

MATHEMATICAL MODELLING OF GAS PRODUCTION IN A COAL SEAM GAS (CSG) FIELD

Steven PSALTIS^{1,2*}, Troy FARRELL^{1,2}, Kevin BURRAGE^{1,2,3,4}, Pamela BURRAGE^{1,2}, Peter MCCABE⁵, Timothy MORONEY^{1,2}, Ian TURNER^{1,2}, Saikat MAZUMDER⁶ and Tomasz BEDNARZ^{1,2,3}

¹ School of Mathematical Sciences, Queensland University of Technology, Brisbane QLD 4000, AUSTRALIA

² ARC Centre of Excellence for Mathematical and Statistical Frontiers, Queensland University of Technology, Brisbane QLD 4000, AUSTRALIA

³ Institute for Future Environments, Queensland University of Technology, Brisbane QLD 4000, AUSTRALIA

⁴ Department of Computer Science, University of Oxford, Oxford OX13QD, U.K

⁵ Australian School of Petroleum, The University of Adelaide, Adelaide SA 5005, AUSTRALIA

⁶ Arrow Energy Pty Ltd, Brisbane QLD 4000, AUSTRALIA

*Corresponding author, E-mail address: steven.psaltis@qut.edu.au

ABSTRACT

Knowledge about the future composition of gas extracted from a coal seam gas (CSG) production well is of vital importance to the CSG industry. In this work we discuss the development of a local model describing the multiphase flow of gaseous species and liquid water within a porous coal seam. Utilising the High Performance Computing (HPC) facilities available at QUT, this local model is validated against production data obtained from Arrow Energy (private communication, 2013) from the Surat Basin in southeast Queensland. By executing the local model over a number of individual production wells, we are able to simulate the gas composition observed at a production facility, and in the near future use visualisation techniques to gain further insight into the outcomes.

NOMENCLATURE

a	matrix width (m)
b	cleat aperture width (m)
b_i^m	Langmuir parameter (1/Pa)
D_i^m	diffusivity of species i in the matrix (m^2/s)
D_i^s	diffusivity of species i in air (m^2/s)
D_i^{eff}	effective diffusivity of species i (m^2/s)
g	gravitational constant (m/s^2)
i	species = CO ₂ , CH ₄ , N ₂
k	intrinsic permeability (m^2)
k_{rg}	gas relative permeability
k_{rw}	water relative permeability
M_i	molecular weight of species i
m	van Genuchten parameter
p_w	water pressure (Pa)
p_g	total gas pressure (Pa)
p_c	capillary pressure (Pa)
p_b	well bottom-hole pressure (Pa)
q_i	volumetric density of adsorbed gas (mol/m^3)
q_i^m	Langmuir parameter (mol/m^3)
R_w	well bore radius (m)
s_g	gas saturation
s_w	water saturation
α	van Genuchten parameter
μ_g	gas viscosity (m^2/s)

μ_w	water viscosity (m^2/s)
ϕ_m	matrix porosity
ϕ	porosity
ρ_i^m	density of species i in the coal matrix (kg/m^3)
ρ_i	density of species i in the cleat network (kg/m^3)
ρ_w	density of liquid water (kg/m^3)
ρ_g	total gas density in the cleat network (kg/m^3)
τ	tortuosity
ω_i	mass fraction of species i

INTRODUCTION

Modern computational fluid dynamics (CFD) software packages are able to simulate a wide range of complicated scenarios and domains, including multiphase flow through porous materials. However, when the structure of the underlying porous material is not well known, or can vary widely across a spatial domain, determining realistic solutions is challenging.

In this work we investigate the mathematical modelling and numerical simulation of the multiphase flow that occurs within a coal seam when subjected to a decreasing pressure at one boundary due to the operation of a pump. This occurs in the production of coal seam gas (CSG), or coal-bed methane, where a well is drilled into a coal seam to allow removal of the trapped water and subsequently the methane. An added complication here is that we wish to be able to simulate gas production across a range of CSG production wells in varying spatial locations. Due to the highly heterogeneous nature of the underlying domain, very little is known about the physical parameters required for the model.

