A mechanistic hydrodynamic model for pressure drop prediction in trickle-bed reactors

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Abstract

A mechanistic hydrodynamic model was developed for representation of two-phase, gas-liquid concurrent down-flow in trickle bed reactors. Starting from the general macroscopic balance equation in a porous media and considering some simplifying hypothesis a set of ordinary differential equations was obtained. Gas-Liquid-Solid interactions were accounted for according to the relative permeability concept. Furthermore, capillary pressure was taken into account using an appropriate correlation available in the literature. Then, the resulting model was integrated step by step from the reactor inlet to its outlet, using a numerical method and MATLAB software for programming. This model, based on the relative permeability concept, provided the hydrodynamic parameters in trickle bed reactors. These parameters were pressure drop, liquid saturation, interstitial gas velocity and interstitial liquid velocity. Next, the case of Hexane-Nitrogen-1.52 mm glass spheres system was studied and leading to the variations of the above mentioned hydrodynamic parameters inside the bed.

Keywords: *mechanistic hydrodynamic model; porous media approach; pressure drop; relative permeability; trickle Bed reactor.*

I. Introduction

Trickle Bed Reactors (TBRS) are Gas-Liquid-Solid contacting devices used in many various fields such as petroleum, petrochemical and chemical industries, in waste water treatment, in biochemical and electrochemical processing, etc. as illustrated by the applications reported by Al-Dahhan et al., (1997) and Ranade (2011) [1, 2].

The external liquid holdup, the pressure drop and the flow regime (flow pattern) are important hydrodynamic parameters which have to be known for the process design of a trickle bed installation.

First of all, the liquid-phase residence time and the degree of wetting of the external catalyst surface are both related to the external liquid holdup. Second of all, the pressure drop determines energy losses: sizing of the compression equipment and often gas-liquid mass transfer parameters are correlated to it as well as to the external liquid holdup. Finally, several flow patterns can be observed in the trickle bed reactor: trickle, pulse, spray and dispersed bubble flow and information on the boundaries between these flow patterns is essential because the pressure drop, the liquid holdup and especially the mass transfer parameters are affected differently in each regime[3, 4].

The commercial concurrent trickle-bed reactors normally operate adiabatically and with superficial gas and liquid velocities of up to 30 and 0.8 cm/s, respectively. To increase the concentration of the ga gaseous reactant in the liquid phase, nearly all commercial process are performed at elevated pressures of up to between 20 and 30 MPa. [5]

II. The porous media approach

Trickle bed reactors are considered as multiphase mediums, which are constituted of a solid phase (porous block) and one or many fluid phases (gas or liquids) occupying the void space. In the porous media approach, both fluid and solid phases are modeled as inter-penetrating continua; as if they co-existed at every point in the packed bed (see Fig. 1).

Actually, it is impossible to describe the complex geometry of the solid block and the topology of the void at the microscopic level. As consequence, limit conditions for a mathematical model could not be known. In addition, it is extremely difficult to measure the state variables at each point of the bed. Then, it is necessary to transform the whole problem from the microscopic level to the macroscopic one.

First of all, the microscopic balances of extensive quantities of fluid phases (mass, momentum and energy) were established. The presence of solid was implicitly represented by a porosity distribution.

Next, the averaging of the obtained microscopic balances equations was made to obtain macroscopic balances equations in terms of averaged microscopic quantities, which had measurable values.

Finally, a system of differential equations was obtained in terms of variables representing the measurable quantities (fluid velocities, saturations and pressures).

