An investigation of the pseudo-steady state approach to modelling inter-porosity flow in fractured geomaterials

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Abstract. This paper examines the assumption of pseudo-steady state inter-porosity mass exchange in dual porosity models of fractured rock. Models of this type rely on the assumption that a pseudo-steady pore pressure distribution prevails in the porous matrix at all times, thereby neglecting transient pressure gradients. The rate of inter-porosity mass exchange is then conveniently expressed as a linear function of the difference between the average pore pressures in the fracture and matrix domains. Whilst providing a relatively simple description of mass exchange, the accuracy of this approach has been debated and it is strictly only valid once the pressure front due to changing conditions in the fracture network reaches the centre of the matrix. The aim of this paper is to compare the pseudo-steady state model of mass exchange with an explicit model of diffusive flow into a rock matrix with parallel-plate geometry. Since the mass exchange coefficient is sometimes described as a function of matrix block geometry and effective diffusivity, an attempt is made to adopt this approach before curve fitting is used. The results indicate that the adopted function underestimates the mass exchange rate compared to the benchmark, although the pseudo-steady state model can provide close agreement if curve fitting is used. It is concluded that the assumption of pseudo-steady state mass exchange may be valid only for cases where calibration of the linear coefficient is possible. Constitutive relationships describing the coefficient should be approached with care, with the possible exception of those considering some level of transiency.

Keywords: Fractured geomaterials, inter-porosity flow, mass exchange, dual porosity.

1 Introduction

Fractures and discontinuities are commonly important features in geological formations and can have a significant bearing on the water and gas flows and reactive chemical transport. They effectively divide a geomaterial into two distinct porosities, namely, the fracture network and the porous rock matrix [1]. A number of modelling techniques are available to allow the heterogeneous pore structure of a dual porosity geomaterial in a form more amenable to numerical treatment. In broad terms, these are discrete fracture network (DFN) models, equivalent continuum models, and dual (or higher) porosity

models [2]. The most appropriate type of model for a given application depends largely on the problem scale/conditions, the available input data, the type of output data required, and the available computational resources [1, 3]. A discussion of the relative merits of each approach can be found in Hosking et al. [4], whilst the work presented here focuses on the dual porosity model and specifically the mass exchange term used to couple the fracture and matrix flows.

Dual porosity models consider the fracture network and porous matrix as distinct continua over the domain. This approach intends to overcome the loss in accuracy of homogenised, equivalent continuum models as the partition between the fracture and matrix flows becomes more apparent. To reflect the material properties of most fractured rocks, it is generally true that the fracture continuum provides the majority of the flow capacity and the matrix continuum provides the majority of the storage capacity. The fracture continuum is then more highly conductive with a lower porosity and the matrix is poorly (or non-) conductive with a higher porosity [5]. Provided representative properties can be assigned to the respective continua, the capability of the model to predict the salient transport behaviour of fractured rock requires an accurate description of the inter-porosity mass exchange.

Mass exchange models relying on the assumption of a pseudo-steady pore pressure distribution in the matrix are common in the study of dual porosity systems, including water and solute transport in structured porous media [6, 7] and gas flow in coal [8, 9]. This assumption neglects transient pressure gradients in the matrix and allows the rate of inter-porosity mass exchange to be conveniently expressed as a linear function of the difference between the average pore pressures in the fracture and matrix domains. Whilst providing a relatively simple description of mass exchange, the accuracy of this approach has been challenged [10, 11] and it is strictly only valid once the pressure front due to changing conditions in the fracture network reaches the centre of the matrix [6].

This paper examine the soundness of assuming pseudo-steady state mass exchange in dual porosity models. The test cases considered deal with the mass exchange of an ideal, inert gas under isothermal conditions in rigid coal with a parallel-plate geometry, with benchmarks provided by an explicit model of diffusive flow into the coal matrix slabs. Since the mass exchange coefficient is sometimes described as a function of matrix block geometry and effective diffusivity, an attempt is made to adopt this approach in preference to curve fitting. The results presented in this work have been obtained using the coupled thermal, hydraulic, chemical and mechanical (THCM) model, COMPASS, developed incrementally at the Geoenvironmental Research Centre [12, 13].

2 Theoretical models for inter-porosity mass exchange

Based on a theoretical formulation that can be described as a mechanistic approach, the coupled THCM model used in this work has a background of high performance simulations of three-dimensional multiphase, multicomponent reactive transport in single porosity geomaterials. Recent developments to this platform, presented by Hosking et

al. [4], have extended the capabilities by introducing a dual porosity framework and non-ideal gas behaviour. These new capabilities are employed here alongside the benchmark simulations, which have been performed using the single porosity model assuming purely diffusive gas flow in the coal matrix. A summary of both formulations is provided in the following sections.

