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A macroscopic model for the description of two-phase flow in structured packings using the concept of effective surface

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Abstract

Columns containing structured packings play an important role in chemical engineering processes involving distillation and gas-liquid separation, such as air distillation or CO_2 absorption. The packings often consist of corrugated plates that significantly increase the exchange surface between gas and liquid phases in the column. The columns are generally operated in a counter-current flow mode: a thin liquid film is driven by gravity and is sheared by the upward gas flow. The structure of the packings may be seen as a porous medium with a large porosity and multi-scale features, with a locally repeating elementary pattern. A pore-scale, associated to the elementary pattern, and a macro-scale assimilated to the packing scale, define the two-scale description. An upscaling approach was used previously to develop a macro-scale law for the gas-phase flow at relatively large Reynolds numbers [?]. At this scale the flow is governed by averaged equations, and information concerning the dynamic of the phase as well as its interactions with the solid structure are embedded in effective parameters. In this model, it was assumed, as a first approximation, that the liquid film is sufficiently thin so that its impact on the flow and the average gas pressure drop can be neglected.

It is well known, however, that the interaction between the two phases plays an important role in the process due to

the development of surface waves at the liquid-gas interface [?]. How much such a non-uniform surface affects the gas flow and the macroscale pressure drop remains to be determined. In this work, we propose to analyze the potential effect of the film wave instabilities on the macroscale flow and pressure drop.

Effective wall law for the gas-liquid interface As mentioned above, the gas phase is driven as a countercurrent flow over the liquid film, resulting in a shear stress at the gas-liquid interface. This leads to the appearance of complex instabilities at the liquid film surface, which can take the form of a train of waves [?]. Modeling of this two-phase flow is a complicated problem, but one that can be greatly simplified using a scaling analysis of the characteristic time and length scales. The liquid film thickness is firstly considerably small compared to the pore size with a ratio between mean thickness about 1 to 100. However, the amplitude of the waves at the liquid surface can be large compared to the film thickness, with a ratio about 1 to 5. The viscosity and density of the gas are also much smaller than that of the liquid whereas the velocity of the gas is much larger than that of the fluid. These assumptions can be used to simplify the equations that govern the flow for the gas phase so that the liquid-gas interface is considered as a wavy rigid interface and gas flow is uncoupled from liquid flow. This assumption is based on the fact that the fluctuations in the gas flowing over the liquid film decay in the same way as those in the gas flowing over a rigid wall.

Even with these approximations the problem remains computationnaly challenging to solve, in particular because of the fluid surface roughness. To circumvent this problem, we first transform the rough no-slip surface into an effective smooth boundary. A wall law, derived using the method of domain decomposition [?], is derived at the smooth surface in order to mimic the effects of the complex rough wall on the gas flow. Fig. 1 is a schematic representation of the liquid-gas system and the effective surface Γ_{eff} . This approach is valid in the limit where the fluctuations induced by the rough wall on the flow are confined into the boundary layer of the gas phase and vanish sufficiently far from the wall. The wall-law is used on Γ_{eff} and consists in a combination of the normal derivatives of the velocity field at the interface. At first order, it is a Navier slip condition. The coefficients present in the wall law are computed by the resolution of closure problems over an elementary pattern of the rough wall, which is refered as Ω_{1_i} in Fig. 1.

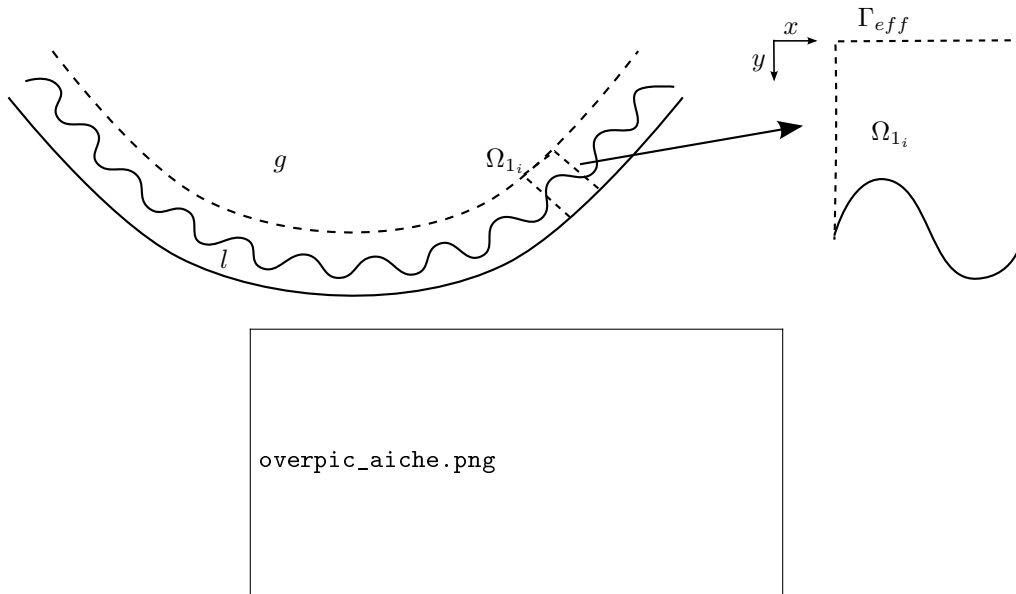


Figure 1: Schematic representation of the effective surface at the liquid-gas interface