III. The general macroscopic balance equation in porous media

The mathematical elaborations concerning the general macroscopic balance equation in porous media may refer the original work reported by Kolditz (2002) [6], wherein the following expression for an α-phase in porous medium:

$$\frac{\partial \varepsilon^{\alpha}\overline{\psi^{\alpha}}}{\partial t} = -\nabla.\left(\varepsilon^{\alpha}\overline{\psi^{\alpha}V^{\alpha}} + \varepsilon^{\alpha}\overline{\psi'^{\alpha}V'^{\alpha}} + \varepsilon^{\alpha}\overline{\Phi^{\psi^{\alpha}}_{Diff}}\right) - \frac{1}{\Omega_0}\int_{S^{\alpha\beta}}\Phi^{\psi^{\alpha}}_{Diff}.dS - \frac{1}{\Omega_0}\int_{S^{\alpha\beta}}\psi^{\alpha}(V-W).dS + q^{\psi^{\alpha}} \quad (1)$$

with: Ω_0 Elementary volume of the porous medium

ε^{α} Volumetric fraction of α-phase within the elementary volume

ψ^{α} Extensive quantity (mass, momentum, energy)

V^{α} Velocity of α-phase

ψ'^{α} Fluctuation of ψ^{α}

V'^{α} Fluctuation of V^{α}

$\Phi^{\psi^{\alpha}}_{Diff}$ Diffusive flux of quantity ψ^{α}

$S^{\alpha\beta}$ Interface between α-phase and β-phase, fluid-fluid interface or fluid-particle interface

W Velocity of the interface

$q^{\psi^{\alpha}}$ Source of ψ^{α}

The bar on the letters means the averaged value of the corresponding quantity within the elementary volume

IV. Case of trickle bed reactor

Fig.1 represents flow in a trickle bed reactor according to the porous media approach, illustrating how the liquid trickles over the wall of the reactor and the gas flows in the remaining void. This image represents well the trickle flow regime (low interaction regime) at low fluid velocities. It can also be seen that solid phase does not appear in the picture because it is implicitly represented by a porosity distribution.

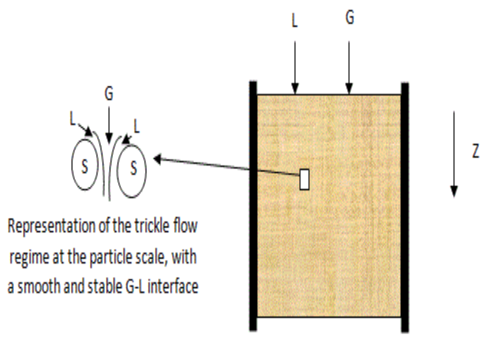

Fig. 1 Schematic representation of TBR according to effective porous media approach(Solid is treated as penetrated continuum)

A. Hypothesis and simplifications:

The following set of hypothesis was considered:

1- Constant bed porosity ($\varepsilon = cte$)
2- We consider a smooth and stable interface between the gas and the liquid
3- Flow is considered steady state: $\frac{\partial \varepsilon^{\alpha}\overline{\psi^{\alpha}}}{\partial t} = 0$

4- Plug flow condition is assumed, then the flow is one-dimensional in the axial direction, Z
5- We neglect the turbulence term: $\varepsilon^{\alpha}\overline{\psi'^{\alpha}V'^{\alpha}}$
6- No mass transfer
7- No reaction
8- Viscous stress forces are neglected
9- Constant liquid density and ideal gas is considered

B. Mass balance equations

Putting$\psi^{\alpha} = \rho^{\alpha}$ and according to the precedent assumptions, Eq. (1) becomes:

$$\frac{1}{P}\frac{dP}{dZ} + \frac{1}{1-\theta}\frac{d(1-\theta)}{dZ} + \frac{1}{U^{G}}\frac{dU^{G}}{dZ} = 0 \quad (2)$$

$$\frac{1}{\theta}\frac{d\theta}{dZ} + \frac{1}{U^{L}}\frac{dU^{L}}{dZ} = 0 \quad (3)$$

θ: is the liquid saturation, and it is defined as:

$$\theta = \frac{\varepsilon^{L}}{\varepsilon} \quad (4)$$

C. Momentum balance equation of α-phase

Putting$\psi^{\alpha} = \rho^{\alpha}V^{\alpha}$, and according to the precedent assumptions, Eq. (1) becomes:

$$\varepsilon^{\alpha}\rho^{\alpha}U^{\alpha}\frac{dU^{\alpha}}{dz} = P^{\alpha}\frac{d\varepsilon^{\alpha}}{dz} - \varepsilon^{\alpha}\frac{dP}{dz} + \varepsilon^{\alpha}\rho^{\alpha}g - F^{\alpha} \quad (5)$$
$$\alpha = G, L$$

F^{α} : is the inter-phase coupling term based on the relative permeability concept and was introduced for the first time by Saez and Carbonell (1985) [7], and adopted recently by Atta and al. (2000) [8] as discussed below.