2.1 Single porosity model for diffusive mass exchange (benchmark case)

Based on the principle of conservation of mass, the temporal derivative of the gas chemical accumulation is equal to the spatial gradient of the relevant fluxes. Gas flow from the fracture network into the fully dry, non-deformable coal matrix is assumed to be driven purely by diffusion, which for an ideal, inert gas yields:

$$n\frac{\partial c_g}{\partial t} = \nabla \cdot \left[D_{e,g}\nabla c_g\right] \tag{1}$$

where n is the matrix porosity, c_g is the gas concentration, and $D_{e,g}$ is the gas effective diffusion coefficient, given by [14]:

$$D_{e,g} = n\tau_g D_g \tag{2}$$

where the tortuosity factor, τ_g, is calculated using the relationship by Millington and Quirk [15]:

$$\tau_g = n^{4/3} \tag{3}$$

The gas pressure, u_g, is calculated from c_g, the temperature, T, and the universal gas constant, R, using the ideal gas law, i.e. $u_g = RTc_g$.

2.2 Dual porosity model with pseudo-steady state mass exchange

Mass exchange for the dual porosity case is handled through the addition of a sink/source term to the mass balance expression given in equation (1). Since this work is concerned with mass exchange and not the bulk flow of gas in the coal, the diffusive flux term is removed, yielding:

$$n_\beta \frac{\partial c_{g,\beta}}{\partial t} = \lambda \Gamma_g \tag{4}$$

where the subscript β is the continuum identifier and becomes F to denote the fracture continuum and M to denote the matrix continuum, Γ_g is the sink/source term for mass exchange, and $\lambda = -1$ if $\beta = F$ or $\lambda = 1$ if $\beta = M$.

The fracture continuum porosity, n_F, is the fraction of the total porosity associated with the fracture network, given by:

$$n_\beta = w_f n_F^L \tag{5}$$

where n_F^L is the local fracture porosity, expressed mathematically as the volume of pores in the fractured network divided by the total volume of the fracture network, i.e.

V_F^P/V_F^T. This becomes 1.0 in a clean fracture, but may be less due to mineral infillings and the presence of altered matrix surrounding the fracture. w_f is the volumetric weighting factor, defined as the total volume of the fracture network divided by the bulk rock volume, i.e. $w_f = V_F^T/V_T$, analogous to the following expression for a parallel-plate geometry:

$$w_f = \frac{a_F}{b_F} \tag{6}$$

where a_F is the fracture aperture and b_F is the fracture spacing.

Equation (5) allows the matrix continuum porosity, n_M, to be expressed in terms of the total porosity, n_T, w_f, and n_F^L, giving:

$$n_M = n_T - w_f \mathrm{n_F^L} \tag{7}$$

Assuming a pseudo-steady state gas pressure distribution in the matrix slabs at all times, Γ_g becomes a first-order mass exchange term expressed in general as [16]:

$$\Gamma_g = \sigma_D\left(c_{g,F} - c_{g,M}\right) \tag{8}$$

where σ_D is the first-order exchange rate, which may be expanded to consider geometrical and material properties, including the coal matrix shape and dimensions and the effective diffusivity of the gas, giving an expression of the form [17]:

$$\sigma_D = \frac{4\psi}{{b_M}^2} D_{e,g,M} \tag{9}$$

where ψ is a dimensionless shape factor related to the geometry of the matrix blocks, ranging from 3 for rectangular slabs (as in the parallel-plate model in this work) to 15 for spherical aggregates [6].

3 Problem conditions

Three coal slab geometries are considered in this work, as shown in Figure 1, taken from Laubach et al. [18] for coal from the San Juan and Black Warrior Basins, USA. Specifically, fracture apertures of 5, 7 and 9 μm have been selected for Tests I, II and III, respectively. The adopted values of fracture spacing correspond to a maximum permeability of 1 mD, giving a_F as 0.013 m, 0.035 m and 0.065 m, respectively. A total porosity of 0.01 was prescribed in each test, with $n_F^L = 1.0$.

