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Incorporating the effect of gas in modelling the impact of CBM extraction on regional groundwater systems

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SUMMARY

Production of Coalbed Methane (CBM) requires extraction of large quantities of groundwater. To date, standard groundwater flow simulators have mostly been used to assess the impact of this extraction on regional groundwater systems. Recent research has demonstrated that predictions of regional impact assessment made by such models may be seriously compromised unless account is taken of the presence of a gas phase near extraction wells. At the same time, CBM impact assessment must accommodate the traditional requirements of regional groundwater modelling. These include representation of surficial groundwater processes and up-scaled rock properties as well as the need for calibration and predictive uncertainty quantification. The study documented herein (1) quantifies errors in regional drawdown predictions incurred through neglect of the presence of a gas phase near CBM extraction centres, and (2) evaluates the extent to which these errors can be mitigated by simulating near-well desaturation using a modified Richards equation formulation within a standard groundwater flow simulator. Two synthetic examples are provided to quantify the impact of the gas phase and verify the proposed modelling approach (implemented in MODFLOW-USG) against rigorous multiphase flow simulations (undertaken using ECLIPSE*). ECLIPSE simulations demonstrate convergence towards a time-asymptotic relationship between water saturation and pressure. This relationship can be approximated using a slightly modified van Genuchten function. Where this function is employed in combination with the modified Richards equation strategy to accommodate near-well desaturation, errors in predicted drawdown are reduced significantly, including in cases where complexities such as sloping coal layers are introduced to the model domain (the latter promoting buoyancy-driven movement of gas). Sensitivity analyses further indicate that only the general properties of the employed desaturation function need to be respected to significantly reduce errors in regional drawdown predictions that would arise if the presence of the near-well gas phase was ignored. These properties can be inferred from reservoir properties and from the outcomes of reservoir model simulations that are available at local CBM operation sites.

1. Introduction

1.1. General

As in many other countries, Coalbed Methane (CBM) production is growing rapidly in Australia. Much of this is focussed on the Surat Basin (Hamawand et al., 2013; Moore, 2012; Queensland-Government, 2013), where CBM development areas are of a significant scale. Up to 40,000 wells will be drilled over the next half century. Water production from each of these is expected to average about 20,000 litres per day (CSIRO, 2013).

Gas companies and governments are required to assess regional impacts of CBM production on overlying/underlying aquifer systems that serve as sources of water for industrial/agricultural/domestic use and that sustain important groundwater-dependent eco-systems. Groundwater modelling is therefore undertaken to develop management and monitoring strategies that mitigate the potential impacts of these developments on regional groundwater systems (CEDA, 2012; Fisher, 2010; Mudd, 2012; QWC, 2012a;

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Commonwealth of Australia, 2014). In most cases of which the authors are aware, standard groundwater flow simulators such as MODFLOW (Harbaugh, 2005) have been employed for the making of these assessments (Meredith et al., 2008; Myers, 2009; Wheaton and Metesh, 2002; QWC, 2012a; Golder Associates, 2009, 2011; and Arrow-Energy, 2012). At the same time, the U.S. National Research Council (Fisher, 2010) states that traditional groundwater modelling has not been able to incorporate the full range of natural complexities in CBM basins and recommends that "uncertainties in groundwater modelling results should be explicitly recognized when the results are used to make produced water management and regulatory decisions". Implied in this recommendation is that errors incurred through failure to simulate important aspects of the coal bed methane extraction process be included in the uncertainties that are computed for predictions made by such models. Two potential sources of error associated with current CBM impact assessment modelling include: (1) the up-scaling of complex coal reservoir units that is required for their representation in regional models, and (2) incorporating the presence of a gas phase in the vicinity of CBM extraction sites. A recent study by Moore et al. (2014) demonstrates the importance of both of these issues in regional CBM impact assessment modelling. It suggests that further research on each of them is urgently required, first separately so that each can be properly understood, and then together as both must operate simultaneously in any regional CBM impact assessment context.

Spatial scales over which regional CBM impact assessments must be made can be very large, this reflecting both the large areal extent of CBM gas fields, and the distances over which drawdowns induced by CBM extraction may propagate. For example the area over which the impact of Surat Basin gas extraction must be assessed is of the order of 550 km $\times$ 660 km (QWC, 2012a), an area equivalent to the size of Germany. Furthermore, some of the aquifers for which impact must be assessed are up to 1.5 km deep. Models whose domains span this area are described by QWC (2012a) and Howell et al. (2013). Groundwater systems within such vast areas are affected not just by gas extraction, but also by historical processes (spanning millions of years) which have determined their present state, these including complex interactions with streams and shallow groundwater systems at recharge and discharge areas, interactions with waters of continental scale aquifers such as those of the Great Artesian Basin, and extraction which has taken place over the last hundred years to support the development of agriculture and other industries prior to the advent of gas extraction. Despite their large domain, models of this type are required to run at reasonable execution speeds so that their parameters can be informed through calibration, and so that their predictions can be subjected to calibration-constrained uncertainty analysis (QWC, 2012b).

The presence of a subsurface gas phase near sites of methane extraction can have a significant impact on these model predictions. Moore et al. (2013, 2014) and Howell et al. (2013) demonstrate that failure to simulate the presence of subsurface gas near CBM extraction wells can lead to severe over-prediction of CBM induced drawdown at distances from those wells that far exceed those over which gas is present as a separate phase. While multiphase reservoir models are regularly employed by CBM operators to study depressurization and gas generation at a local scale, the use of such models in regional scale impact assessment is rare, the only instance of which the authors are aware being that of QGC (2014). While a reservoir model can indeed accommodate the effects of near-well gas desorption as part of a regional scale impact assessment, it may not always be the preferred option for a range of practical reasons. Current reservoir simulation software is not specifically designed for regional groundwater impact assessment. Its limitations in this capacity include a lack of steady-state capabilities and reduced number of modules through which inflows and outflows to and from a groundwater system can be represented compared with those offered by standard groundwater simulators (QGC, 2014). Furthermore, the use of reservoir simulators, which are often expensive and closed-source, requires high levels of expertise and complex material property data sets that might not be available to those undertaking the impact assessment modelling. Furthermore the multiphase flow equations embodied in such simulators may not provide adequate descriptions of these processes when these are applied to the necessarily up-scaled representation of coal measures that a regional model requires.

In summary, as recognized by Commonwealth of Australia (2014), a unique challenge to CBM groundwater impact assessment modelling is the need to account for the presence of gas near CBM extraction centres while maintaining computational speed and simulation integrity as it pertains to other processes, some of which are operative on a regional scale, that must be represented in the making of such assessments.

The purpose of this paper is to:

(1) report the outcomes of a series of numerical experiments in which errors incurred by neglecting the presence of gas on simulated drawdowns are examined in a controlled modelling environment;
(2) discuss strategies for inclusion of the effects of near-well gas in models built for the purpose of regional CBM impact assessment; and
(3) propose an efficient, practical methodology for incorporating the impact of a near-well gas phase on regional drawdown assessments made using a traditional, single-phase groundwater model, and verify this approach against rigorous multiphase modelling.

A short description of flow dynamics associated with CBM production is first provided. This is followed by a brief overview of previous groundwater modelling studies that have been undertaken in support of regional CBM impact assessment. Finally, a modified groundwater flow modelling approach is presented with verification problems to address the issue of gas phase presence on assessment of regional groundwater impacts of CBM production.

1.2. CBM production – basics

CBM production can be divided into three stages, namely (1) the dewatering stage, (2) the production stage, and (3) the decline stage. During the dewatering stage coalbeds are depressurised by extraction of water. When sufficiently depressurised, gas starts to desorb from the coal matrix. As dewatering continues, gas concentrations in coalbed fractures/cleats start to increase. This leads to increased gas mobility, which allows gas to migrate down pressure gradients to CBM extraction wells. During the dewatering phase, gas production rates generally increase over time while water production rates generally decrease, this ushering in the production phase. Eventually gas production rates start to decline due to depletion of gas in depressurised coal seams that are connected to the well. Type curves provided in publications such as Seidle (2011) and Moore (2012) depict gas and water production rates for these three stages, and illustrate their variability between different gas fields.

