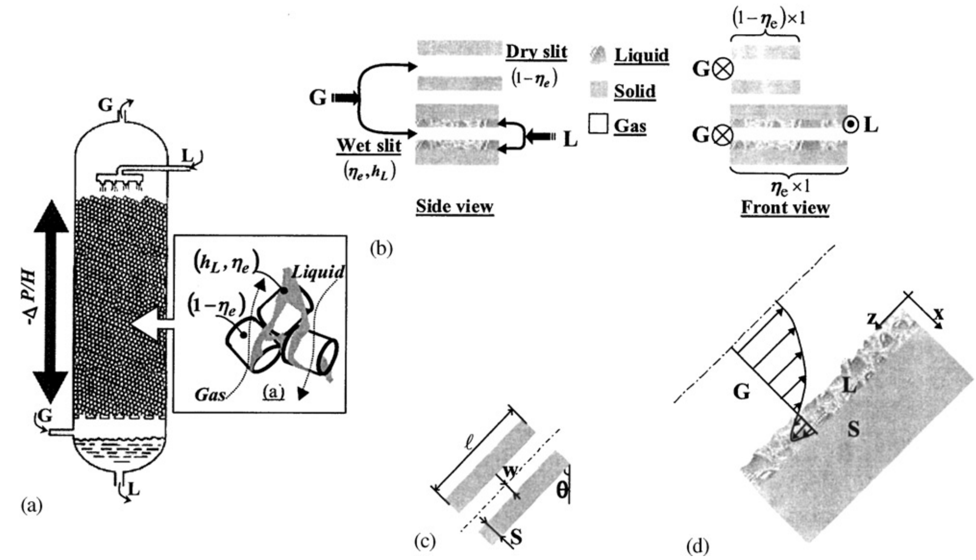

Fig. 1. (a) Actual, (b) conceptual two-phase flow pattern in partially wetted counter-current random packed-bed columns, (c) slit geometrical characteristics, (d) gas–liquid structure in the wet slit.

liquid films over the packing, the packing-scale partial wetting dealt with here is an effective wetting that is averaged over time and ensemble-averaged over the tower domain.

It is thus easy to figure out that deep in the pre-loading zone at low flow rates, the counter-current gas–liquid flow structure over partially wetted packing elements in a randomly packed tower, can be decomposed into two elementary contacting patterns:

- A dry-packing region having a fractional area $1-\eta_e$ with gas–solid contacting.
- A wet-packing region having a fractional area equal to η_e with direct liquid–solid contacting between packing and liquid film contributing to the holdup, h_L.

This dichotomy of the local flow structure highlights the interplay between several hydrodynamic features, prediction of which is key for the description of the tower hydraulics. According to Fig. 1a, there are three hydrodynamic variables in counter-current flow packed-bed columns that are interlinked to each other, these are the packing fractional wetted area, η_e, the total liquid hold-up, h_L, and the overall irrigated pressure drop, $-\Delta P/H$.

3. Packed bed geometrical approximation model

In an attempt to predict these three variables, a two-zone one-dimensional hydrodynamic model is developed which consists first in simplifying the actual local bed geometry and gas–liquid structure by assuming an idealized *double-slit* architecture shown in Fig. 1b. This so-called slit approximation has proved fruitful in the past in modeling the hydrodynamics of co-current down-flow trickle-bed reactors (Holub, Duduković, & Ramachandran, 1992; Iliuta, Larachi, & Al-Dahhan, 2000) and recently in modeling two-phase flow in structured-packing containing columns (Iliuta & Larachi, 2001). It is extended here to model the hydrodynamics of dumped-packing containing towers with counter-current gas–liquid flow.

The approach states that the bed-scale macroscopic hydrodynamics can be mapped from knowledge of the gas–liquid flow distribution and hydrodynamics inside an idealized double-slit. The latter is an assemblage of two parallel inclined and interconnected slits:

- A gas slit representing the dry region $a_s(1-\eta_e)$ is fed upwards by a fraction of the gas flow rate.
- A wet slit representing the wetted region $a_s\eta_e$ is fed downwards by the liquid flow rate in the form of a constant thickness film, and upwards in the center by the remaining gas flow rate part.