Upscaling at the packing-scale As a second step, we use the method of volume averaging to upscale mass and momentum balance equations from the pore to the packing-scale (Fig. 2). The pore-scale model consists in Navier-Stokes equations at moderate Reynolds numbers (no turbulence model is considered) with the effective boundary condition derived at the first step. The resulting macro-scale momentum equation is a generalized Darcy-Forchheimer equation with correction tensors that can be calculated locally over a unit-cell. For $Re \ll 1$, the macro-scale equation reduces to the classic Darcy's law, where the intrinsic permeability captures the rough geometry of the medium via the concept of effective condition. The method is first applied to a channel flow for which we compare the pressure drop computed from a direct numerical simulation of the wavy wall with the case of effective conditions prescribed at smooth walls. The method is also applied to the elementary pattern of structured packings, where the wavy pattern on the walls represents the wavy liquid-gas interface. This model allows us to describe how the roughness impacts the apparent permeability at the packing-scale via the concept of effective boundary condition.

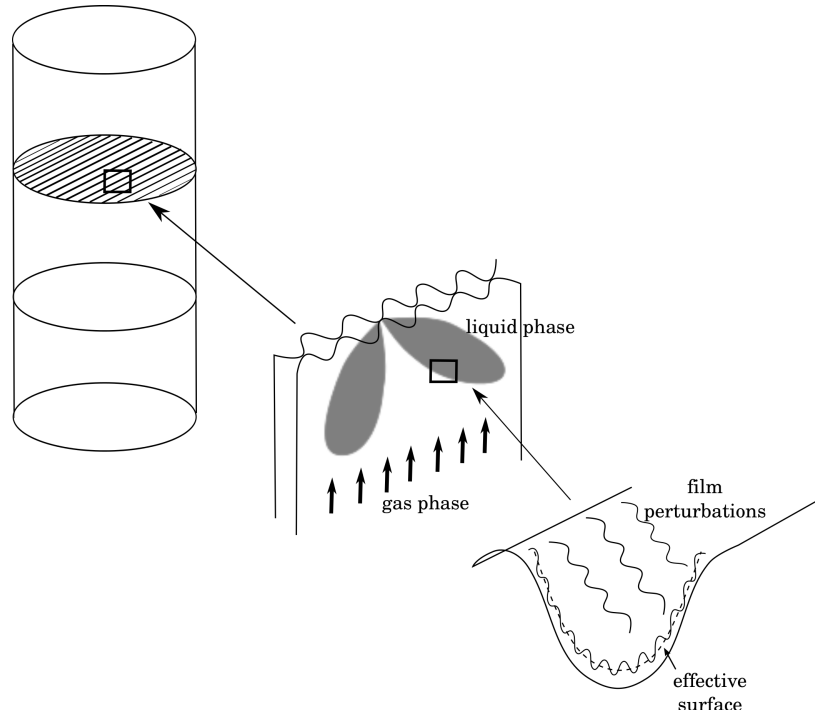


Figure 2: Schematic representation of the upscaling process : from the pore-scale to the packing-scale

Computation of the macroscale system at the column-scale At the column-scale, a multiphase system of macro-scale equations based on the effective surface model can be used to model the liquid and gas phases in structured packings. These averaged equations can predict the pressure drop in the column, as well as the liquid spreading. The macro-scale momentum equation for the gas phase is a Darcy-Fochheimer law with effective tensors. These tensors take into account a coupling with the liquid film through the concept of effective surface, where the effective surface replaces the complex liquid-gas interface. The liquid phase is assimilated to a thin gravity film flowing downward according to an effective angle θ^* . Following the idea suggested by Mahr et al. [?] and extended by Soulaine et al. [?], the liquid film is separated into two distinct phases in order to capture the radial spreading of the liquid phase into the column. The two resulting films are not independent and exchange mass at the contact points between the corrugated sheets. This yields a two equations system for the liquid phases, with multiphase permeability tensors [?]. The resulting macro-scale system for the liquid-gas system is then a three equations model that involves effective permeability tensors, relating the superficial velocities to the pressure gradients.

Our model extends previous works on modeling flow in distillation columns in the following way

- We have proposed a method to evaluate the potential pressure drop in distillation process induced by the surface waves at the liquid-gas interface.
- We have developed a three-scale analysis of the problem allowing us to compute numerically the effective parameters of the model. This is essentially done using the concept of effective surface that greatly reduces the mesh element number.

These advances in the model will allow us to pursue the development of the three equations model, particularly regarding the saturation dependency of the effective properties.

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