D. Relative permeability model to account for the drag force F^{α}

There are two approaches for CFD modeling of multi phase flows in trickle bed reactors: Fluid-fluid interaction model and porous media concept. Fluid-fluid interaction model, uses inter phase drag forces to define the interaction between phases and it was well developed in the work of Attou and al. (1999) [9]. However, in porous zone the relative permeability concept was used to specify the effect phases on each other. For a porous medium, relative permeability concept seems to be appropriate to account for the drag forceF^{α}, because it is less computationally demanding.

The approach to be used in this work was based on the assumption that flow domain (fixed bed with catalyst particles) could be described as porous media (as illustrated in fig.1)

The relative permeability concept was first proposed by Saez and Carbonell (1985) for predicting the two-phase hydrodynamics (pressure drops and liquid holdups) of trickle flow in packed beds.

The concept of relative permeability used an expression for the drag for single-phase flow, which was re-scaled to account for the second phase. This parameter, known as the relative permeability was defined as the ratio of the drag force per unit volume under one-phase flow condition to the drag force per unit volume under two-phase flow conditions at the same superficial velocity of a given phase as expressed by:

$$k^{\alpha} = \frac{(F^{\alpha}/\varepsilon^{\alpha})^{0}}{(F^{\alpha}/\varepsilon^{\alpha})} \quad (6)$$

Using an Ergun-type equation for the single-phase pressure drop, the two-phase flow pressure drop could be written in the form:

$$\frac{F^{\alpha}}{\varepsilon^{\alpha}} = \frac{1}{k^{\alpha}}\left[\frac{E_1\mu^{\alpha}(1-\varepsilon)^2}{d_P^2\varepsilon^2}V^{\alpha} + \frac{E_2\rho^{\alpha}(1-\varepsilon)}{d_P\varepsilon^3}V^{\alpha 2}\right] (7)$$

Where:

V^{α}: is the superficial velocity of α-phase

μ^{α}: is the dynamic viscosity of α-phase

d_P: is the equivalent diameter of catalytic solid particles

E_1 and E_2 are the Blake-Kozeny-Carman and Burke-Pulmmer constants, respectively.

Saez and Carbonell (1985) [7] obtained optimal expressions for the gas- and liquid-phase relative permeability based on holdup and pressure drop data taken from the literature. In the calculations, the constants E_1 and E_2 were set equal to 180 and 1.8, respectively, as recommended by Macdonald et al. (1979) Mentioned in [10].

Actually, the relative permeability took into account the blockage of flow in pores as a result of the presence of a second phase. As a result, the relative permeability for a given phase considered a function only of the fraction of the pore volume occupied by that phase, and then their expressions were written as functions of the reduced liquid-phase saturation and the gas-phase saturation:

(From the phase indicators are written as indices)

$$k_L = \delta_L^{2.43} \quad (8)$$

$$k_G = S_G^{4.8} \quad (9)$$

δ_L: is the ration of effective volume of flow of liquid phase to the available volume of flow considering that the static liquid holdup (ε_L^0) represents a portion of the void fraction occupied by stagnant liquid. Thus:

$$\delta_L = \frac{\varepsilon_L - \varepsilon_L^0}{\varepsilon - \varepsilon_L^0} \quad (10)$$

S_G: is the gas saturation and it is defined as:

$$S_G = \frac{\varepsilon - \varepsilon_L}{\varepsilon} \quad (11)$$

Using the expressions from (8) to (11), the drag force expressions for two-phase flow in a trickle bed, can then be obtained:

$$\frac{F_G}{\varepsilon_G} = (\frac{\varepsilon}{\varepsilon - \varepsilon_L})^{4.8}[\frac{E_1\mu_G(1-\varepsilon)^2}{d_P^2\varepsilon^3}V_G + \frac{E_2\rho_G(1-\varepsilon)}{d_P\varepsilon^3}V_G^2] \quad 12)$$

$$\frac{F_L}{\varepsilon_L} = (\frac{\varepsilon - \varepsilon_L^0}{\varepsilon_L - \varepsilon_L^0})^{2.43}\left[\frac{E_1\mu_L(1-\varepsilon)^2}{d_P^2\varepsilon^3}V_L + \frac{E_2\rho_L(1-\varepsilon)}{d_P\varepsilon^3}V_L^2\right] \quad (13)$$