Knowledge of coal permeability is essential for estimation of gas and water extraction rates, as well as for assessment of the impact of CBM production on regional groundwater systems. Coal permeability is determined by the properties of its fracture system (i.e. by the system of coal cleats). The hydraulic properties of the coal cleats systems have been well-documented in publications such as Laubach et al. (1998), Palmer (2009) and Pan and Connell

(2012). The overall permeability of coal beds is generally low compared to that of aquifers, ranging from less than 1 milliDarcy (mD) to 1000 mD (Seidle, 2011). (Note that 1 mD is equivalent to a hydraulic conductivity of about 1.25×10^{-3} m/day for freshwater at 40 °C.) During CBM production the relative permeabilities of gas and water alter in accordance with their respective saturations. The relationship between relative permeability and saturation is often described using a power function; see Brooks and Corey (1964). Though neglected in the present study, total coal permeability can change as gas production progresses as an outcome of changes to effective stress, and through coal shrinkage and swelling. See, for example, Klinkenberg (1941) and Pan and Connell (2012) for further details. Typically, coalbeds exhibit greatest permeability parallel to bedding, this giving rise to significant vertical anisotropy (Laubach et al., 1998). Vertical connectivity of cleat networks is generally limited by the termination of small cleats at interfaces between coal types, and large cleats at coal-non-coal bed interfaces (Laubach et al., 1998).

Coal seams are generally neither evenly distributed nor laterally continuous throughout a coal measure sequence. In the Surat Basin, Australia, thicknesses of individual coal seams vary between less than 10 cm to over 10 m (bhpbilliton, 2012). Most individual seams are less than 3 km in lateral extent (Ryan et al., 2012). Coal seams are generally separated by relatively impermeable siltstones and claystones – these often being referred to as interburden. Because of the limited connectivity of coal seams, many wells must be drilled to depressurise large enough areas to support production of economic quantities of gas. Sometimes hydraulic fracturing is used to enhance connectivity between CBM production wells and coal seams, and between seams themselves.

1.3. CBM-related regional groundwater modelling

To date, assessments of the effect of CBM extraction on regional groundwater systems has received little attention in the scientific literature. Meredith et al. (2008), Myers (2009), and Wheaton and Metesh (2002) discuss modelling carried out in the Powder River Basin (USA) for the purpose of impact assessment; the groundwater flow simulator, MODFLOW, was employed in all cases. While modelling carried out to date in the Surat Basin (Australia) has not been reported in scientific journals, it has been discussed extensively in company reports, and in technical conferences. See QWC (2012a), Golder Associates (2009, 2011), ArrowEnergy (2012) and QGC (2014). All but the last of these employed MODFLOW as their simulation platform; QGC (2014) employed the ECLIPSE (Schlumberger, 2012) reservoir simulator.

1.4. Regional modelling and gas phase impacts

In a comprehensive study focussed on flow conditions close to a semi-synthetic CBM extraction well-field, Moore et al. (2013, 2014) compares pressures calculated by a traditional (single-phase) groundwater flow model with those calculated by a multiphase reservoir simulator. The model domain used in their study was comprised of a complex lithological realization of thin coal and interburden layers that is typical of certain Surat Basin gas fields. The study demonstrated that drawdowns calculated by a standard groundwater flow model can significantly exceed those calculated by a multiphase reservoir model, both close to extraction well fields and at large distances from well fields. Similar conclusions were drawn by Golder Associates (2012) in a study undertaken to assess the impact of oil-sand mining on regional groundwater systems in Canada.

As outlined by Moore et al. (2013, 2014) there are two principal reasons why use of a standard groundwater model leads to over-prediction of pressure drawdown. As gas desorbs from the coal matrix because of coal seam depressurization, its presence in the cleat system through which fluid flow takes place instigates a reduction in the relative permeability of the water phase. This reduced water phase permeability hinders the outward propagation of the extraction-induced cone of depressurization. At the same time, water is displaced from the coal cleat system by gas. Even where coal porosity is low, the volume of water released by gas generation in cleats is far greater than that released from elastic storage, which further mitigates the transient outward propagation of extraction-induced drawdown.

Means through which it may be possible to take these effects into account in regional impact modelling include (1) use of a detailed multi-phase reservoir simulator for regional impact assessment, and (2) implementation of a hybrid approach in which the above effects are approximated in a modified single-phase groundwater flow model designed for regional scale impact assessment. The former approach is taken by QGC (2014); the latter approach is the subject of the present paper.

The proposed formulation described in the present paper employs a modified Richards equation to characterize water desaturation arising from the presence of gas in coal cleats. It has been coded into the public domain groundwater flow code MODFLOW-USG (Panday et al., 2013). Its use is demonstrated using two synthetic models which embody simplified representations of CBM reservoirs. These models simulate extraction from a single homogeneous coal seam on the one hand, and CBM extraction from a more complex sequence comprised of two homogeneous coal seams separated by an interburden layer and overlain by a water-bearing formation on the other hand. First, errors in predicting drawdown incurred by ignoring the presence of gas are investigated by comparing pressures calculated using the ECLIPSE reservoir simulator with those calculated using the standard MODFLOW-USG simulator. Second, two alternative strategies are investigated for mitigating drawdown over-prediction by a groundwater simulator. The first of these alternatives employs MODFLOW-USG as a traditional groundwater flow model; however its water extraction rates are pre-calculated by the reservoir simulator ECLIPSE. The second alternative acknowledges the existence of a gas phase by simulating desaturation using a modified Richards equation functionality coded into MODFLOW-USG.

2. Methodology

The equations for two-phase flow of gas and water that are now briefly presented find numerical expression in commercial CBM production simulators such as ECLIPSE (Schlumberger, 2012) and SIMEDWin (CSIRO, 2014), as well in open source-codes such as those described by Thararoop et al. (2012) and Manik et al. (2002). Secondary effects such as alterations to coal permeability with pressure and gas content, and the low-level solubility of methane in water are neglected.

The amount of methane that can be stored in the coal matrix through adsorption, and its variation with pressure, is described by a nonlinear Langmuir isotherm:

$$L = L_m\left(\frac{p}{p + p_L}\right) \tag{1}$$

where:

L, is the coal gas content (volume of gas under standard conditions per volume of coal) (–);
L_m, is the gas sorption capacity of coal (–);
p, is the pressure (M/LT^2); and
p_L, is the Langmuir pressure constant (M/LT^2).

When pressure in a coal seam is reduced to the point where methane concentration exceeds the capacity of the coal matrix to

adsorb it, methane is released. It then diffuses through the coal matrix to the cleat system, where it displaces water to exist as its own phase and flow with water to extraction wells.

Flow of water and gas through an isotropic porous medium can be described by the following equation.

$$\nabla \cdot \left[k \frac{k_{ri}}{\mu_i B_i} \nabla (p_i + \rho_i g z) \right] = \frac{\partial}{\partial t} \left(\frac{\phi S_i}{B_i} \right) - q_i \tag{2}$$

where:

k, is the permeability of the medium (L^2);
k_{ri}, is the relative permeability of phase i (–);
μ_i, is the viscosity of phase i (M/LT);
B_i, is the formation volume factor of phase i (volume of phase under formation conditions per volume of phase under standard conditions) (–);
p_i, is the pressure of phase i (M/LT^2);
ρ_i, is the density of phase i (M/L^3);
g, is acceleration due to gravity (L/T^2);
z, is elevation (L);
t, is time (T);
ϕ, is porosity (–);
S_i, is the saturation of phase i (–); and
q_i, is the source strength density of phase i expressed as volume (under standard conditions) of phase i introduced to the medium per unit volume of the medium ($1/T$).

where there are two phases, modelling must solve for four unknowns, these being p_i and S_i for $i = g$ (i.e. gas) and $i = w$ (i.e. water). The above two equations must therefore be supplemented by another two equations. These are:

$$p_g - p_w = p_c \tag{3}$$

and

$$S_g + S_w = 1 \tag{4}$$

where p_c is the (saturation-dependent) capillary pressure (M/LT^2). In CBM reservoir modelling this is usually assumed to be zero; hence p_g is assumed to equal p_w.