The two inclined slits are geometrically similar (Fig. 1c) except for their width which is dictated by the extent of wetting (front view of Fig. 1b). Further relationships are needed to ensure the mapping of the slits' geometry features into those of the bed. These are based on the following assumptions:

- The slits have identical half-wall thickness, S, half-void thickness, w, and slit length ℓ (Fig. 1c). The widths of the dry and wet slits are proportional to $1-\eta_e$ and η_e, respectively.
- The solid surface area per unit solid volume is uniform across the slits and equal to that of the bed:

$$S = \frac{1-\varepsilon}{a_s}. \tag{1}$$

- The void-to-solid and the liquid-to-solid volume fractions within the slits and the bed are equal:

$$\frac{w}{S} = \frac{\varepsilon}{1-\varepsilon} \quad \text{for both slits,} \tag{2}$$

$$\frac{\delta\eta_e}{S} = \frac{h_L}{1-\varepsilon} \quad \text{for the wet slit.} \tag{3}$$

- The slits are inclined by an angle θ with respect to the vertical axis (Fig. 1c). It is related to the bed tortuosity, T, by $\cos\theta = 1/T$ (Holub et al., 1992). T is a measure of the ratio between an effective flow path and vertical bed height.
- An estimate of θ (or T) is inferred from measurements of single-phase pressure drop across the dry bed, through the so-called Ergun creeping and inertial constants, E_1 and E_2, respectively. These latter, actually measured, reflect at the bed level, the average inclination of the randomly oriented interstices in the porous bed. These constants are given as (Holub et al., 1992)

$$E_1 = \frac{72}{\cos^2\theta}, \tag{4}$$

$$E_2 = \frac{6f_w}{\cos^3\theta}. \tag{5}$$

4. Two-phase pressure drop—liquid holdup—wetted fractional area model

Beside these hypotheses, to make the slit flow dynamics representative of the flow in the packed tower, further assumptions on the nature of the gas–liquid flow are also laid down:

- The flow regime in the bed corresponds to the *pre-loading zone*. Therefore, no ripples (or waves) occur at the gas–liquid interface leading thus to a smooth and stable liquid film (Fig. 1d). Note that these ripples and interfacial instabilities are more likely to occur in the *loading zone* where the packing wetting phenomenon is no longer an issue.
- The dominant liquid texture components are contributed by films and rivulets which will be referred to as "liquid film" throughout this paper. This structure far outweighs the droplet contribution so that the packing fractional wetted area, (η_e), is tantamount to the effective gas–liquid interfacial area (a_e):

$$\eta_e = \frac{a_e}{a_s}. \tag{6}$$

Therefore,

$$h_L = a_s\eta_e\delta = a_e\delta. \tag{7}$$

- The (Newtonian) liquid film and gas flows remain steady-state and acceleration-free.
- The intrinsic phase velocities are the same in the bed and in the representative slits, leading to

$$\text{dry slit}: \quad u_G = \frac{v_{SG}}{\varepsilon\cos\theta}, \tag{8}$$

$$\text{wet slit}: \quad u_G = \frac{\eta_e v_{SG}}{(\eta_e\varepsilon - h_L)\cos\theta}, \quad u_L = \frac{v_{SL}}{h_L\cos\theta}. \tag{9}$$

- The friction factor (f_i) at the gas–liquid interface and the wall friction factor (f_w) at the gas–solid interface are equal (Holub et al., 1992):

$$f_i = f_w. \tag{10}$$

- There is no discontinuity in the velocity and shear stress profiles at the gas–liquid interface:

$$u_{i,G} = u_{i,L}, \quad @\, x = 0, \tag{11}$$

$$\tau_{i,L} = -\mu_L \frac{\mathrm{d}u_L}{\mathrm{d}x} = \tau_{i,G} = -\mu_G \frac{\mathrm{d}u_G}{\mathrm{d}x}, \quad @\, x = 0. \tag{12}$$