To this end, we have developed our own numerical simulation code and embedded it within a population of models (POMs) framework (Marder and Taylor, 2011), to allow us to explore the variability in results across a range of parameters.

Coal seams are typically characterised as a dual-porosity media (Warren and Root, 1963), as shown in Figure 1. They are comprised of a porous coal matrix separated by a

cleat network through which transport occurs. The cleats are typically highly saturated with water, with only a limited amount of gas. As shown in Figure 1, the vast majority of the gas is adsorbed to the surface of the porous coal matrix.

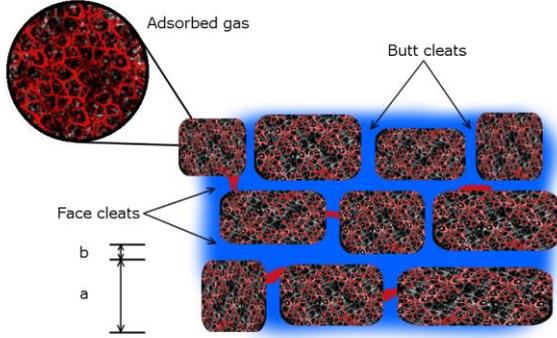


Figure 1: Schematic of coal seam

When a well begins operation, water is pumped from the coal seam, thereby reducing the pressure in the cleat network between the coal matrices. This causes the adsorbed gas in the coal matrix to desorb and diffuse into the cleats. The gas can then be transported through the cleat network to the well boundary where it is removed from the seam.

MODEL DESCRIPTION

We assume a one-dimensional radially symmetric domain with the well-bore located at the centre, as seen in Figure 2. We will consider a model where a single coal seam of thickness 1 m is intersected by a well. In reality, a well will often intersect with a number of seams and produce gas from each of these, and this introduces a source of error between our model and observational data. A model that accounts for production from multiple seams would introduce significant computational overhead that we do not wish to account for in this work.

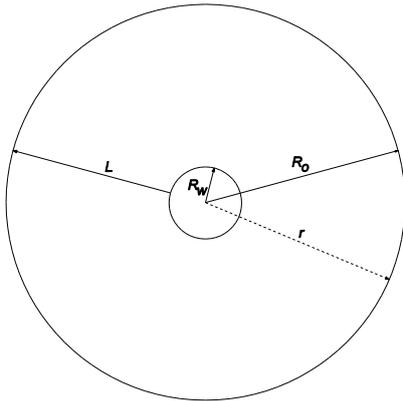


Figure 2: Schematic diagram of computational domain.

The mathematical model describes multiphase flow of water, methane, carbon dioxide and nitrogen through the cleat networks and the diffusion and adsorption of the gaseous species in the coal matrix. (Psaltis et al., 2015) (Cui, 2006)

Coal Matrix

Within the coal matrix, we assume that only gaseous species are present and that water is unable to penetrate the microscopic pores due to their small size scale (Harpalani and Chen, 1997) and the capillary pressure that would exist. The conservation of gas species in the matrix is given by (Psaltis et al., 2015)

$$\frac{\partial}{\partial t}(\varphi_m \rho_i^m) + (1 - \varphi_m) M_i \frac{\partial q_i}{\partial t} = -\nabla \cdot \mathbf{N}_i, \quad (0.1)$$

where an approximation for the diffusion of gas species from the coal matrix to the cleat network is used (Yang, 1987), namely,

$$\nabla \cdot \mathbf{N}_i = \frac{8\pi\varphi_m D_i^m}{a^2} (\rho_i^m - \rho_g). \quad (0.2)$$

The total gas density in the cleats, ρ_g , is given by the sum of the individual species densities,

$$\rho_g = \sum_i \rho_i, \quad (i = \text{CO}_2, \text{CH}_4, \text{N}_2). \quad (0.3)$$

