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Numerical Modeling of Non-Isothermal Compositional Compressible Gas Flow in Soil and Coupled Atmospheric Boundary Layer

Ondřej Pártl[1,*], Michal Beneš[1], Radek Fučík[1] and Tissa Illangasekare[2]

[1] *Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Trojanova 13, 120 00 Prague 2, Czech Republic.*
[2] *Center for the Experimental Study of Subsurface Environmental Processes, Department of Civil and Environmental Engineering, Colorado School of Mines, Golden, CO 80401, Colorado, USA.*

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Abstract. Compositional gas flow in a heterogeneous porous medium and in the coupled atmospheric boundary layer above the porous medium surface is of interest in many applications, which requires reliable numerical tools for modeling of very complex physical processes. But there are still many important effects which are very often ignored in contemporary models of this flow. One of them is compressibility. So far, no models of non-isothermal compositional compressible gas flow in a porous medium and in the coupled atmospheric boundary layer above its surface has been reported in the literature. Therefore, we propose mathematical and numerical models for the description of the above scenario. In order to assess the reliability of our numerical model, we analyze its convergence by quantitative computational studies. We also present several qualitative computational studies which present the dynamics of the non-isothermal compositional compressible gas flow in free flow–porous medium flow interaction.

AMS subject classifications: 76N99, 76S99

Key words: Compressible flow, non-isothermal flow, compositional flow, porous medium, free flow, coupling conditions.

Nomenclature

Greek letters

α_{BJ} Beavers-Joseph coefficient $[-]$ (introduced in (2.39), page 355)

*Corresponding author. *Email addresses:* ondrej.partl@fjfi.cvut.cz (O. Pártl), michal.benes@fjfi.cvut.cz (M. Beneš), radek.fucik@fjfi.cvut.cz (R. Fučík), tillanga@mines.edu (T. Illangasekare)

α_{EOC}	coefficient defined on page 372
$\Gamma^{\alpha}_{i,j}$	side of V^{α}_{i} (defined on page 361)
$\Gamma_{f,\theta}$	part of $\partial\Omega^{pm}$, where $\theta \in \{\text{Dir}, \text{Neu}, \text{out}\}$ and $f \in \{p, X_n, T\}$
Γ^{ff}_{θ}	part of $\partial\Omega^{ff}$, where $\theta \in \{\text{left}, \text{right}, \text{top}_1, \text{top}_2, \text{side}\}$
Γ_i, Γ^b_i	parts of ∂V_i (defined on page 357)
$\Gamma^e_{i,j}$, $\Gamma^b_{i,j}$	parts of ∂V_i (defined on page 357)
Γ^{pm}_{θ}	part of $\partial\Omega^{pm}$, where $\theta \in \{\text{wall}, \text{gap}_1, \text{gap}_2, \text{right}\}$
$\delta_{i,j}$	Kronecker delta
κ	ratio of specific heats $[-]$
λ	thermal conductivity $[\text{kg}\cdot\text{m}\cdot\text{s}^{-3}\cdot\text{K}^{-1}]$
Λ^e, Λ_i	sets of indices (defined on page 357)
Λ^e_i, Λ^b_i	sets of indices (defined on page 357)
$\Lambda_{i,j}$, Λ^n_i	sets of indices (defined on page 357)
$\Lambda^b_{f,\theta,i}$	set of indices related to function f, where $\theta \in \{\text{Neu}, \text{out}\}$ (defined on page 357)
μ	dynamic viscosity $[\text{kg}\cdot\text{m}^{-1}\cdot\text{s}^{-1}]$
ν	output time step [s] (introduced in (4.4), page 372)
ρ	density $[\text{kg}\cdot\text{m}^{-3}]$
τ	time step in the numerical scheme from Section 3.1 [s]
τ_{cou}	time step for the coupling of the numerical schemes from Section 3 [s]
ϕ	porosity $[-]$
φ_i	basis function associated with node $\boldsymbol{x}_i$ of $\mathcal{T}$
Ω	spatial domain
$\tilde{\Omega}^{ff}$	extension of Ω^{ff} (defined on page 360)

Latin letters

a	longitudinal dispersion coefficient [m]
c_p	specific heat at constant pressure $[\text{m}^2\cdot\text{s}^{-2}\cdot\text{K}^{-1}]$
$c_{p,\sigma}$	specific heat at constant pressure of component σ $[\text{m}^2\cdot\text{s}^{-2}\cdot\text{K}^{-1}]$
c_s	specific heat capacity of the solid matrix $[\text{m}^2\cdot\text{s}^{-2}\cdot\text{K}^{-1}]$
c_V	specific heat at constant volume $[\text{m}^2\cdot\text{s}^{-2}\cdot\text{K}^{-1}]$
$c_{V,\sigma}$	specific heat at constant volume of component σ $[\text{m}^2\cdot\text{s}^{-2}\cdot\text{K}^{-1}]$
D	diffusion coefficient $[\text{m}^2\cdot\text{s}^{-1}]$
$D_{\sigma,\gamma}$	multicomponent diffusion coefficient $[\text{m}^2\cdot\text{s}^{-1}]$
D_n	diffusion coefficient of the NAPL vapor $[\text{m}^2\cdot\text{s}^{-1}]$