- The slipless condition holds at the slit walls:

$$u_L = 0, \quad @\, x = \delta \text{ (wet slit)}, \tag{13}$$

$$u_G = 0, \quad @\, x = w \text{ (dry slit)}. \tag{14}$$

- The total pressure gradient is the same across the bed and the idealized slit network:

$$-\frac{\Delta P}{H} - \rho_G g = \frac{1}{\cos\theta}\left(-\frac{\mathrm{d}P}{\mathrm{d}z} - \rho_G g\right) = \rho_G g \Psi_G, \tag{15}$$

$$-\frac{\Delta P}{H} + \rho_L g = \frac{1}{\cos\theta}\left(-\frac{\mathrm{d}P}{\mathrm{d}z} + \rho_L g\right) = \rho_L g \Psi_L, \tag{16}$$

$$1 + \Psi_G = \frac{\rho_L}{\rho_G}(\Psi_L - 1). \tag{17}$$

Based on the above assumptions, the gas and liquid momentum balance equations over the slits are

$$-\frac{\mathrm{d}P}{\mathrm{d}z} - \rho_G g\cos\theta = \frac{\eta_e\tau_{i,G} + (1-\eta_e)\tau_{w,G}}{(w-\delta)\eta_e + w(1-\eta_e)}, \tag{18}$$

$$-\frac{\mathrm{d}P}{\mathrm{d}z} + \rho_L g\cos\theta = \frac{\tau_{w,L} - \tau_{i,L}}{\delta}, \tag{19}$$

where $\tau_{i,\alpha}$ is the shear stress on the α-phase side of the gas–liquid interface, and $\tau_{w,\alpha}$ is the wall shear stress exerted by the slit wall on the α-phase. Eq. (18) was obtained through combination of the streamwise projections of the gas-phase momentum balances in the dry and wet slits:

$$(1-\eta_e)\tau_{w,G} = \left(-\frac{\mathrm{d}P}{\mathrm{d}z} + \rho_G g\cos\theta\right) w(1-\eta_e), \tag{20}$$

$$\eta_e\tau_{i,G} = \left(-\frac{\mathrm{d}P}{\mathrm{d}z} + \rho_G\, g\cos\theta\right)(w-\delta)\eta_e. \tag{21}$$

The gas–liquid interfacial, the wall–liquid and the wall–gas shear stresses possess laminar and turbulent contributions and were related using a friction factor formulation

(Holub et al., 1992):

$$\tau_{i,G} = 2\,\frac{(u_G + u_{i,G})\mu_G}{w-\delta} + f_i\rho_G(u_G + u_{i,G})^2, \tag{22}$$

$$\tau_{w,L} = 2\,\frac{u_L\mu_L}{\delta} + f_w\rho_L u_L^2, \tag{23}$$

$$\tau_{w,G} = 2\,\frac{u_G\mu_G}{w} + f_w\rho_G u_G^2. \tag{24}$$

The local momentum balance equation at location (x,z) for the liquid in the wet slit is

$$\rho_L g\cos\theta - \frac{\mathrm{d}P}{\mathrm{d}z} = -\mu_L\frac{\mathrm{d}^2u_L}{\mathrm{d}x^2} \tag{25}$$

subject to the boundary conditions Eqs. (11), (13) and

$$\tau_{L,xz} = \left(-\frac{\mathrm{d}P}{\mathrm{d}z} - \rho_G g\cos\theta\right)(w-\delta), \qquad @\,x=0. \tag{26}$$

Double integration of Eq. (25) yields the velocity distribution of the liquid in the wet slit:

$$u_{L,z}(x) = \frac{\delta^2}{2\mu_L}\left[1-\left(\frac{x}{\delta}\right)^2\right]\left(-\frac{\mathrm{d}P}{\mathrm{d}z} + \rho_L g\cos\theta\right) + \frac{\delta(w-\delta)}{\mu_L}\left(1-\frac{x}{\delta}\right)\left(-\frac{\mathrm{d}P}{\mathrm{d}z} - \rho_G g\cos\theta\right). \tag{27}$$

Similarly, the liquid-film average or intrinsic velocity, u_L, is obtained as

$$u_L = \frac{1}{\delta}\int_0^\delta u_{L,z}(x)\,\mathrm{d}x = \frac{\delta^2}{3\mu_L}\left(-\frac{\mathrm{d}P}{\mathrm{d}z} + \rho_L g\cos\theta\right)x + \frac{(w-\delta)\delta}{2\mu_L}\left(-\frac{\mathrm{d}P}{\mathrm{d}z} - \rho_G g\cos\theta\right). \tag{28}$$

By replacing $x = 0$ in Eq. (27) and after using the slit-to-bed mapping equations (1)–(10) and (15)–(17), one obtains the expression for the liquid (or gas) interfacial velocity (Eq. (11)):

$$u_{i,L} = \frac{72}{E_1}\frac{gh_L}{\eta_e^2 a_s^2\mu_L}\left\{\frac{1}{2}\Psi_L\rho_L h_L + \Psi_G\rho_G(\eta_e\varepsilon - h_L)\right\}. \tag{29}$$