Gas is adsorbed to the surface of the coal structure, and the adsorption/desorption behaviour is described by the Langmuir competitive adsorption isotherm (Ottiger, Pini, Storti, and Mazzotti, 2008), namely,

$$q_i = \frac{q_i^m b_i^m p_i^m}{1 + \sum_j b_j^m p_j^m}. \quad (0.4)$$

Coal Cleat Network

Within the cleat network transport of water is assumed to be governed by Darcy's law (Cui, 2006), while the transport of the different gas species is governed by both diffusion and Darcy's law (Cui, 2006; Harpalani and Chen, 1997). This leads to equations for the conservation of gas species,

$$\frac{\partial}{\partial t}(s_g \varphi \rho_i) + \nabla \cdot \mathbf{F}_i = (1 - \varphi) \nabla \cdot \mathbf{N}_i \quad (0.5)$$

where the flux of each species is given by

$$\mathbf{F}_i = -s_g \varphi \rho_g D_i^{\text{eff}} \nabla \omega_i - \rho_i \frac{k_{rg} k}{\mu_g} \nabla p_g, \quad (0.6)$$

and for water,

$$\frac{\partial}{\partial t}(s_w \varphi \rho_w) + \nabla \cdot \mathbf{F}_w = 0, \quad (0.7)$$

where the water flux is defined by

$$\mathbf{F}_w = -\rho_w \frac{k_{rw} k}{\mu_w} \nabla p_w. \quad (0.8)$$

The gas saturation is related to water saturation via

$$s_g = 1 - s_w. \quad (0.9)$$

Auxiliary Equations

We also require a number of additional auxiliary equations to describe the variables in the system. We introduce the capillary pressure, p_c , and relate it to the gas and water pressure by $p_w = p_g - p_c$, where p_g is the total gas pressure,

$$p_g = \sum_i p_i, \quad (i = \text{CO}_2, \text{CH}_4, \text{N}_2), \quad (0.10)$$

p_c is given by,

$$p_c = \rho_w \frac{g}{\alpha} (s_w^{-1/m} - 1)^{1-m}, \quad (0.11)$$

and the individual species' pressures are given by the ideal gas law,

$$p_i = \frac{\rho_i R_i T}{M_i}. \quad (0.12)$$

Relative permeabilities are calculated based on saturation using the van Genuchten relations (van Genuchten, 1980), namely,

$$k_{rg} = (1 - s_w)^{1/2} (1 - s_w^{1/m})^{2m}, \quad (0.13)$$

and

$$k_{rw} = s_w^{1/2} \left(1 - \left[1 - s_w^{1/m}\right]^m\right)^2. \quad (0.14)$$

We calculate the effective diffusivity of each gas species within the cleat network via (Bear, 1972)

$$D_i^{eff} = \tau D_i^s (\phi s_g)^{3/2}, \quad (0.15)$$

where τ is the tortuosity. The intrinsic permeability is related to the cleat aperture width, b , the matrix width, a , and the tortuosity via

$$k = \frac{b^3 \tau}{4a}, \quad (0.16)$$

while the porosity depends on the cleat aperture width and the matrix width, that is,

$$\phi = \frac{3b}{a}. \quad (0.17)$$

Boundary and Initial Conditions

To simulate the action of a well extracting gas and water we define flux boundary conditions for water and gas species at the centre of the domain, namely

$$\mathbf{F}_w = -\rho_w \frac{k_{rw} k}{\mu} \nabla p_w, \quad (0.18)$$

and

$$\mathbf{F}_{gi} = -\rho_i \frac{k_{rg} k}{\mu} \nabla p_g. \quad (0.19)$$

The resolution of the gradients ∇p_w and ∇p_g in Equations (0.18) and (0.19) will be discussed in the next section.

At the far end of the domain, $r = R_o$, we assume the boundary to be impermeable and we therefore set no flow conditions. To close the system we specify that the system is at equilibrium initially, where the densities in the coal matrix and cleat network are assumed equal and are set via the initial pressure. The initial pressure is set via an empirical relationship between pressure and the depth of the seam.

