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Modeling flow in porous media with rough surfaces: Effective slip boundary conditions and application to structured packings

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HIGHLIGHTS

- An upscaling methodology is proposed to characterize fluid flow in porous media with rough surfaces.
- The no-slip condition on the rough surface is replaced with a tensorial slip condition on a fictive smooth surface.
- The permeability decreases significantly, even for small amplitudes of the roughness.
- The pressure drop is accurately predicted for structured packings used in separation processes.
- Different regimes are identified in the transition from creeping flow to the onset of unsteady inertial flow.

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ABSTRACT

Understanding and modeling flows in columns equipped with structured packings is crucial to enhance the efficiency of many processes in chemical engineering. As in most porous media, an important factor that affects the flow is the presence of rough surfaces, whether this roughness has been engineered as a texture on the corrugated sheets or is the result of hydrodynamic instabilities at the interface between a gas and a liquid phase. Here, we develop a homogenized model for flows in generic porous media with rough surfaces. First, we derive a tensorial form of an effective slip boundary condition that replaces the no-slip condition on the complex rough structure and captures surface anisotropy. Second, a Darcy-Forchheimer model is obtained using the volume averaging method to homogenize the pore-scale equations with the effective slip condition. The advantage of decomposing the upscaling in these two steps is that the effective parameters at the Darcy-scale can be calculated in a representative volume with smooth boundaries, therefore considerably simplifying mesh construction and computations. The approach is then applied to a variety of geometries, including structured packings, and compared with direct numerical solutions of the flow to evaluate its accuracy over a wide range of Reynolds number. We find that the roughness can significantly impact the flow and that this impact is accurately captured by the effective boundary condition for moderate Reynolds numbers. We further discuss the dependance of the permeability and generalized Forchheimer terms upon the Reynolds number and propose a classification into distinct regimes.

1. Introduction

Structured packings are widely used in industrial processes for phase separation such as distillation or post-combustion CO_2 capture. These often consist of parallel corrugated sheets packed together in a way that maintains a large void fraction and surface area, therefore maximizing transfers between phases. Prediction of the pressure drop in columns equipped with such packings is a major concern for users and manufacturers alike. Recent developments in computational fluid dynamics (CFD), along with the advent of high performance computing, are providing the necessary basis to better understand flow in these complex structures and, ultimately, to optimize their design.

Column-scale computations of the flow at the pore-scale, however, is still not feasible. Most simulations focus on a restricted part of the domain, for instance a representative elementary volume (REV) of structured packings. Calculations over a REV are useful to understand the micro-scale physics and evaluate effective parameters that apply to the packing and the column-scale, while being small enough to allow for accurate simulations resolving the smallest scales of the flow. This strategy, inspired from approaches

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Nomenclature

Greek symbols

γ	fluid phase
σ	solid phase
ρ_γ	density of the phase γ
μ_γ	dynamic viscosity of the phase γ
λ	wavelength of the roughness
$\mathcal{A}$	amplitude of the roughness
$\mathcal{V}$	volume
Ω	domain
ϕ	volume fractions of the domains Ω
Ω_{w_i}	small domain over a unit rough element
κ	curvature of the interface Γ_{ws}
$\Gamma_{\gamma\sigma}$	surface of the rough porous medium
Γ_{ws}	interface between the two sub-domains Ω_w and Ω_s
$\Gamma_{\gamma\sigma}^{\text{smooth}}$	surface of the smooth domain Ω_{smooth} positioned at the mean position of the roughness

Roman symbols

l	characteristic length-scale of the pores
l_w	distance between the rough wall and the effective surface
L	characteristic length associated with the averaging domain Ω
d	diameter of the cylinders
H	characteristic length for the 2D channel and for structured packings
$p_\gamma,\ p_s,\ p_w$	pressure defined respectively in $\Omega_\gamma,\ \Omega_s,\ \Omega_w$
$\mathbf{u}_\gamma, \mathbf{u}_s, \mathbf{u}_w$	fluid velocity defined respectively in the domain $\Omega_\gamma, \Omega_s, \Omega_w$
$\mathbf{a}, \mathbf{A}$	couple of mapping variables for pressure and velocity in Ω_{w_i}
$\mathbf{b}_s, \mathbf{B}_s$	couple of mapping variables for pressure and velocity in Ω_s
$\mathbf{F}$	inertial correction tensors
$\mathbf{K}^\star$	apparent permeability
$k^\star$	dimensionless permeabilities
$\mathbf{g}$	gravitational acceleration
g_p	global pressure gradient
g_s	global dissipation rate
Re_d	Reynolds number with d as characteristic length