Combining Eq. (28) with Eqs. (7) and (9) and using the same slit-to-bed mapping yields the final expression for the fractional wetted area:

$$\eta_e = \frac{\phi^2h_L^2}{2E_1\varepsilon^2}\left(\Psi_L - 1 - \frac{\rho_G}{\rho_L}\right)\frac{Ga_L}{Re_L} + \sqrt{\frac{\phi^2h_L^3}{E_1\varepsilon^3}}\sqrt{\frac{Ga_L}{Re_L}}\left\{\frac{\phi^2}{4E_1}\frac{h_L}{\varepsilon}\frac{Ga_L}{Re_L}\left(\Psi_L - 1 - \frac{\rho_G}{\rho_L}\right)^2 + \frac{\rho_G}{\rho_L} - \frac{\Psi_L}{3} + 1\right\}^{1/2}. \tag{30}$$

Finally by substituting Eqs. (22)–(24) in Eqs. (18), (19) and using the mapping definitions given by Eqs. (15)–(17) yields the final forms of the dimensionless pressure drop in the bed framework:

$$\Psi_G = \frac{\varepsilon^3\eta_e^3}{(\varepsilon\eta_e - h_L)^2(\varepsilon - h_L)}\left\{\frac{E_1}{\eta_e\phi^2}\frac{\eta_e Re_G + (\eta_e\varepsilon - h_L)Re_i}{Ga_G} + \frac{E_2}{\eta_e^2\phi}\frac{[\eta_e Re_G + (\eta_e\varepsilon - h_L)Re_i]^2}{Ga_G}\right\} + \frac{\varepsilon(1-\eta_e)}{\varepsilon - h_L}\left\{\frac{E_1}{\phi^2}\frac{Re_G}{Ga_G} + \frac{E_2}{\phi}\frac{Re_G^2}{Ga_G}\right\}, \tag{31}$$

$$\Psi_L = \frac{\varepsilon^3\eta_e^3}{h_L^3}\left[\frac{E_1}{\eta_e\phi^2}\frac{Re_L}{Ga_L} + \frac{E_2}{\eta_e^2\phi}\frac{Re_L^2}{Ga_L}\right] - \frac{\varepsilon\eta_e - h_L}{h_L}\left(\Psi_L - 1 - \frac{\rho_G}{\rho_L}\right). \tag{32}$$

5. Discussion

Eqs. (30)–(32) establish the non-linear implicit mechanistic model as a set of three coupled algebraic equations and three unknowns, i.e., $-\Delta P/H$, h_L and η_e. The input variables to be fed to this model are the fluid superficial velocities, the fluid physical properties, the bed and packing characteristics, the Ergun constants, determined from single-phase flow experiments, and the interfacial velocity given by Eq. (27). Provided all these variables are known a priori, the model therefore requires *no adjustable* parameters. The non-linear model is solved using an iterative Newton–Raphson algorithm.

To validate the proposed model, literature data relative to the irrigated pressure drop (Sarchet, 1942; Schoenborn & Dougherty, 1944; Andrieu, 1974; Wu & Chen, 1987; Stichlmair et al., 1989; Billet, 1995; Wagner, Stichlmair, & Fair, 1997), the dry pressure drop, the total liquid holdup (Shulman, Ulrich, Wells, Proulx, & Zimmerman, 1955; Charpentier, Prost, van Swaaij, & Le Goff, 1968; Linek, Benes, Sinkule, & Krlvsky, 1978; Spedding, Munro, & Jones, 1986; Billet, 1989; Miyahara, Ogawa, Nagano, Hirade, & Takahashi, 1992) and the gas–liquid interfacial area (Linek, Petricek, & Benes, 1984; Linek, Sinkule, & Brekke, 1995; Rizzuti & Brucato, 1989) in the pre-loading zone at ambient conditions has been collected for columns containing the following dumped packings: Raschig rings, Bialecki rings, Cascade mini-rings, Berl saddles, Mitsui Nutter rings, Hiflow rings and Pall rings (Table 1). E_1 and E_2 constants fitted by applying Ergun equation on the dry pressure drop data are also given in Table 1. The gas–liquid systems included in the database are: air/ water, air/nitrogen, air/water + sucrose, air/water + ethanol, air + CO_2/water + NaOH, air + CO_2/water + K_2CO_3 + $KHCO_3$. The experimental conditions included superficial liquid velocities from 0.0007 to 0.0222 m/s, and superficial gas velocities varying between 0.007 and 3.6 m/s. The gas–liquid interfacial areas correspond to partially and fully wetted beds, $\eta_e \leqslant 1$.