The geometrical parameters described above were used to define the terms of the dual porosity equations (4) to (9). The domain for the dual porosity simulations was arbitrary since no bulk flow occurs (only mass exchange via the sink/source term). Owing to the symmetry of the parallel-plate model, the 2-dimensional domains for the benchmark diffusive mass exchange simulations were formed using 0.001 m wide sections of coal slab with thicknesses of $0.5(b_F - a_F)$, i.e. the half width of a single slab. The coal matrix initially contains no gas with the fracture containing gas at a pressure of 100 kPa. The simulation period in each Test corresponded to the time taken for the coal matrix pressure to equilibrate with the prescribed fracture pressure.

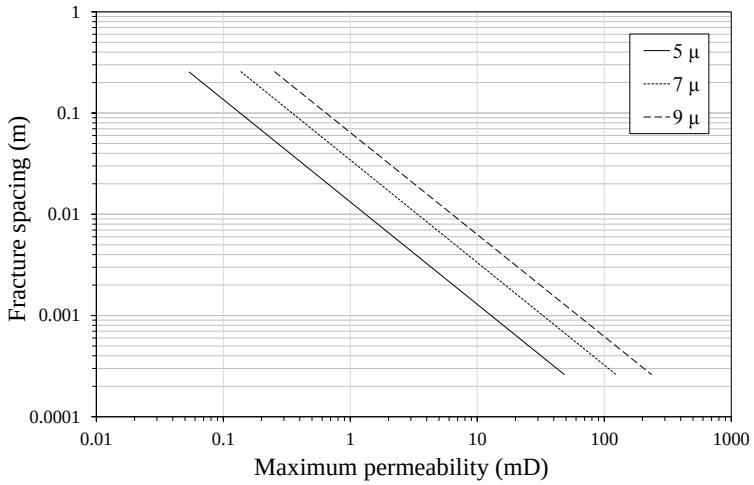

Figure 1 Relationship between coal permeability and fracture spacing for the three fracture apertures considered in this work (adapted from Laubach et al. [18]). The values of fracture spacing used in the test cases correspond to a maximum permeability of 1 mD.

4 Results and discussion

The results for Tests I, II and II are shown in Figure 2, Figure 3 and Figure 4, respectively. Markers are used to denote the results of the benchmark tests in which diffusive mass exchange into the matrix slabs was considered explicitly. These results show the evolution of gas pressure at the mid-point of the domain, i.e. a quarter into the matrix slab thickness. The dual porosity results for case A used equation (9) to define the mass exchange rate, σ_D, whereas for case B the best-fit values were used.

As expected, the benchmark results follow the same trend in each test, reflecting the transient gas pressure gradient in the matrix slab as it tends towards equilibrium with the fracture pressure. The only notable difference is in the time scale, which naturally increases with the thickness of the matrix slabs. It can be seen that in all three tests case A underestimated the rate of mass exchange by a considerable margin relative to the benchmark. The results for case B show that the pseudo-steady state model yielded a close agreement with the benchmark only when the values of σ_D from case A were increased by in the region of 2 orders of magnitude.

These findings imply that the assumption of pseudo-steady state mass exchange may be valid only for cases where calibration of the linear coefficient is possible. In other words, σ_D appears to be a largely empirical value. The use of constitutive relationships describing the coefficient should be approached with care, with the possible exception of those considering some level of transiency, such as those reviewed by Hassanzadeh et al. [10]. Transiency is typically included by taking ψ in equation (9) as a function of time. In effect, the rate of mass exchange is increased substantially at early times and decays towards the pseudo-steady state at late times. Referring to the findings in this work, the use of such a transient function would lead to an improved agreement between

case A and the benchmark. However, whether this approach improves the theoretical robustness of σ_D beyond being a largely empirical factor is debatable, depending on the exact definition used. Suitable functions may consider different boundary conditions at the fracture-matrix interface (pressure- or flux-dependent), different geometries, and the properties of the solid and pore fluid, including multiphase flow.