used in porous media sciences, was first introduced by Petre et al. (2003), who modeled the gas flow within four REVs in the viscous and turbulent regimes. Once effective parameters, such as the permeability tensor, have been evaluated in this REV, the whole column can be treated as a homogenized porous medium. For instance, momentum transport at the column-scale can be described by Darcy-Forchheimer's law, which can then be solved numerically on a coarse mesh. This approach yields results that are generally more accurate than earlier empirical correlations, such as those proposed by Brunazzi and Paglianti (1997), Olujic (1999) and Rocha et al. (1993).

A recent contribution that uses the porous media approach to study flow and pressure drop in gas-liquid distillation columns is the work by Mahr and Mewes (2008). The authors introduced a flow resistance tensor that depends on the velocity magnitude, which can be used to predict the pressure drop for any flow direction. Soulaine and Quintard (2014) further investigated anisotropy generated at the micro-scale by inertial flow and proposed an upscaling methodology to determine a correction tensor in the Darcy-Forchheimer's law. Their conclusion, for 45° inclined corrugations, is that the non-diagonal terms in the effective second-order tensors can be neglected in comparison to the diagonal ones.

In addition to inertial effects and anisotropy, an important factor that affects the gas pressure drop in these columns is the potential presence of rough surfaces. For instance, the corrugated sheets may be textured to increase the efficiency of distillation processes (McGlamery, 1988) or hydrodynamic instabilities may develop at the liquid-gas interface as a result of the steep flowing angle of the film and the high contrast in velocity between the two phases (Zapke and Kröger, 2000; Dietze and Ruyer-Quil, 2013). Those instabilities, which can manifest as soliton structures, are likely to generate dramatic changes of the pressure drop and contribute to the flooding of the column for a large flow rate of the gas phase (Trifonov, 2010). Based on the contrasts in density, viscosity and velocity between the two phases, one often assumes that the gas flow can be treated as a single-phase flow over a rigid rough surface. For this to be accurate, the velocity in the gas phase must be much larger than the velocity in the liquid phase so that we can use a no-slip boundary condition (see also (Vellingiri et al., 2013) for additional details). The trains of waves can then be treated as a surface roughness for the pressure drop in the gas-phase. This is also consistent with previous works that treat the pressure drop of the gas phase *a posteriori*, by considering the liquid film hold-up for the calculation of the interstitial gas velocity (Raynal and Royon-Lebeaud, 2007).

Here, we propose a multi-scale approach to evaluate the impact of rough surfaces on the macro-scale properties of momentum transport. We develop a systematic methodology for a generic porous medium, independently of the initial nature of the roughness, which is based on the idea that the rough surface can be replaced by an effective boundary condition over a smooth surface, to reduce computation time and limit issues with the mesh construction. To this end, we start by describing the pore-scale system of equations in Section 2, along with the domain decomposition method leading to the derivation of an *effective slip boundary condition* that replaces the rough surface. We then go on to upscale these equations in Section 3 using the *volume averaging with closure technique* to obtain the macro-scale equations that describe momentum transport along with the closure problems that are used to calculate effective parameters. In Section 4, we apply this generic approach to a variety of geometries including a representative element of structured packings. We evaluate the accuracy of our approach and the impact of the roughness on the effective parameters. Finally, in Section 5, we discuss the limitations of the framework and provide ideas for future improvements.

2. Derivation of an effective slip condition

As discussed in Section 1, the goal of this paper is to develop an upscaling methodology that can be used to evaluate the impact of rough surfaces in porous media. To this end, we will use the method of volume averaging with closure, which has been widely documented since the early work of Whitaker (1986). This method usually yields a macro-scale model involving effective parameters that are computed by solving closure problems over a REV. An important implication of rough surfaces is that computations of the closure problems over a REV may not be tractable if the characteristic amplitude, $\mathcal{A}$, and wavelength, λ, of the roughnesses are small compared to the pore-scale, l. If this is the case, i.e. if $\frac{\mathcal{A}}{l} \ll 1$