The parity plot diagrams, shown in Figs. 2a–c, provides the ability to compare the model prediction by

Table 1
Packing and column properties

Packing type	a_s (m^{-1})	ε (%)	ϕ	[a]E_1	[a]E_2	Nominal ∅ (mm)
Glass Raschig ring	518	74	0.359	440.3	4.40	10
Porcelain Raschig ring	310	73.5	0.434	360.0	3.14	15
	381	60.5	0.497	154.7	3.04	12.7
Clay Raschig ring	190	68	0.427	1501	2.47	25
Carbon Raschig ring	696	55	0.598	292.1	2.60	6
Cascade mini-ring	235	96.2	0.102	513.0	1.34	25
Metal Bialecki ring	220	94	0.11	751.7	2.46	25
Porcelain Berl saddle	205	69.5	0.427	67.5	1.64	25
Mitsui Nutter ring	213	97.7	0.078	1165	1.18	17
Plastic Hiflow ring	109	93.2	0.141	1258	1.32	50
Metal Pall ring	105	95.6	0.104	514.8	1.50	50
Plastic Pall ring	212	89.7	0.187	432.8	1.95	25

[a]Fitted using $\Psi_G = \frac{E_1}{\phi^2}\frac{Re_G}{Ga_G} + \frac{E_2}{\phi}\frac{Re_G^2}{Ga_G}$ on dry pressure drop data.