NUMERICAL TECHNIQUES

To solve the above equations we have utilised the finite volume method (Patankar, 1980; Versteeg and Malalasekera, 2007) to discretise Equations (0.5) to (0.8) in one dimension. We have assumed here a radially symmetric domain with the well-bore located in the centre of the coal seam, as shown in Figure 2.

The gradients ∇p_w and ∇p_g in Equations (0.18) and (0.19) are evaluated using a one-sided finite difference operation (Burden and Faires, 2001). The value of each pressure at the well boundary is set equal to the boundary pressure, p_b .

To calculate p_b we utilise the provided water data to fit an equation of the form

$$f_w(t) = \sum_{i=1}^n a_i \exp\left(-\left(\frac{t-b_i}{c_i}\right)^2\right), \quad (0.20)$$

where $f_w(t)$ is the volumetric water production and n can range from 1 to 10. This model allows us to obtain a good representation of the water production data. Figure 3 shows the resulting fitted water curve for Well 25. We can see that we recover the initial peak water production, and the general trend of the water data. Note that here the experimental water data has been smoothed using standard techniques (Cleveland, 1979).

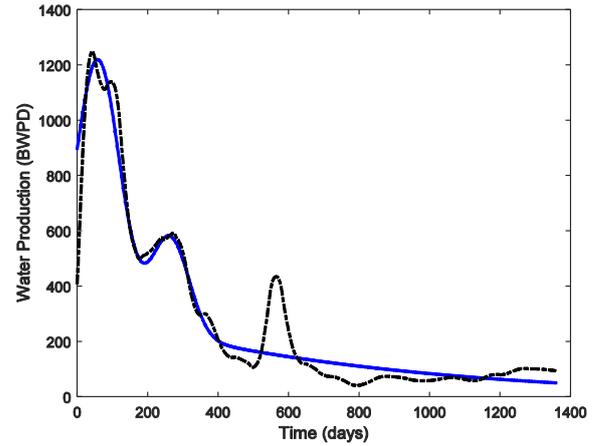


Figure 3: Water production for Well 25; (---) Water production data; (—) Fitted water production.

To implement the numerical solution of the model described above we have developed our own code in Matlab. This was done due to the fact that our industry partners required the ability to run the simulations, and that the numerical solution needed to be embedded within a population of models (POMs) (Marder and Taylor, 2011; McKay, Beckman, and Conover, 1979) framework to allow us to investigate plausible values of unknown parameters. Without these constraints, this model could be implemented in the sophisticated CFD software packages available today.

The use of POMs with Latin Hypercube Sampling (LHS) allows us to search a multidimensional parameter space in a constrained way. To do this we specify the parameters that we wish to search over, and a suitable range for each parameter. These ranges are then subdivided a specified number of times, and samples are taken from each division such that the combination of divisions being sampled is a Latin hypercube. By way of example, in two-dimensional parameter space (only two parameters are searched over) a Latin square requires there to be only one sample in each row and column of divisions, as shown in Figure 4. Sampling in this way guarantees good coverage of parameter space.

To execute the simulations across the wells in a production field the Matlab code has been compiled on the SGI Altix XE Cluster with 128 compute nodes available at QUT. This allows us to run simulations across each of the wells simultaneously.

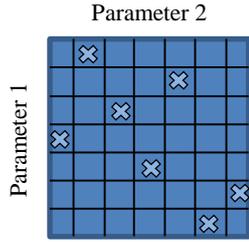


Figure 4: Representation of LHS in 2D parameter space.

RESULTS

We now consider the gas production results for a specific well in the production field. We have generated a family of simulation results utilising POMs for Well 25. We compare the total gas production in both instantaneous and time cumulative form, where the gas production data has been smoothed using standard techniques. To select a simulation result as being a successful match we require the relative error between the data and simulation (in cumulative form) at five equally spaced points to be less than 50%. This is a large tolerance, however here we are interested in examining the variability in the gas production over a range of parameter values.

