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Effective surface and boundary conditions for heterogeneous surfaces with mixed boundary conditions

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ABSTRACT

To deal with multi-scale problems involving transport from a heterogeneous and rough surface characterized by a mixed boundary condition, an effective surface theory is developed, which replaces the original surface by a homogeneous and smooth surface with specific boundary conditions. A typical example corresponds to a laminar flow over a soluble salt medium which contains insoluble material. To develop the concept of effective surface, a multi-domain decomposition approach is applied. In this framework, velocity and concentration at micro-scale are estimated with an asymptotic expansion of deviation terms with respect to macro-scale velocity and concentration fields. Closure problems for the deviations are obtained and used to define the effective surface position and the related boundary conditions. The evolution of some effective properties and the impact of surface geometry, Péclet, Schmidt and Damköhler numbers are investigated. Finally, comparisons are made between the numerical results obtained with the effective models and those from direct numerical simulations with the original rough surface, for two kinds of configurations.

1. Introduction

Transport phenomena taking place over heterogeneous and rough surfaces can be found in a wide range of processes, such as dissolution, drying or ablation to cite a few. The surface characteristic length-scale (linked to the heterogeneities) is generally much smaller than the scale of the global mechanism. In these circumstances, direct numerical simulations (DNSs) become difficult to achieve in practical applications. Indeed, DNSs are only possible when the two length-scales have more or less the same order of magnitude. To overcome this difficulty, a traditional way of solving such problems is to incorporate the micro-scale behaviors into a boundary condition over a smooth, “homogenized” or effective surface.

In [1–3], domain decomposition and multi-scale asymptotic analysis were first introduced to develop an effective surface and the associated boundary conditions for the flow over a rough solid–liquid surface. Later, the effective surface concept was used to describe ablation processes in aerospace [30] and nuclear safety [15] contexts. Different from these works which employed asymptotic method, Wood et al. [33] obtained a spatially smoothed jump condition for the originally non-uniform surface with volume averaging technique. For sake of simplicity, most of the previous studies ignored the geometry changes

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Nomenclature

Roman symbols

$\mathbf{A}$	closure variable for the velocity (dimensionless)	
a	closure variable for the concentration (dimensionless)	
$A_{\beta\gamma}$	surface area of the soluble material in Ω_i	m^2
$A_{\beta\sigma}$	surface area of the insoluble material in Ω_i	m^2
$\mathbf{B}$	closure variable for the velocity	m
b	closure variable for the concentration	m
b_r	roughness width	m
c	concentration of the dissolved species defined in Ω	$kg\,m^{-3}$
c_{eq}	thermodynamic equilibrium concentration of the dissolved species	$kg\,m^{-3}$
c_i	concentration of the dissolved species defined in Ω_i	$kg\,m^{-3}$
$\tilde{c}_i$	concentration deviation of the dissolved species in Ω_i	$kg\,m^{-3}$
c_0	concentration of the dissolved species defined in Ω_0	$kg\,m^{-3}$
D	diffusion coefficient of the dissolved species	$m^2\,s^{-1}$
Da	Damköhler number (dimensionless)	
$\mathrm{Da}^v_{\mathrm{eff}}$	effective Damköhler number at Σ^v_{eff} (dimensionless)	
$\widehat{\mathrm{Da}}$	mean Damköhler number over surface Σ (dimensionless)	
$\mathbf{e}_1$	unit normal vector linked to x (dimensionless)	
$\mathbf{e}_2$	unit normal vector linked to y (dimensionless)	
h_r	roughness height	m
k	reaction rate coefficient at Σ	$m\,s^{-1}$
k_γ	reaction rate coefficient at $\Sigma_{\beta\gamma}$	$m\,s^{-1}$
k_σ	reaction rate coefficient at $\Sigma_{\beta\sigma}$	$m\,s^{-1}$
k^0_{eff}	effective reaction rate coefficient at $y=0$	$m\,s^{-1}$
k^c_{eff}	effective reaction rate coefficient at Σ^c_{eff}	$m\,s^{-1}$
k^v_{eff}	effective reaction rate coefficient at Σ^v_{eff}	$m\,s^{-1}$
k^w_{eff}	effective reaction rate coefficient at $y=w$	$m\,s^{-1}$
$\hat{k}^v$	surface average reaction rate coefficient at Σ^v_{eff}	$m\,s^{-1}$
l	micro-scale characteristic length	m
l_i	width of Ω_i	m
L	macro-scale characteristic length	m
m	closure variable for the pressure	$Pa\,s\,m^{-1}$
$\mathbf{n}_{ls}$	unit normal vector on Σ pointing towards the solid (dimensionless)	
$\mathbf{n}_{0,i}$	unit normal vector on $\Sigma_{0,i}$ pointing towards the wall (dimensionless)	
p	pressure defined in Ω	Pa
p_0	pressure defined in Ω_0	Pa
p_i	pressure defined in Ω_i	Pa
Pe_l	micro-scale Péclet number (dimensionless)	
$\tilde{p}_i$	pressure deviation defined in Ω_i	Pa
Re_l	micro-scale Reynolds number (dimensionless)	
Re_L	macro-scale Reynolds number (dimensionless)	
s	closure variable for the pressure	Pa s
Sc	micro-scale Schmidt number (dimensionless)	
$\mathbf{u}$	fluid velocity defined in Ω	$m\,s^{-1}$
$\mathbf{u}_i$	fluid velocity defined in Ω_i	$m\,s^{-1}$
$\tilde{\mathbf{u}}_i$	fluid velocity deviation in Ω_i	$m\,s^{-1}$
$\mathbf{u}_0$	fluid velocity defined in Ω_0	$m\,s^{-1}$
U	magnitude of macro-scale velocity	$m\,s^{-1}$
w^c_x	distance between Σ_0 and Σ^c_{eff}	m
w^v_x	distance between Σ_0 and Σ^v_{eff}	m
x	abscissa	m
y	ordinate	m

Greek symbols

β	subscript referring to the fluid phase	
δ	effective surface position	m
δ_c	position of effective surface under thermodynamic equilibrium (dimensionless)	
δ_v	position of effective surface with no-slip condition (dimensionless)	
γ	subscript referring to soluble phase	
σ	subscript referring to insoluble phase	
μ	fluid dynamic viscosity	Pa s
Ω	global domain	
Ω_0	subdomain associated with length scale L	
Ω_i	pseudo-periodic unit cell	
ρ	fluid density	$kg\,m^{-3}$
ρ_γ	density of soluble medium	$kg\,m^{-3}$
ρ_σ	density of insoluble material	$kg\,m^{-3}$
Σ	rough solid–liquid interface	
$\Sigma_{\beta\gamma}$	interface between β and γ phases	
$\Sigma_{\beta\sigma}$	interface between β and σ phases	
Σ_0	fictitious surface separating Ω_0 and Ω_i	
$\Sigma_{0,i}$	restriction of Σ_0 in Ω_i	
Σ_e	upper surface of Ω	
Σ^c_{eff}	effective surface under thermodynamic equilibrium	
Σ^v_{eff}	effective surface with no-slip boundary condition	
Σ_l	lateral surface of Ω	
$\Sigma_{l,i}$	periodic surface lateral surface of Ω_i	