An injection/extraction well constitutes a point source/sink of fluid, and can thus be represented in the q_i term of Eq. (2). However in most contexts of CBM extraction, well pressure eventually falls to a level which is then maintained for the rest of the life of the well. A well then constitutes a constant pressure boundary condition.

As a coal seam is being depressurized another source of fluid comes into existence as gas is desorbed from the coal matrix. Once the pressure declines to a point where, according to the governing Langmuir isotherm, gas is desorbed, it diffuses from the matrix to the cleat system in accordance with Fick's law. This takes place under a concentration gradient equal to the difference between its current bulk concentration and the Langmuir concentration at current pressure. Diffusion creates a time delay between desorption of gas and its functioning as the q_g term in Eq. (2). The time constant τ of this delay is given by:

$$\tau = \frac{1}{\sigma D_c} \tag{5}$$

where:

D_c, is the diffusion coefficient (L^2/T); and
σ, is a shape factor (see Kazemi et al., 1976) which describes the assumed geometry of the matrix-fracture interface within the coal seams (L^{-2}).

For both phases, k_{ri} is a function of S_i. A Brooks–Corey formulation (Brooks and Corey, 1964) is often used to describe this function. For water, effective water saturation is defined as:

$$S_e = \frac{S_w - S_r}{1 - S_r} \tag{6}$$

where S_r is residual water content (–). k_{rw} (–) is then expressed as:

$$k_{rw} = S_e^n \tag{7}$$

where n is chosen appropriately for the porous medium under consideration. A similar formula is employed for k_{rg}.

Where fluid flow is horizontal (as is approximately the case in CBM extraction), then over that part of the model domain where pressures are low enough for gas to be released, Eq. (2) can be approximated for the gas and water phases respectively, as:

$$\nabla \cdot \left[k \frac{k_{rg}}{\mu_g B_g} \left(\nabla p + g z \nabla \rho_g \right) \right] = \phi \frac{\partial}{\partial t} \left(\frac{S_g}{B_g} \right) + \frac{dL}{dp} \frac{\partial p}{\partial t} \tag{8a}$$

and

$$\nabla \cdot \left[k \frac{k_{rw}}{\mu_w} \nabla p \right] = \phi \frac{\partial S_w}{\partial t} \tag{8b}$$

Use of Eq. (8) implies that:

- Capillary pressure is zero so that pressure of gas and water are the same, this allowing the subscript on p to be dropped.
- Water is incompressible so that B_w is unity.
- The matrix is incompressible so that ϕ is constant.
- Diffusion time of desorbed gas from matrix to cleats is small enough to be ignored.

Eqs. (8) and (4) form a system of three equations which can be solved for p, S_w and S_g. S_g appears in Eq. (8a) through its influence on k_{rg}, while S_w is expressed in Eq. (8b) through both the storage term and its influence on k_{rw}. These equations become de-coupled if S_w (and hence S_g) can be expressed as a function of p alone. Hence, as will be suggested later in this paper, if the behaviour of a dual-phase system under certain configurations and boundary conditions is such that S_w can be approximately considered to be a function p, then the second of the above equations can be solved independently of the first for p_w. Solution of Eq. (8b) independently of Eq. (8a) is a matter of great convenience in CBM impact assessment modelling as this impact is mostly defined in terms of drawdowns induced by gas production, often at considerable distances from pumping centres, and hence far from the locations where gas is extracted and desaturation occurs. The purpose of the present study is to inquire whether separation of the gas and water flow equations is justified in the CBM impact assessment context, notwithstanding the obvious shortcomings of such a strategy in other contexts, especially those whose focus is on processes close to gas extraction centres where the flow of two separate phases must be explicitly represented (e. g. reservoir production forecast studies).

In traditional unsaturated modelling of water movement, dual-phase flow of water and air in the vadose zone is often described by a single equation pertaining to flow of water alone, this being referred to as the Richards Equation. The assumption here is that gas flow is instantaneous, with the gas phase rapidly equilibrating to atmospheric pressure conditions ($p_g = 0$). Thus the capillary pressure, which is not neglected in such simulations, is the negative of the water pressure as per Eq. (3). In vadose zone modelling the dependence of S_w on p is often described by the van Genuchten function (van Genuchten, 1980). This provides a general S-shaped curve in which the α and β parameters (see below) are adjusted to define the soil's capillary characteristics at a particular site. In the present paper we employ a modified form of this function, though not to define capillarity (which is often ignored in CBM simulations), but rather to describe the time-asymptotic

dependence of S_w on p that emerges from CBM-induced water desaturation processes that have been described above. The modified van Genuchten equation is:

$$S_e = \frac{S_w - S_r}{1 - S_r} = [1 + \{\alpha(h_b - h)\}^{\beta}]^{-\gamma} \quad \text{for } (h_b - h) > 0 \tag{9}$$

The term γ (–) is computed as:

$$\gamma = 1 - 1/\beta \tag{10}$$

while water head h (L) is computed as:

$$h = \frac{p}{\rho_w^g} \tag{11}$$

In Eq. (9), α (L^{-1}) and β (–) are fitting parameters. h_b is the bubble point pressure head [L], this being the pressure head at which water desaturation induced by gas desorption commences. The introduction of this term marks the only departure of equation 9 from the standard van Genuchten equation. It allows water desaturation to commence at a pressure of the user's choice. If it is set to zero then equation 9 becomes the standard van Genuchten equation wherein desaturation commences as water pressure falls below atmospheric pressure. In a CBM production context desaturation commences at pressures that are much greater than atmospheric pressure. h_b therefore represents the height of a column of water that corresponds to the pressure at which gas starts to be released by the coal matrix.

It is important to note that our use of a modified van Genuchten equation in the CBM context does not imply that physical processes in that context are the same as those in the vadose zone. In particular, capillary pressure is assumed to be zero in simulations described herein. Its use is based partly on the fact that the modified van Genuchten equation replicates water desaturation computed by a dual-phase reservoir simulator reasonably well. Its use is also based on its availability in MODFLOW-USG. The authors did, in fact, test other analytical formulations of the dependence of water saturation on water head; however no improvements over the above formulation were found.

Reservoir simulators typically provide a high degree of flexibility in definition of well emplacement and pumping rates from wells. In the current study, a target pumping rate is set for each individual well; extraction from each well continues at this rate until the pressure in the well (referred to as bottom-hole pressure) falls to a level at which it is then constrained (at 73.5 psia in the present study) to fall no further. This representation of extraction wells is common in CBM reservoir simulation. For an individual well, the rate of water production q_w is calculated as:

$$q_w = W(p - p_{well}) \tag{12}$$

where the well productivity index, W (L^4T/M), is computed using Peaceman's formula (Peaceman, 1983); this is a function of well radius, grid size, permeability of the model cell perforated by the well, and an optional skin factor (assumed to be zero in the present study). Where an individual well taps multiple layers, extraction is divided between them in such a manner as to maintain either hydrostatic conditions within the well, or a pressure drop that accounts for fluid flow within the well column. In MODFLOW-USG similar functionality is available through the connected linear network (CLN) package. Slight modifications were made to the coding of this package for the present study in order to allow identical definition of bottom-hole pressure constraints to that employed by reservoir simulators.