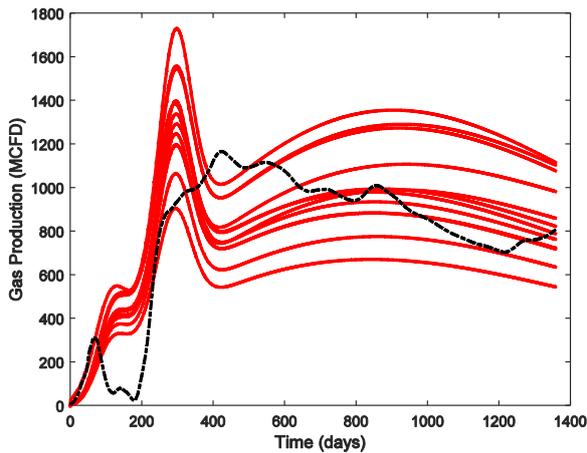


Figure 5: Gas production for Well 25; (---) Gas production data; (—) Simulated gas production.

When comparing the instantaneous data to the simulations as shown in Figure 5, we see that there is a large discrepancy in the period from approximately 100 to 200 days, and we note that the peak in the simulations at approximately 300 days is also significantly larger than the data. We also note that the multiple peaks observed in the data may be due to gas being produced from multiple coal seams located at different depths. However, our simulations appear to recover the rate of gas production and the behaviour at later times, and this gives us confidence that our model may be able to recover the gas production data when the tolerance is tightened and more determination of suitable parameter ranges is performed.

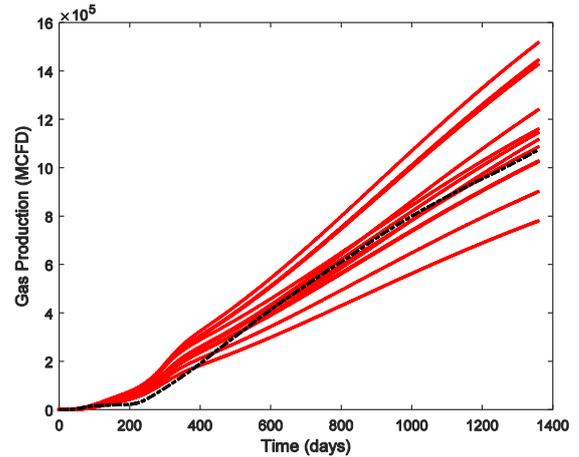


Figure 6: Cumulative gas production for Well 25; (---) Gas production data; (—) Simulated gas production.

Figure 6 shows a comparison between the cumulative gas production data and the simulations. We see here that our model is able to recover the observed cumulative gas production, and the family of simulation results all exhibit the same general trend.

VISUALISATION

Currently, we are in the process of preparing visualisation tools to drive the process of visual inspection and comparison of compute results versus field measurements. This is in the preliminary stage, but we are undertaking two approaches: (a) web based visualisation utilizing visual analytics methodologies (Thomas and Cook, 2005); (b) expanding to 3D immersive visualisation (Billen et al., 2008) of a coal seam. The first approach is to visualise geospatial data on a structure similar to a map, where users can click on a specific well and see basic underlying information about that well. On the right hand side of the dashboard, the user will be able to see information visualisations of simulation results versus field measurements, and also see the physical parameters used to drive the simulation. Additionally, we will also have a slider that allows us to progress through the transient development of gas production for that location. This will allow users to visually inspect and verify progress and the quality of the simulation. The second approach will use more sophisticated visualisation techniques, to present similar data but in 3D space. The idea is that the user is placed in the immersive environment to enable them to get closer to a specific well in virtual reality, and observe the effect of different model parameters.

DISCUSSION AND CONCLUSION

In this work we have presented a mathematical model describing the multiphase flow of gaseous species and liquid water through the porous structure of a coal seam. We have shown that our model is able to obtain good agreement with observed data from a well currently under operation. The use of a population of models framework allows us to observe the variability in the model as key parameters are varied.