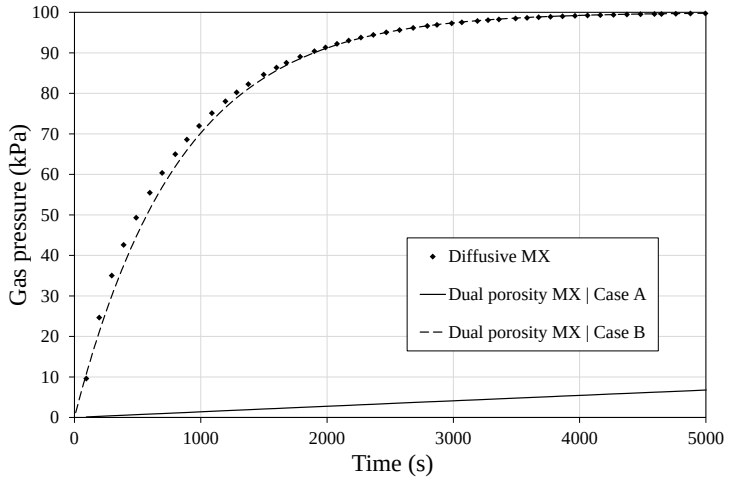

Figure 2 Results for Test I with $a_F = 5\mu$m and $b_F = 0.013$m, giving $w_f = 3.84 \times 10^{-4}$. Case A used equation (9) to give $\sigma_D = 1.4 \times 10^{-5}$ s^{-1}, with case B using the best fit value of $\sigma_D = 1.5 \times 10^{-3}$ s^{-1}.

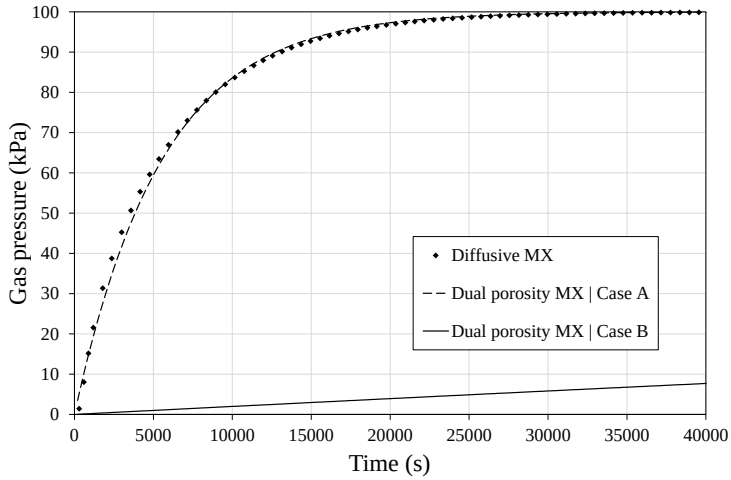

Figure 3 Results for Test II with $a_F = 7\mu$m and $b_F = 0.035$m, giving $w_f = 2.00 \times 10^{-4}$. Case A used equation (9) to give $\sigma_D = 2.0 \times 10^{-6}$ s^{-1}, with case B using the best fit value of $\sigma_D = 1.8 \times 10^{-4}$ s^{-1}.

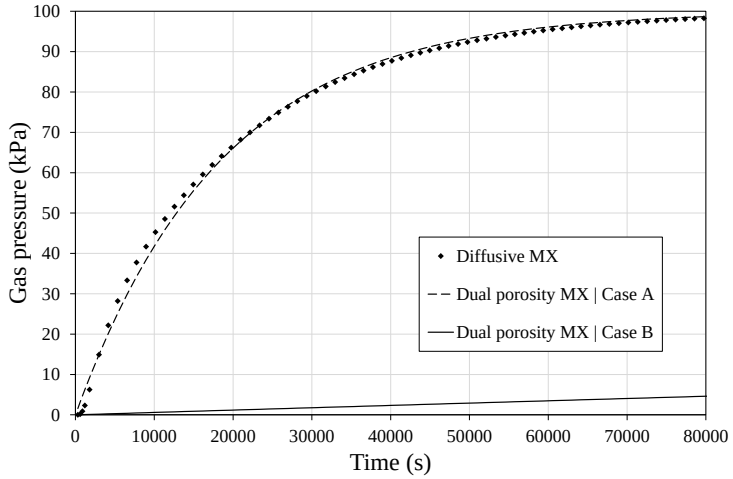

Figure 4 Results for Test III with $a_F = 9\mu$m and $b_F = 0.065$m, giving $w_f = 1.38 \times 10^{-4}$. Case A used equation (9) to give $\sigma_D = 5.9 \times 10^{-7}$ s^{-1}, with case B using the best fit value of $\sigma_D = 5.4 \times 10^{-5}$ s^{-1}.

5 Conclusions

This paper has investigated the soundness of assuming a pseudo-steady rate of inter-porosity (fracture-matrix) mass exchange in dual porosity numerical models. Three test scenarios have been presented for coal covering a range of fracture apertures and matrix slab thicknesses assuming a rigid parallel-plate geometry. Each test considered the inter-porosity (fracture-matrix) flow of an ideal, inert gas under isothermal conditions. The predicted pseudo-steady state mass exchange rates have been compared with benchmarks provided by explicitly modelling diffusive flow into the coal matrix slabs, thereby taking into account the transient pressure gradient neglected in the pseudo-steady state approach. Since the mass exchange coefficient is sometimes described as a function of matrix block geometry and effective diffusivity, an attempt was made to adopt this approach (case A) before curve fitting was used (case B).