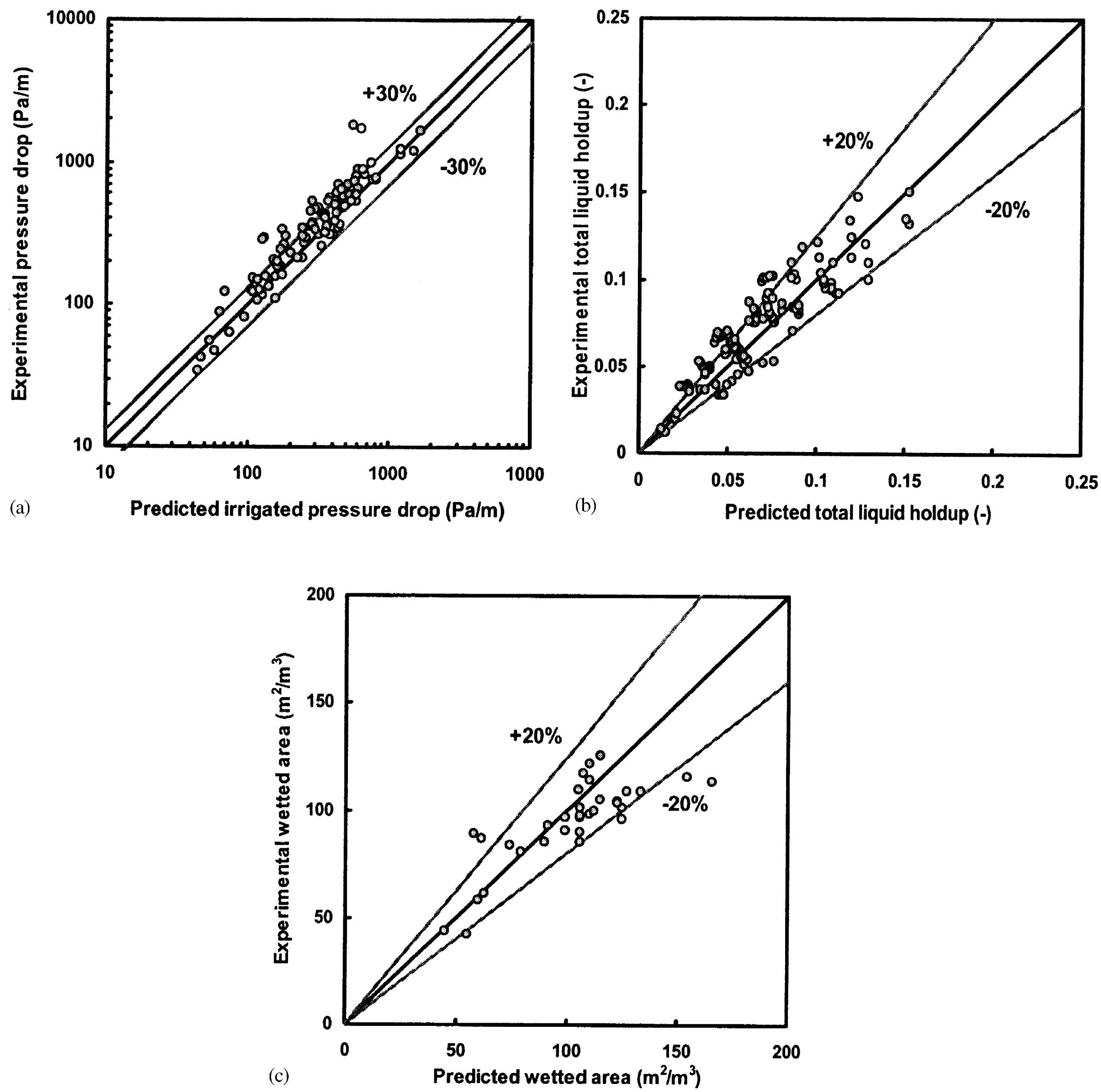

Fig. 2. Predicted versus experimental (a) irrigated two-phase pressure drop, (b) total liquid holdup, (c) packing wetted area (data belongs to pre-loading zone).