The static liquid holdup (ε_L^0) can be calculated by the following correlation given by Saez and Carbonell (1985) [7]:

$$\varepsilon_L^0 = \frac{1}{(20 + 0.9Eo^*)} \quad (14a)$$

Where

$$Eo^* = \frac{\rho_L g d_P^2 \varepsilon^2}{\sigma_L(1-\varepsilon)^2} \quad (14b)$$

Eo^*: is the Eötvös number, and it indicates the effect of surface tension on the liquid flow inside the bed.

E. The final form of the mathematical model

The final mathematical model describing the trickle flow regime in trickle bed reactor based on the effective porous medium approach (relative permeability concept) is represented by the differential equations system (15):

$$\frac{1}{P}\frac{dP}{dZ} + \frac{1}{1-\theta}\frac{d(1-\theta)}{dZ} + \frac{1}{U_G}\frac{dU_G}{dZ} = 0$$

$$\frac{1}{\theta}\frac{d\theta}{dZ} + \frac{1}{U_L}\frac{dU_L}{dZ} = 0$$

$$\frac{dP}{dZ} = \left(\frac{P}{1-\theta}\right)(\frac{d\theta}{dz}) - (P/RT)U_G\frac{dU_G}{dZ} - (\frac{1}{1-\theta})^{4.8}\left[\frac{E_1\mu_G(1-\varepsilon)^2}{d_P^2\varepsilon^3}V_G + \frac{E_2(P/RT)(1-\varepsilon)}{d_P\varepsilon^3}V_G^2\right] + (P/RT)g$$

$$\frac{dP}{dZ} = -\left(\frac{P-P_c}{\theta}\right)\left(\frac{d\theta}{dz}\right) - \rho_L U_L\frac{dU_L}{dZ} - \left(\frac{1-\theta^0}{\theta-\theta^0}\right)^{2.43}\left[\frac{E_1\mu_L(1-\varepsilon)^2}{d_P^2\varepsilon^3}V_L + \frac{E_2\rho_L(1-\varepsilon)}{d_P\varepsilon^3}V_L^2\right] + \rho_L g \quad (15)$$

Such that $\theta^0$is the static liquid saturation, and is defined by the following expression

$$\theta^0 = \frac{\varepsilon_L^0}{\varepsilon} \quad (16)$$

and $P_c$is the capillary pressure which is calculated by the correlation proposed by Attou and Freschneider (2000) [11] (see Appendix)

The system of equations (15) is a set of four differential equations, and it contains four unknown variables, which are:

P: is the gas pressure

θ : is the liquid saturation

U_G: is the gas interstitial velocity

U_L: is the liquid interstitial velocity

For a given operating conditions (fluids superficial velocities, operating pressure, operating temperature), fluids properties (densities, viscosities and liquid surface tension) and packing characteristics (particle diameter, and bed porosity), this model is integrated step by step starting from the inlet up to the outlet of the trickle bed reactors by means of the fourth order Runge-Kutta algorithm.

V. Simulation of the model

By resolving the equations set (15), the variation of gas pressure, fluid interstitial velocities and liquid saturation along the bed might be obtained. Herein after, simulations based on the model were performed with the following operating conditions, fluid properties and packed bed characteristics:

a- Operating conditions:

- Liquid superficial velocity: V_L=0.085 m.s^{-1}
- Gas superficial velocity: V_G=0.01 m.s^{-1}

- Pressure: P=0.31 MPa
- Temperature: T=298 K

b- Fluid properties [12]:

- Hexane
  $(\rho_L = 663\ kg.m^{-3}, \mu_L = 3.07.10^{-4} Pa.s, \sigma_L = 17.89\ mN.m^{-1})$
- Nitrogen
  $(\rho_G = \frac{P}{RT} kg.m^{-3}, \mu_G = 1.78.10^{-5} Pa.s, R = 296.73\ J.kg^{-1}.K^{-1})$

The liquid dynamic viscosity is inversely dependent to its density. As the liquid density was supposed to be constant, then its dynamic viscosity was assumed to be constant. For ideal gas, the dynamic viscosity is independent to pressure. ([13], [14])

c- Bed characteristics:

- Porosity: $\varepsilon = 0.412$
- Particle equivalent diameter: $d_P = 1.52\ mm$
- Bed length: $L = 51.61\ cm$

A. Limit conditions:

It was considered that at the inlet of the bed that the velocities profile and the liquid saturation were flat i.e.

$$\frac{dP}{dz} = \frac{dU_G}{dz} = \frac{dU_L}{dz} = \frac{d\theta}{dz} = 0 \qquad (17)$$

By replacing expressions (17) in the equations set (15), the following algebraic equation with one variable (θo) was obtained:

$$(\frac{1}{1-\theta o})^{4.8}\left[\frac{E_1\mu_G(1-\varepsilon)^2}{d_P^2\varepsilon^3}V_G + \frac{E_2(P/RT)(1-\varepsilon)}{d_P\varepsilon^3}V_G^2\right] + (P/RT)g = (\frac{1-\theta^0}{\theta o-\theta^0})^{2.43}\left[\frac{E_1\mu_L(1-\varepsilon)^2}{d_P^2\varepsilon^3}V_L + \frac{E_2\rho_L(1-\varepsilon)}{d_P\varepsilon^3}V_L^2\right] + \rho_L g \qquad (18)$$

θo: is the liquid saturation at the bed inlet

The algorithm of Newton-Raphson was used to solve Eq. (18) and the inlet liquid saturation might be obtained:

Inlet liquid saturation: $\theta o = 0.7867$

Then, the use of the definitions of interstitial liquid and gas velocity inside the bed led to the following numerical data:

Inlet liquid interstitial velocity: $V_{L0}=V_L/(\theta_0\varepsilon)$= 0.2622 m/sec

Inlet gas interstitial velocity: $V_{G0}=V_G/(\varepsilon(1-\theta_0))$= 0.1138 m/sec

Finally, the inlet pressure was set to be the following:

Inlet Pressure: P_0=310000 Pa

B. Results:

The following graphs show the evolution of gas pressure, liquid saturation, liquid interstitial velocity and gas interstitial velocity along the bed.

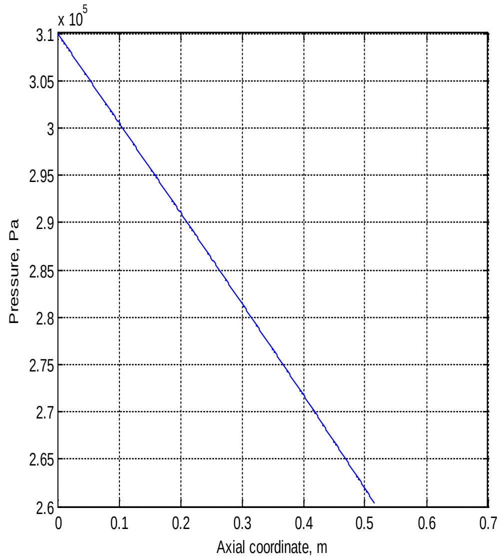

Figure 2. Pressure variation along the bed

Fig. 2 illustrates the pressure variation along the bed, it can be seen clearly that the pressure drop was equal to 4.9704e+04Pa. Actually, the pressure drop is a lost energy from the fluids internal energy due to flow resistance because of the trickle bed reactor topology.