3. Numerical models

In a series of numerical experiments which are now described, pressures and saturations induced by CBM extraction are calculated throughout the domains of two different models, a simple model in which a single coal seam is represented, and a more complex model comprised of multiple coal seams. The latter model also includes boundary conditions which enable exchange of water with neighbouring formations. In both cases CBM extraction is simulated using both a reservoir simulator (ECLIPSE) and a groundwater flow simulator (MODFLOW-USG). The purpose of the experiments is to test, in a controlled numerical environment, whether a single-phase groundwater flow simulator, configured for accommodation of CBM-induced water desaturation, can be used for the purpose of regional CBM impact assessment. Specifications of the two models are now provided; variations are introduced later.

3.1. Single layer model

Fig. 1 shows a simulation grid comprised of 368 rows and 368 columns. Row and column widths vary from 15 m at the centre of the model domain (where pumping takes place) to 1 km at its periphery, with a cell width multiplication factor of 1.1 at intermediate distances. The dimensions of the overall model domain are

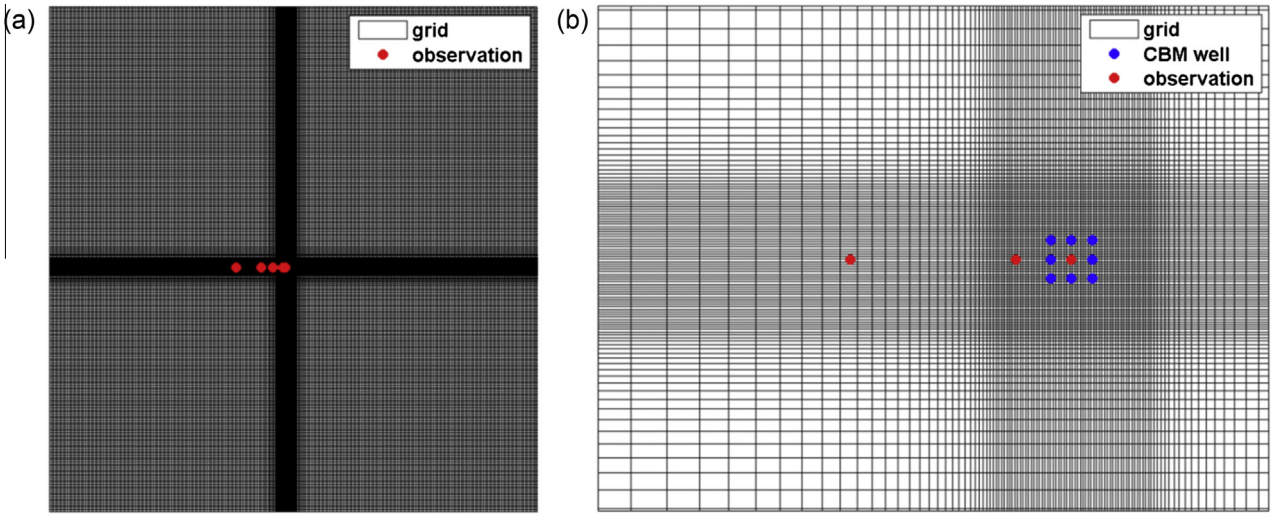

Fig. 1. (a) Grid used for the single layer model. The red dots are a row of observation wells. 9 pumping wells are located in the centre of the model domain. (b) Setup of CBM extraction wells (blue) and monitoring wells (red). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

about 244 km × 244 km. The grid contains one coal layer of 1 m thickness.

A regular array of 9 CBM extraction wells is placed at the centre of the model domain. These are spaced 375 m apart; each has a diameter of 0.25 m. Each of these wells is specified to pump at a water rate of 200 stb/day (i.e. 31.80 m^3 per day), subject to a limiting bottom-hole pressure constraint of 73.5 psia (41.34 m of water) at the elevation of the centre of the grid block from which each well pumps. CBM production takes place for 20 years; the following 20 years of drawdown recovery are also simulated. No-flow conditions are applied at all model boundaries.

Properties of coal comprising the single model layer are provided in Table 1. These are similar to those employed by Moore et al. (2014) and are representative of parts of the Surat Basin. In MODFLOW-USG elastic storage is accommodated using the specific storage parameter. This is calculated to be $1.1 \times 10^{-6}\ m^{-1}$ based on the porosity provided in Table 1, with water and rock compressibilities assumed to be $4.4 \times 10^{-6}\ m^{-1}$ and $2.8 \times 10^{-5}\ m^{-1}$ respectively. Relative permeability functions pertaining to the water and gas phases are depicted in Fig. 2a (only the former is used by MODFLOW-USG whereas both are required by ECLIPSE). S_r in Eq. (6) is assigned a value of 0.2 while the Brooks–Corey exponent used in Eq. (7) is assigned a value of 2.

The gas compressibility function (expressed as a gas formation volume factor) is depicted in Fig. 2b while the Langmuir isotherm is depicted in Fig. 2c; both of these are used by ECLIPSE. Re-adsorption of gas upon cessation of pumping is assumed to be governed by the same properties as desorption. The capillary pressure between gas and water is set to zero.

An initial pressure of 900 psia at an elevation of 0.0 m (this corresponding to the top of the coalbed layer) is assumed. This is equivalent to a head of 623 m. The initial gas content is set to $1.0 \times 10^{-2}\ Msm^3/m^3$.

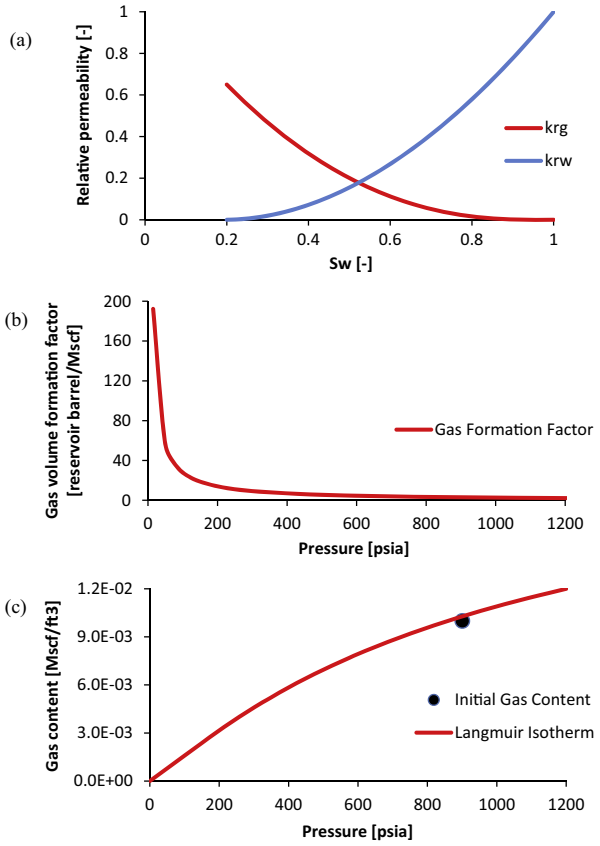

Fig. 2. (a) Relative permeabilities, (b) gas volume formation factor, and (c) Langmuir isotherm, used in ECLIPSE simulations.

3.2. Six layer model

Simulation grid specifications are provided in Table 2. Once again, the grid is comprised of 368 rows and 368 columns. Row and column widths vary between 50 m and 100 m; dimensions of the total model domain are roughly 30 km × 30 km. The grid contains 6 layers. Layers 1 and 2 represent overburden material while layers 3–6 represent a coal measure sequence comprising two separate, continuous coal seams (layers 4 and 6) overlain by continuous interburden layers (layers 3 and 5). Layer thicknesses are provided in Table 3.