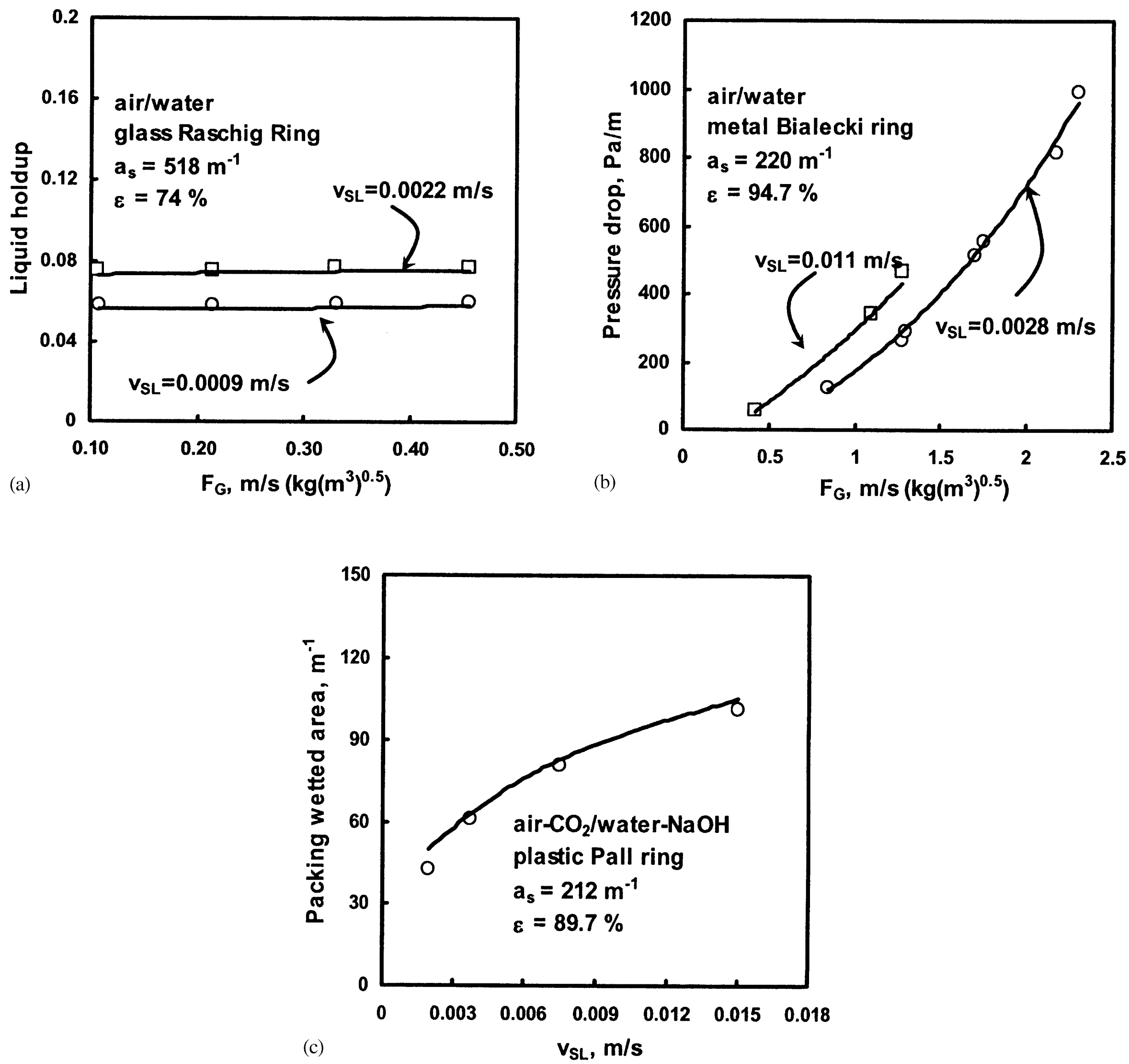

Fig. 3. Effect of gas capacity factor and liquid superficial velocity on the total liquid holdup (a), the irrigated pressure drop (b), the packing wetted area (c). Lines show simulated behavior using Eqs. (30)–(32) and the symbols refer to experimental data points.

Eqs. (30)–(32) with the experimental data pertinent to the pre-loading zone. It should be noted that the irrigated pressure drop, the liquid holdup and packing wetted area are predicted with a mean absolute relative error of 19.4%, 17.3% and 14.6%, respectively.

Owing to its mechanistic nature, the model can be a helpful tool in exploring variations in the irrigated pressure drop, liquid holdup and packing wetted area as a function of changes in the operation conditions of the packed bed columns. As shown in Figs. 3a–c, the simulated effects of gas and liquid loads on the liquid holdup, the irrigated pressure drop and the fractional wetted area in the pre-loading zone for various types of packings match very well the measured values. The model predicts the increase with liquid load of liquid holdup, as well as the very weak influence of gas capacity factor. It also predicts the correct trend between the gas and liquid loads and the two-phase pressure drop (Fig. 3b) and the fractional wetted area (Fig. 3c).

6. Conclusion

A two-zone phenomenological model was developed to predict two-phase pressure drop, total liquid holdup and packing fractional wetted area in gas–liquid counter-current columns containing random packings and operated in the pre-loading zone. The model was an offshoot of the well-known single-slit mechanistic approach of the co-current down-flow trickle-bed reactors. It mimicked the actual bed void by means of two hypothetical and geometrically similar inclined slits consisting of a dry and a wet slits. This mechanistic model required *no single* adjustable parameter, from two-phase flow conditions, and proved powerful in the prediction of the column hydraulics under various operational conditions.

Notation

a_s	specific surface area of packing (surface/bed volume), m^2/m^3
d_p	equivalent diameter based on a sphere of equal volume, m
$E_{1,2}$	Ergun constants
f_i, f_w	interfacial and wall friction factors
g	gravity acceleration, m/s^2
Ga_α	Galileo number, $Ga_\alpha = d_p^3 g \varepsilon^3 \rho_\alpha^2/\mu_\alpha^2(1-\varepsilon)^3$
h_L	liquid holdup
Re_i	interfacial Reynolds number, $Re_i = u_{i,G}\rho_G d_p/\mu_G$
Re_α	Reynolds number, $Re_\alpha = v_{S\alpha} d_p \rho_\alpha/\mu_\alpha(1-\varepsilon)$
u_α	velocity of α-phase in the slit, m/s
$u_{i\alpha}$	interfacial velocity of α-phase, m/s
$v_{S\alpha}$	superficial velocity of α-phase, m/s

Greek letters

α	subscript standing for gas (G) or liquid (L)
δ	liquid film thickness, m
ε	bed void fraction
ϕ	sphericity factor
η_e	packing fractional wetted area
μ_α	viscosity of α-phase, kg/m s
ρ_α	density of α-phase, kg/m^3
$\tau_{i,\alpha}$	shear stress on α-phase, Pa
Ψ_α	α phase dimensionless body force

Subscripts

i	gas–liquid interface
G	gas
L	liquid
w	wall

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