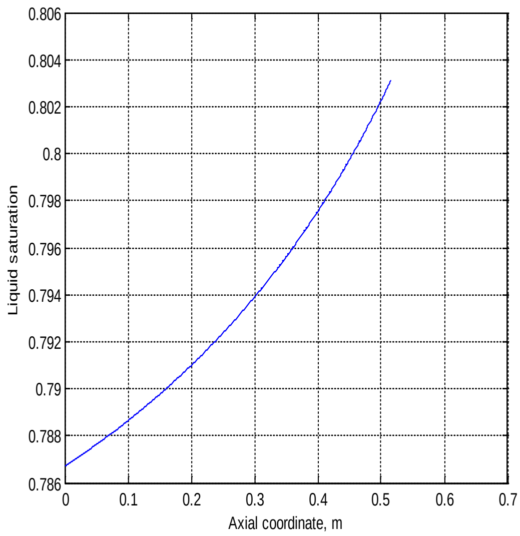

Figure3. Liquid saturation variation along the bed

Fig. 3 illustrates the liquid saturation variation along the bed, it can be seen clearly that the liquid saturation was increasing along the bed. In fact, capillary pressure presented an additional resistance for liquid flow, so that liquid tended to be accumulated inside the bed and this was represented by an increase in liquid fraction going down in the bed.

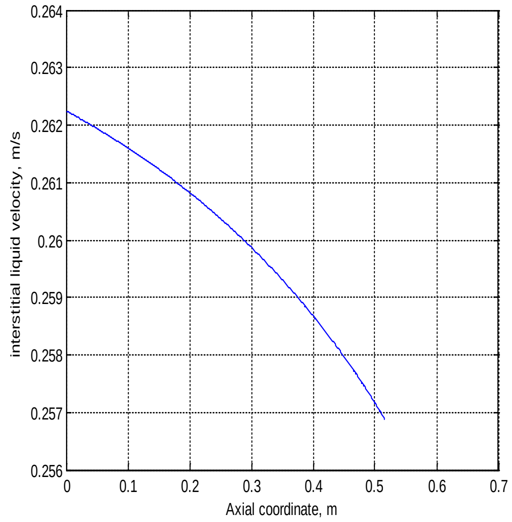

Figure 4. Interstitial liquid velocity variation along the bed

Fig. 4 shows that the interstitial liquid velocity was decreasing along the bed. Here also, for the case of the interstitial liquid velocity, the capillary pressure effect appeared. The additional resistance due the capillary effect, curbed the liquid flow, thus a decreasing in liquid velocity inside the bed was observed. Truly, an opposite effect on liquid saturation was observed.

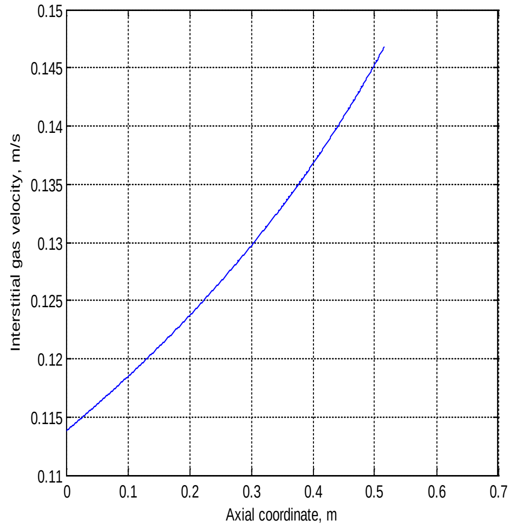

Figure5. Interstitial gas velocity variation along the bed

Fig. 5 presents an increasing profile of the gas interstitial velocity along the bed. Really, a decrease of gas pressure, due to the pressure drop, thermodynamically, leads to an increase of its flow rate

VI. Conclusions:

A 1D-model was developed describing flow inside trickle bed reactors. A systematic approach was adopted to establish the model, starting from the general balance equation in porous media and relying on a set of hypothesis, the mass balance and momentum balance equations for a trickle bed reactor were derived. Closure relationships for capillary pressure and drag forces were needed. The model was integrated step by step from the reactor inlet to its outlet and the hydrodynamic parameters profiles along the bed were plotted.

This model predicted the pressure drop and liquid distribution inside the bed which are key hydrodynamic parameters for trickle bed reactor design.