Extraction takes place through a regular array of 25 wells separated by 750 m (a typical well separation in the Surat Basin (Arrow-Energy, 2012; QGC, 2012). Well diameters are 0.25 m; pumping specifications are 600 stb/day (95.4 m^3/day) of water with a bottom-hole pressure constraint of 73.5 psia at the centre of the top coal seam. Pumping takes place for 20 years; this is followed by a recovery period of 20 years. Screens are open to both of the coal layers in all wells; extraction is distributed automatically between these two layers in the manner described above. A constant pressure condition equal to the initial pressure is applied at all lateral boundaries. Rock properties are listed in Table 3.

Table 1
Specifications of the single layer model.

Parameters	Petroleum units	Metric units
Grid extent	ca. 800.000 ft × 800.000 ft	ca. 244 km × 244 km
Grid dimensions	1 layer, 368 columns, 368 rows	
Grid cell size	49.2 ft–3280 ft	15 m–1 km
Thickness of coal seam	3.28 ft	1 m
Porosity	1%	
Permeability	200 mD	0.25 m/d
Matrix gas content at initial pressure	0.01 Mscf/ft^3	0.01 Msm^3/m^3
Sorption capacity at initial pressure	0.012 Mscf/ft^3	0.012 Msm^3/m^3
Diffusion coefficient of coal matrix	0.01 Mscf/ft^2	0.01 Msm^3/m^3
Initial pressure	900 psia	622.59 m H_2O
Number of wells	9	
Duration of production phase	7305 days	
Duration of recovery phase	7305 days	
Target water extraction rate	200 bbl/day	31.80 m^3/d
Bottom-hole pressure constraint	73.5 psia	41.35 m H_2O
Model boundaries	No flow	

4. Numerical simulations

4.1. Single layer model

4.1.1. Verification

Prior to undertaking any of the numerical experiments documented below, a number of ECLIPSE simulations were undertaken under similar pumping conditions to those described above, but with gas concentrations set to zero; single-phase flow was thereby simulated. ECLIPSE-calculated pressures were converted to heads and compared with heads calculated by MODFLOW-USG under the same pumping regime. Differences between corresponding model outputs were found to be minimal.

4.1.2. Errors incurred by neglecting desaturation

First ECLIPSE was used to simulate water and gas extraction under the conditions described in Section 3.1 The black line in

Table 2
Specifications of the six layer model. Specifications not provided below are the same as those in Table 1.

Property	Petroleum units	Metric units
Grid extent	98.400 ft × 98.400 ft	30 km × 30 km
Depth	98.4 ft	30 m
Grid dimensions	6 layers, 368 columns, 368 rows	
Grid cell size	164 ft–328 ft	50 m–100 m
Number of wells	25	
Distance between wells	2460 ft	750 m
Target water extraction rate	600 bbl/day	95.4 m^3/d
Bottom-hole pressure constraint	73.5 psia	41.35 m H_2O
Model boundaries	MODLFOW-USG: GHB boundary at edges of layers 1–6; ECLIPSE: "AQUFETP" layers 1–6	

Table 3
Layer thicknesses and rock properties used by six layer model.

Layer	Unit	Thickness (m)	Porosity (–)	K_h (m/d)	K_z (m/d)
1	Aquitard	1	0.15	1.3×10^{-2}	1.3×10^{-5}
2	Aquitard	9	0.15	1.3×10^{-2}	1.3×10^{-5}
3	Interburden	9	0.05	1.3×10^{-3}	1.3×10^{-6}
4	Coal	1	0.01	2.5×10^{-1}	1.3×10^{-5}
5	Interburden	9	0.05	1.3×10^{-3}	1.3×10^{-6}
6	Coal	1	0.01	2.5×10^{-1}	1.3×10^{-5}

Fig. 3 shows ECLIPSE-simulated drawdowns at 6 different distances from the centre of the extraction well field; note that pumping is assumed to commence at the beginning of year 2000. Close to the wells, drawdowns of up to 500 m are sustained during the 20 years of CBM production. Maximum drawdowns diminish to around 80 m at a distance of 24,390 m from the production centre. Near the wells the bottom-hole pressure limited maximum drawdown is achieved within a year. Further from the wells drawdowns increase steadily during the CBM production period; far from the wells these continue to increase even after CBM production has ceased. When pumping ceases, drawdown recovery close to the wells is initially rapid as residual gas is re-adsorbed into the coal matrix and replaced (in coal cleats) by nearby water. This is followed by a period of more gradual recovery as water flow within the model domain attempts to establish a new hydrostatic equilibrium. Because boundary conditions are such that the model domain is essentially a "closed box", initial pressures are not re-attained. At larger distances from the CBM well cluster recovery is

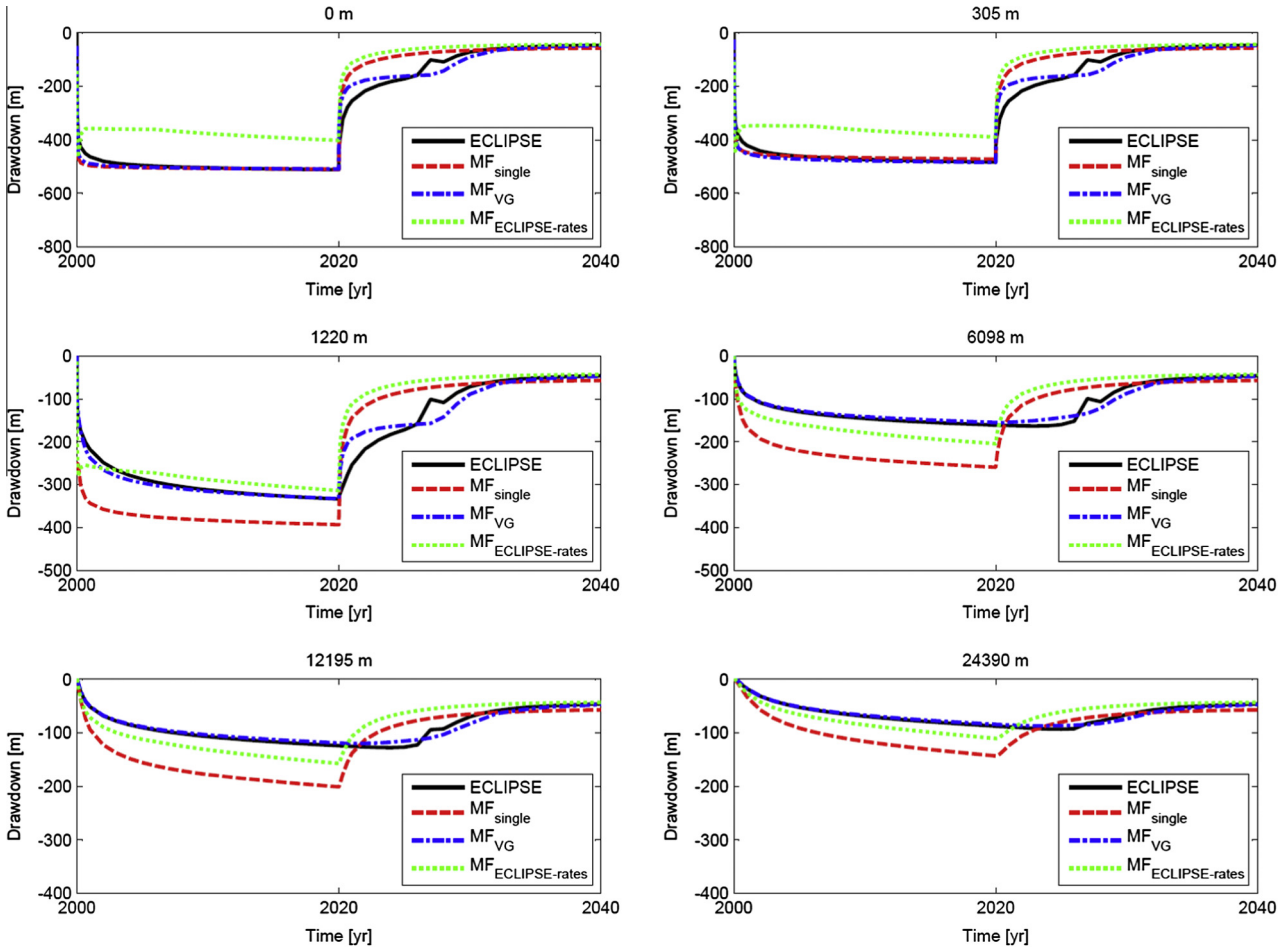

Fig. 3. Drawdown calculated by ECLIPSE (solid black lines), MF_{single} (red dashed lines), $MF_{ECLIPSE\text{-}rates}$ (green lines) and MF_{VG} (blue lines). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

more gradual, though is essentially complete at distances of up to 12,195 m from the pumping centre by the year 2030.