To begin extending this work we will consider the development of a multiple seam model, as in reality a single CSG well intersects with and produces gas from many coal seams. This multi-seam model will utilise the

one-dimensional model presented here, however some simplifications may be required to make the solution computationally feasible.

We will also consider moving to a higher dimensional domain, with the aim being a three dimensional model. This will allow us to utilise sophisticated visualisation techniques to examine the behaviour of the flow through the coal seam. To do this, however, we must explore the use of GPGPU compute abilities to accelerate the solution process. OpenCL can be utilised to redevelop sections of code to execute not only on the GPU but across many other platforms as well. This will potentially provide a significant speedup of the code.

Accelerating the code will also allow us to run POMs over a large number of wells in finite time. This is important to be able to gain accurate insights into the future behaviour of a production facility that is fed by a large number of wells.

ACKNOWLEDGEMENTS

The authors wish to acknowledge Arrow Energy for funding and access to staff and data, and the ARC Centre of Excellence for Mathematical and Statistical Frontiers. Computational resources and services used in this work were provided by the HPC and Research Support Group, Queensland University of Technology, Brisbane, Australia.

REFERENCES

- BEAR, J. (1972). *Dynamics of fluids in porous media*. New York: American Elsevier.
- BILLEN, M. I., KREYLOSA, O., HAMANNA, B., JADAMECA, M. A., KELLOGG, L. H., STAADTA, O., and SUMNERA, D. Y. (2008). A geoscience perspective on immersive 3D gridded data visualization. *Computers and Geosciences*, 34(9), 1056-1072.
- BURDEN, R. L., and FAIRES, J. D. (2001). *Numerical Analysis* (7 ed.). Pacific Grove, CA: BROOKS/COLE.
- Cleveland, W. S. (1979). Robust Locally Weighted Regression and Smoothing Scatterplots. *Journal of the American Statistical Association*, 74, 829--836.
- CUI, X. B., R MARC. (2006). Controls of Coal Fabric on Coalbed Gas Production and Compositional Shift in Both Field Production and Canister Desorption Tests. *Society of Petroleum Engineers Journal*, 11.
- HARPALANI, S., and CHEN, G. (1997). Influence of gas production induced volumetric strain on permeability of coal. *Geotechnical and Geological Engineering*, 15, 303-325.
- MARDER, E., and TAYLOR, A. L. (2011). Multiple models to capture the variability in biological neurons and networks. *Nature Neuroscience*, 14, 133-138.
- MCKAY, M. D., BECKMAN, R. J., and CONOVER, W. J. (1979). A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. *Technometrics*, 21, 239-245.
- OTTIGER, S., PINI, R., STORTI, G., and MAZZOTTI, M. (2008). Measuring and Modeling the Competitive Adsorption of CO₂, CH₄, and N₂ on a Dry Coal. *Langmuir*, 24, 9531-9540.
- PATANKAR, S. (1980). *Numerical Heat Transfer and Fluid Flow*: Taylor and Francis.

PSALTIS, S., FARRELL, T., BURRAGE, K., BURRAGE, P., MCCABE, P., MORONEY, T., . . . MAZUMDER, S. (2015). Mathematical modelling of gas production and compositional shift of a CSG (coal seam gas) field: Local model development. *Energy*. doi:10.1016/j.energy.2015.05.107

THOMAS, J. J., and COOK, K. A. (Eds.). (2005). *Illuminating the Path: The Research and Development Agenda for Visual Analytics*. Los Alamitos, CA: IEEE Computer Society Press.

VAN GENUCHTEN, M. T. (1980). A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Sci Am J*, 44, 892-898.

VERSTEEG, H. K., and MALALASEKERA, W. (2007). *An Introduction to Computational Fluid Dynamics: The Finite Volume Method* (2 ed.). New York: Pearson Education.

WARREN, J. E., and ROOT, P. J. (1963). The behavior of Naturally Fractured Reservoirs. *Society of Petroleum Engineers*, 245-255.

YANG, R. T. (1987). Rate Processes in Adsorbors *Gas Separation by Adsorption Processes* (pp. 101-133). London: Imperial College Press.