It was found that in all three tests case A underestimated the rate of mass exchange by a considerable margin relative to the benchmark. The results for case B showed that the pseudo-steady state model yielded a close agreement with the benchmark only when the values of the mass exchange rate from case A were increased by in the region of 2 orders of magnitude.

It is concluded that the assumption of pseudo-steady state mass exchange may be valid only for cases where calibration of the linear coefficient is possible. Constitutive relationships describing the coefficient should be approached with care, with the possible exception of those considering some level of transiency.

References

1. Bear, J., ed. *Modeling flow and contaminant transport in fractured rocks*. Flow and contaminant transport in fractured rock, ed. B.e. al. 1993, Academic Press, Inc. 1-38.
2. Therrien, R. and E.A. Sudicky, *Three-dimensional analysis of variably-saturated flow and solute transport in discretely-fractured porous media.* Journal of Contaminant Hydrology, 1996. **23**(1-2): p. 1-44.
3. Samardzioska, T. and V. Popov, *Numerical comparison of the equivalent continuum, non-homogeneous and dual porosity models for flow and transport in fractured porous media.* Advances in Water Resources, 2005. **28**(3): p. 235-255.
4. Hosking, L.J., H.R. Thomas, and M. Sedighi, *A dual porosity model of high pressure gas flow for geoenergy applications.* Submitted to Canadian Geotechnical Journal, 2017.
5. Xu, T.F. and K. Pruess, *Modeling multiphase non-isothermal fluid flow and reactive geochemical transport in variably saturated fractured rocks: 1. Methodology.* American Journal of Science, 2001. **301**(1): p. 16-33.
6. Gerke, H.H. and M.T. van Genuchten, *A Dual-Porosity Model for Simulating the Preferential Movement of Water and Solutes in Structured Porous-Media.* Water Resources Research, 1993. **29**(2): p. 305-319.
7. Ma, D.H. and M.G. Shao, *Simulating infiltration into stony soils with a dual-porosity model.* European Journal of Soil Science, 2008. **59**(5): p. 950-959.
8. Wu, Y., et al., *Dual poroelastic response of a coal seam to CO2 injection.* International Journal of Greenhouse Gas Control, 2010. **4**(4): p. 668-678.
9. Chen, D., et al., *Modeling and Simulation of Moisture Effect on Gas Storage and Transport in Coal Seams.* Energy & Fuels, 2012. **26**(3): p. 1695-1706.
10. Hassanzadeh, H. and M. Pooladi-Darvish, *Effects of fracture boundary conditions on matrix-fracture transfer shape factor.* Transport in Porous Media, 2006. **64**(1): p. 51-71.
11. Lemonnier, P. and B. Bourbiaux, *Simulation of Naturally Fractured Reservoirs. State of the Art-Part 2–Matrix-Fracture Transfers and Typical Features of Numerical Studies.* Oil & Gas Science and Technology–Revue de l'Institut Français du Pétrole, 2010. **65**(2): p. 263-286.
12. Thomas, H.R. and Y. He, *Modelling the behaviour of unsaturated soil using an elasto-plastic constitutive relationship.* Géotechnique, 1998. **48**(5): p. 589-603.
13. Sedighi, M., H.R. Thomas, and P.J. Vardon, *Reactive Transport of Chemicals in Unsaturated Soils: Numerical Model Development and Verification.* Canadian Geotechnical Journal, 2016. **53**(1): p. 162-172.
14. Cussler, E.L., *Diffusion: mass transfer in fluid systems*. 2nd Edition ed. 1997, Cambridge: Cambridge University Press.
15. Millington, R. and J.P. Quirk, *Permeability of Porous Solids.* Transactions of the Faraday Society, 1961. **57**(8): p. 1200-&.
16. Gwo, J., et al., *A multiple-pore-region concept to modeling mass transfer in subsurface media.* Journal of Hydrology, 1995. **164**(1-4): p. 217-237.
17. Schwartz, R.C., A.S.R. Juo, and K.J. McInnes, *Estimating parameters for a dual-porosity model to describe non-equilibrium, reactive transport in a fine-textured soil.* Journal of Hydrology, 2000. **229**(3-4): p. 149-167.
18. Laubach, S.E., et al., *Characteristics and origins of coal cleat: A review.* International Journal of Coal Geology, 1998. **35**(1-4): p. 175-207.