The simulation was then repeated using MODFLOW-USG. Identical pumping conditions (including target well extraction rates and bottom-hole pressure constraints) were imposed on extraction wells as were used in the above ECLIPSE simulation. However MODFLOW-USG was employed as a "traditional groundwater model" as no desaturation was allowed to occur; hence extracted water is sourced from elastic storage only, and there is no permeability reduction that would occur due to the presence of gas. We refer to simulations under these conditions as "MF_{single}" (where "single" stands for "single-phase flow" as is assumed in standard groundwater models). Simulated drawdowns are shown as dashed red lines in Fig. 3. At the production wells maximum MF_{single} and ECLIPSE drawdowns are very similar as both models encounter the same bottom-hole pressure constraint. However MF_{single} encounters this constraint at an earlier time than does ECLIPSE. At 1220 m from the production centre ECLIPSE and MF_{single} drawdowns deviate significantly from each other, with MF_{single} overestimating drawdown by more than 100 m. At larger distances this discrepancy increases; at the same time MF_{single} drawdowns propagate faster outwards from the well field than do ECLIPSE drawdowns. As has already been discussed, MF_{single}'s overestimation of drawdown is an outcome of two factors, namely (1) its reliance on elastic storage as its only source of water to supply the demands of extraction whereas ECLIPSE draws on pore water that is displaced by gas, and (2) its failure to reduce relative permeability with drawdown as MF_{single} allows no desaturation.

Further discrepancies are encountered when comparing total volumes of extracted water calculated by the two simulators. Over 20 years of production ECLIPSE extracts 8.52×10^5 m^3 of water while MF_{single} extracts 1.16×10^6 m^3 of water; the latter therefore overestimates water production by 36%.

Significant differences in simulated recovery are also observed, with MF_{single} recovery being much faster than that of ECLIPSE. The redistribution of water that is necessary to attain a new equilibrium can happen much more quickly when there is no desaturation, and groundwater flow therefore takes place under fully saturated and confined conditions.

4.1.3. Error mitigation through use of ECLIPSE pumping rates

The green dashed line in Fig. 3 shows drawdowns calculated using MODFLOW-USG, once again run as a traditional groundwater model, but this time using pumping rates calculated by ECLIPSE; this run is referred to as $MF_{ECLIPSE\text{-}rates}$. A similar strategy was followed by Moore et al. (2013) to ensure that the same amount of water is extracted in the groundwater model as is extracted from the ECLIPSE model during the entire simulation period. Close to the wells $MF_{ECLIPSE\text{-}rates}$ underestimates drawdown by up to 100 m. However drawdown propagates faster for $MF_{ECLIPSE\text{-}rates}$ than it does for ECLIPSE (black lines in Fig. 3), as coal hydraulic diffusivity (Bear, 1972) is higher because of larger hydraulic conductivity and a smaller storage coefficient, these resulting from the assumption of a fully confined, water-saturated system. Underestimation of drawdown therefore becomes overestimation of drawdown (by up to 50 m) at distances of over 6098 m from the pumping centre. Drawdown recovery rates are overestimated by $MF_{ECLIPSE\text{-}rates}$ as they are for MF_{single}. Note that, in contrast to the present study, simulations carried out by Moore et al. (2013) did not indicate underestimation of drawdown close to the well when employing MODFLOW with ECLIPSE-generated pumping rates (though drawdowns were indeed overestimated far from the well). However, their simulations were conducted in a model domain that is far more complex and heterogeneous than that employed in the present study; cause/effect relationships are therefore unclear.

4.1.4. Error mitigation through inclusion of desaturation

Inclusion of desaturation functionality in a modified Richards equation model as a strategy for mitigation of drawdown overestimation requires that parameters be supplied for the modified van Genuchten relationship of Eq. (9). As is now demonstrated, these parameters may be obtainable from local multiphase reservoir models constructed by CBM operators at their extraction sites.

Fig. 4 (solid black lines) shows plots of water saturation versus time calculated by ECLIPSE at a number of distances from the pumping centre. These distances are smaller than those depicted in Fig. 3 since desaturation extends a far smaller distance from the pumping centre than pumping-induced drawdown. In fact the maximum lateral extent of desaturation is about 7 km from the pumping centre, whereas significant drawdowns are computed at distances of more than 25 km.

It is apparent from Figs. 3 and 4 that while pressures fall monotonically near production wells (until encountering the bottom-hole pressure constraint), the variation of near-well water saturation with time is not monotonic. Close to wells rapid desaturation occurs shortly after pumping commences as gas is quickly desorbed from the coal matrix in response to sharp pumping-induced pressure reductions. Saturation then recovers to some extent as water replaces gas in near-well void space as both of these fluids

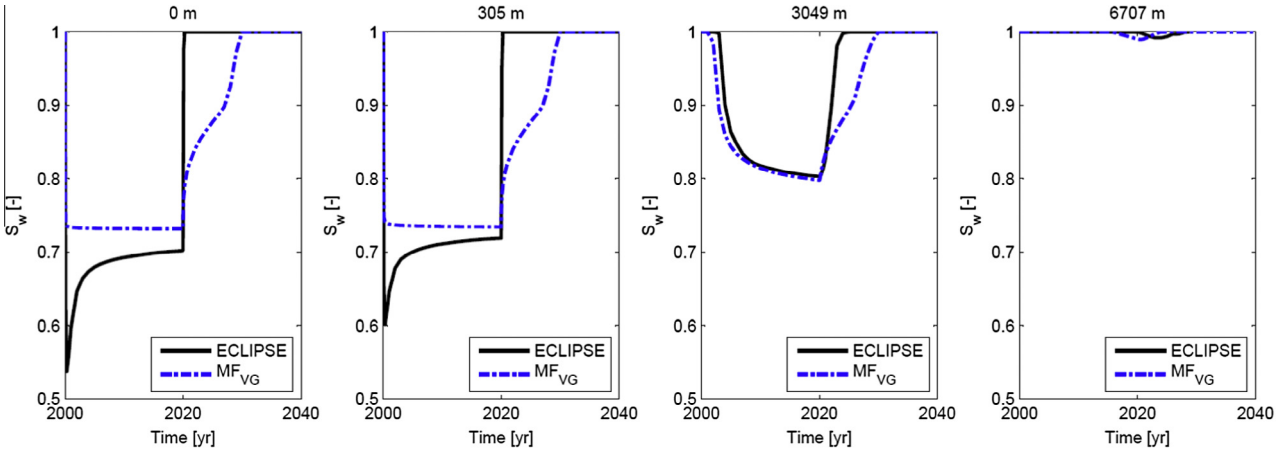

Fig. 4. Simulated water saturations at different distances from the pumping centre calculated by ECLIPSE (solid black lines) and by MF_{VG} (dashed blue lines). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