A one step is remaining to adopt this model, is to study its validity by comparing simulated results with experimental data. Whether the developed model gives precise results or not, it represents a fundamental and a comprehensive approach for trickle bed hydrodynamic modeling.

Acknowledgment

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List of symbols

$\boldsymbol{d_P}$ Equivalent diameter of catalytic solid particles

$\boldsymbol{E_1}$ and $\boldsymbol{E_2}$ Blake-Kozeny-Carman and Burke-Pulmmer constants, respectively.

$\boldsymbol{F^\alpha}$ Resultant forces acting on α-phase

g Gravitational force

G Gas phase

H Bed length

$\boldsymbol{k^\alpha}$Relative permeability of α-phase

L Liquid phase

P Pressure, Pa

$\boldsymbol{P_c}$ Capillary pressure, Pa

R Relative ideal gas constant, $\mathrm{J.kg^{-1}.k^{-1}}$

$\boldsymbol{S}$ Solid phase

$\boldsymbol{S^{\alpha\beta}}$ Interface between α-phase and β-phase, fluid-fluid interface or fluid-particle interface

$\boldsymbol{S_\alpha}$α-phase saturation

$\boldsymbol{T}$ Temperature, k

$\boldsymbol{V^\alpha}$Velocity of α-phase

$\boldsymbol{V'^\alpha}$Fluctuation of V^α

$\boldsymbol{V_\alpha}$Superficial velocity of α-phase

$\boldsymbol{U^\alpha}$α-phase interstitial velocity

$\boldsymbol{W}$ Velocity of the interface

$\boldsymbol{q^{\psi^\alpha}}$Source of ψ^α

Greek letters

$\boldsymbol{\varepsilon}$: Bed porosity

$\boldsymbol{\varepsilon^\alpha}$ Volumetric fraction of α-phase within the elementary volume

$\boldsymbol{\varepsilon_L^0}$ Static liquid holdup

$\boldsymbol{Eo}^*$Eötvös number

$\boldsymbol{\Omega_0}$ Elementary volume of the porous medium

$\boldsymbol{\theta}$: is the liquid saturation

$\boldsymbol{\theta^0}$ Static liquid saturation

$\boldsymbol{\Phi_{Diff}^{\psi^\alpha}}$Diffusive flux of quantity ψ^α

$\boldsymbol{\psi^\alpha}$Extensive quantity (mass, momentum, energy)

$\boldsymbol{\Phi_{Diff}^{\psi^\alpha}}$Diffusive flux of quantity ψ^α

$\boldsymbol{\rho^\alpha}$$\alpha$-phase density

$\boldsymbol{\varepsilon_G}$ Volumetric fraction of gas-phase

$\boldsymbol{\varepsilon_L}$ Volumetric fraction of liquid-phase

$\boldsymbol{\mu^\alpha}$ Dynamic viscosity of α-phase

$\boldsymbol{\sigma_L}$Liquid surface tension

Subscripts

$\boldsymbol{\alpha}$Gas/liquid phase

$\boldsymbol{G}$Gas phase

$\boldsymbol{L}$Liquid phase

$\boldsymbol{0}$Inlet condition

Superscripts

$\boldsymbol{\alpha}$Gas/liquid phase

$\boldsymbol{G}$Gas phase

$\boldsymbol{L}$Liquid phase

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Appendix

Capillary pressure correlation (correlation of Attou and freschneider (2000))

The capillary pressure is defined as:

$$P_c = P - P_L$$

Where:

$P=P_G$: is the gas pressure

P_L: is the liquid pressure

$$P_c = 2\sigma\left(\frac{1-\varepsilon}{1-\varepsilon_G}\right)^{1/3}\left(\frac{1}{d_P}+\frac{1}{d_{min}}\right)F(\frac{\rho_G}{\rho_L})$$

Where

$$d_{min} = (\frac{\sqrt{3}}{\pi} - \frac{1}{2})^{1/2} d_P$$

And

$F\left(\frac{\rho_G}{\rho_L}\right) = 1 + 1.88\left(\frac{\rho_G}{\rho_L}\right)$, for $\frac{\rho_G}{\rho_L} < 0.025$