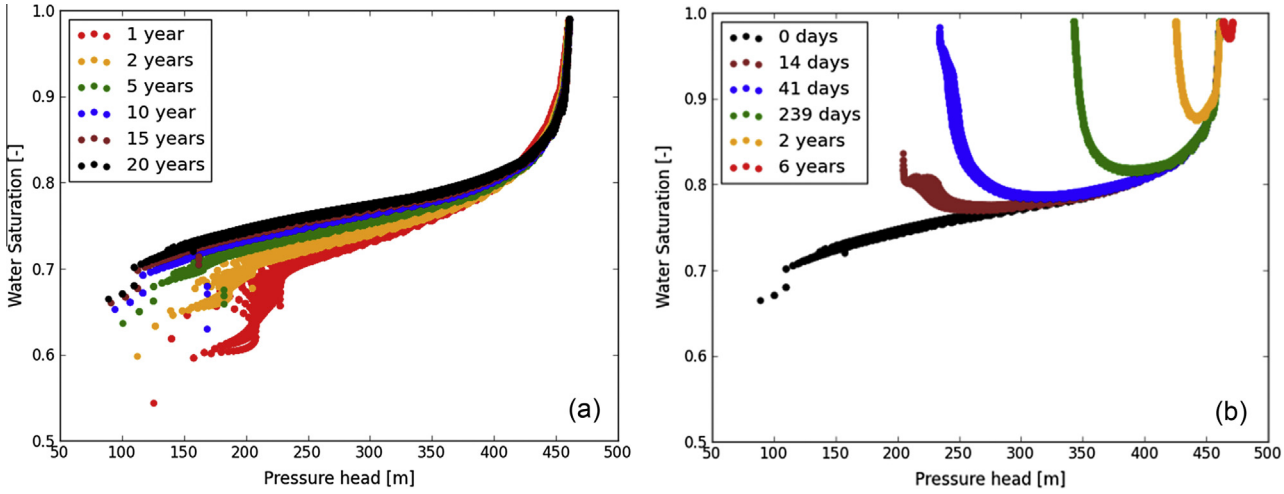

Fig. 5. (a) S_w vs. p at various times during CBM production. (b) S_w vs. p during recovery after CBM production. Time labels in 5b represent time elapsed since cessation of pumping.

flow towards the wells. An immediate repercussion of the non-monotonic behaviour of saturation with time is that the same water saturation can occur at multiple pressures; the notion of pseudo-equilibrium conditions in which saturation is pressure-dependent as expressed by Eq. (9) is thus violated at these early times.

Fig. 5a provides a scatterplot of water saturation versus pressure head (referred to as S_w vs. p) calculated during the CBM production phase of the ECLIPSE simulation. All cells for which desaturation occurs in this simulation are featured in this plot. Points within the plot are colour-coded according to simulation time. Points at the left of the plot are those nearest to the production wells where pressure reduction is greatest. It is apparent from these plots that while the relationship between S_w and p is hardly stationary with time, it evolves over time to a curve where time-stationarity appears to be attained. Fig. 5b shows S_w and p scatterplots during recovery. No stable relationship between S_w and p exists over this time; complete resaturation occurs after approximately 6 years of recovery.

The shape of the time-asymptotic curve of Fig. 5a suggests the attainment of a dynamic pseudo-equilibrium state. Except for locations in the immediate vicinity of the extraction wells, water saturation appears to decreases in a regular way as pressure falls. Meanwhile cones of drawdown and desaturation increase in area and perimeter as gas and water production continue. Water is made available for transmission to wells through desaturation itself. At the same time, gas is made available because reduction in pressure induces gas desorption from the coal matrix in amounts described by the Langmuir isotherm; see Eq. (1). Ever increasing amounts of both of these become available as the cone of pressure decline expands. The perimeter of the cone of water desaturation, where saturation falls from a value of unity, marks the location where pressure falls below the threshold at which, according to the Langmuir isotherm, gas can be released to the flow system. Meanwhile, between the desaturation perimeter and the extraction wells, gas and water are continuously released from storage as pressure and saturation continue to fall. Close to the wells themselves, however, the rate of gas desorption falls to zero as a constant pressure condition is maintained there.

It is obvious from Fig. 5b that as soon as pumping ceases and the recovery process commences, saturation cannot be considered, even approximately, to be a function of pressure despite the fact that such a relationship had been established prior to cessation of pumping. Fig. 4 indicates that water re-saturation is almost immediate near switched-off extraction wells where pressure gradients are steepest. Here down-gradient flow of water that was previously collected by wells now fills cleats as low pressure gas rapidly re-enters the matrix where, with very little rise in pressure, its re-adsorption is readily accommodated by the Langmuir isotherm. Meanwhile, further from pumping wells where pressures are higher and gradients are lower, recovery of the pressure necessary for readsorption of gas to occur is slower. However re-adsorption does indeed occur, progressing from low pressure areas near the well to higher pressure areas further from the well, forming a ring of desaturation whose internal radius expands until it meets its almost static external radius when desaturation had ceased.

Parameters α and β of the modified van Genuchten equation (Eq. (9)) used by MODFLOW-USG were obtained by fitting this equation to the S_w vs. p scatterplot of Fig. 5a. In fitting this curve h_b (the bubble point pressure head) was assumed to be the same as the gas desorption threshold calculated using the same Langmuir isotherm as that used by ECLIPSE. The residual water saturation was also adopted from the ECLIPSE simulation. Fig. 6 shows the resulting curve; best-fit parameters are listed in Table 4.

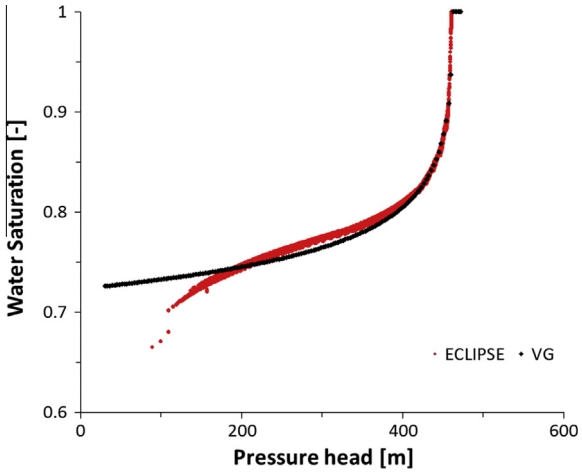

Fig. 6. S_w vs. p after 20 years of CBM production (red dots). The black curve shows the estimated modified van Genuchten function. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 4
Estimated modified van Genuchten parameters for the single layer model.

Parameter	Value
S_r (–)	0.2
α (m^{-1})	0.22
β (–)	1.073
n (–)	2
h_b (m)	463

Equipped with the modified van Genuchten relationship derived in this manner, MODFLOW-USG was used to simulate the evolution of water pressure and saturation during extraction and recovery. The same pumping conditions (i.e. a target extraction rate together with a bottom-hole pressure constraint) and relative permeability function for water were provided to MODFLOW-USG as were provided to ECLIPSE; hence MODFLOW-USG calculates appropriate pumping rates itself once the bottom-hole pressure constraint is encountered. Pressures resulting from this simulation are labelled MF_{VG} in Fig. 3; see the dashed blue lines. It is apparent that drawdowns calculated by MF_{VG} provide a very good match to those calculated by ECLIPSE over the 20 year production period. However drawdowns at very early simulation times close to extraction wells are over-estimated. More significant differences between MF_{VG} and ECLIPSE drawdowns occur over the 20 year recovery period where MF_{VG} slightly underestimates drawdowns calculated by ECLIPSE during part of the recovery period, and slightly overestimates ECLIPSE drawdowns during the other part. Nevertheless the fit with ECLIPSE-drawdowns during this recovery period is far better than that attained by either MF_{single} or $MF_{ECLIPSE\text{-}rates}$.

Water saturations calculated by ECLIPSE and MF_{VG} are compared in Fig. 4. Despite the attainment of a relatively good pressure match during the recovery phase, ECLIPSE saturation behaviour during recovery is poorly matched by MF_{VG}; in particular, the near-instant resaturation attained through gas re-adsorption cannot be reproduced by MF_{VG}. During the 20 year pumping period, the match between ECLIPSE and MF_{VG} saturations is reasonable, except for early times close to the extraction centre where the transient desaturation peak calculated by ECLIPSE cannot be reproduced by MF_{VG}.

Total extracted water volume calculated by MF_{VG} matches that computed by ECLIPSE reasonably well, the former being only 2% higher than the latter.

In summary, drawdowns calculated by MF_{VG} track those calculated by ECLIPSE well, with the greatest departures being at early times in close proximity to pumping wells, and during the recovery period. MF_{VG}'s ability to reproduce ECLIPSE-calculated water saturations is not as good. However, this is of secondary importance, as the purpose of the present study is to assess MF_{VG}'s ability to act in regional CBM impact assessment where the primary goal of modelling is to predict regional water-pressure drawdown and

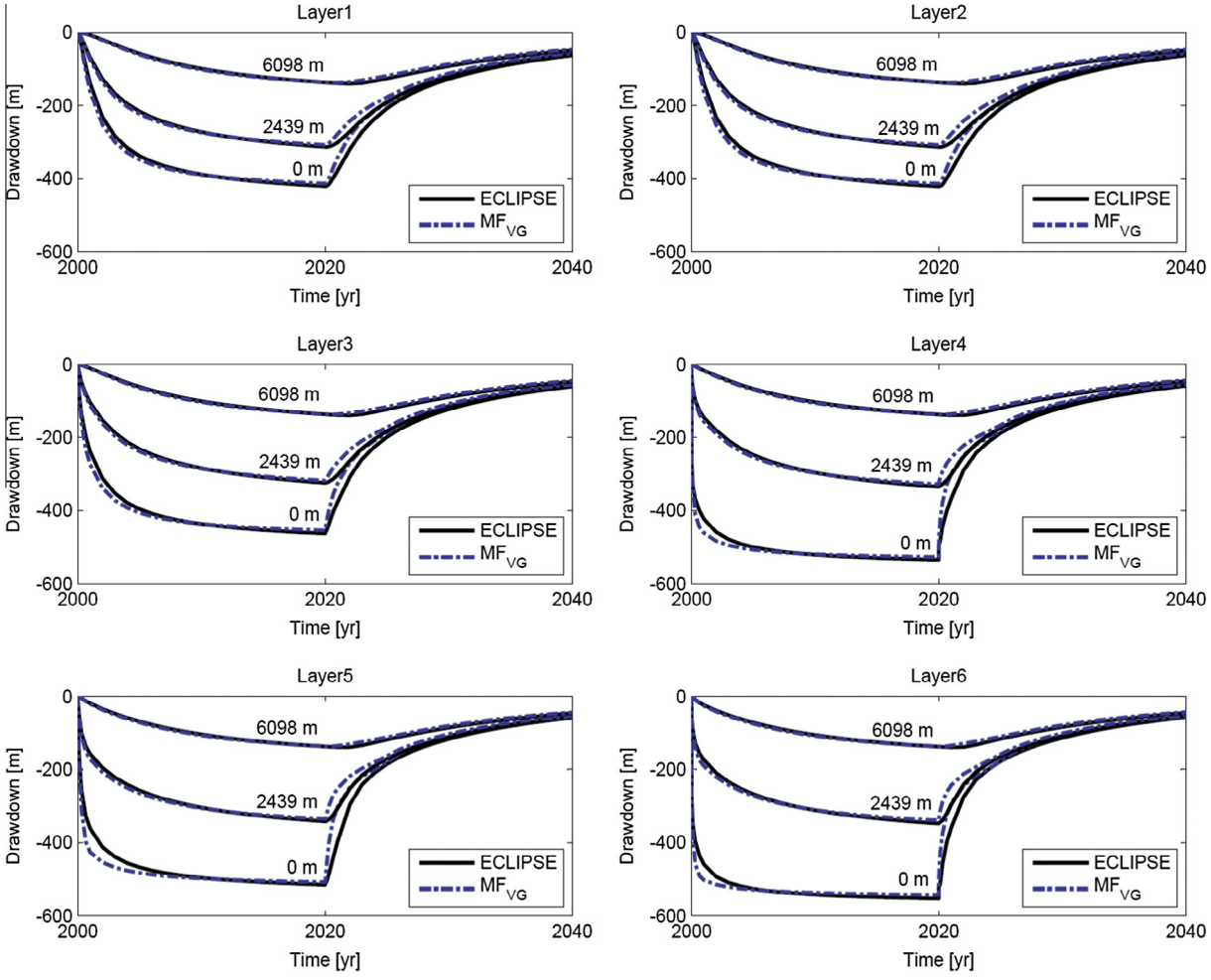

Fig. 7. Drawdowns calculated for the six layer model. Each subplot represents a different layer of the model. In contrast to Figs. 3 and 4, drawdowns at different distances from the well cluster are shown for the pertinent layer within each subplot. Black lines represent drawdowns calculated by ECLIPSE and blue lines represent drawdowns calculated by MF_{VG}. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

global water production figures rather than near-well water saturation or gas production figures.

Though not reported herein, similar numerical experiments were performed using variations of the above model in which permeability, porosity, relative permeability, layer thickness, and Langmuir isotherm characteristics were all varied. In all cases a stable asymptotic S_w vs. p curve was attained in the ECLIPSE simulations. In all cases MF_{VG} replicated ECLIPSE-calculated drawdowns very well during the extraction phase of the simulation, and moderately well during recovery, when using a modified van Genuchten function that matches the asymptotic S_w vs. p curve computed by ECLIPSE.

4.2. Six layer model

4.2.1. Flat layers

The six layer model was described in Section 3.2. Recall that this model features two overburden layers, two coal layers and two interburden layers. It is also laterally enclosed by fixed pressure boundary conditions.

ECLIPSE-calculated drawdowns for the six layer model are shown as solid black lines in Fig. 7 wherein drawdown curves in each layer at three different distances from the well are provided. Largest drawdowns of about 500 m are incurred near the extraction wells in the coal seam layers (i.e. layers 4 and 6). Total extracted water over 20 years of production is 7.02×10^6 m^3.

As provision of ECLIPSE-calculated pumping rates to a MODFLOW-USG model that does not allow desaturation does not yield accurate prediction of drawdown for the single layer model, the "$MF_{ECLIPSE\text{-}rates}$"-modelling strategy is not repeated for the six layer model. Only the performance of MF_{VG} is discussed.

Scatterplots of S_w vs. p for layer 4 at different simulation times are depicted in Fig. 8; those for layer 6 are similar. In both cases a time-stationary S_w vs. p curve is approached at high simulation times (see Fig. 8a). The modified van Genuchten curves fitted to both of these are shown in Fig. 8b; fitted parameters used by this equation are listed in Table 5. Drawdowns calculated by MF_{VG} when using these parameters are shown in blue in Fig. 7. As for the single layer case, drawdowns calculated by MF_{VG} match those calculated by ECLIPSE well, except at early simulation times and during recovery. The rate of recovery is slightly overestimated by MF_{VG}. MF_{VG} extracts a total of 6.71×10^6 m^3 of water; in doing so it underestimates total ECLIPSE water extraction by 4%.

Table 5
Estimated modified van Genuchten parameters for layers 4 and 6 of the six layer model.

Parameter	Layer 4	Layer 6
S_r (–)	0.2	0.2
α (m^{-1})	0.40	0.51
β (–)	1.053	1.047
n (–)	2	2
h_b (m)	468	473

Differences in water saturations calculated by ECLIPSE and MF_{VG} are illustrated in Fig. 9. At early times near the production wells, saturations calculated by ECLIPSE are significantly lower than those calculated by MF_{VG} where, as already discussed, the latter is unable to simulate the high levels of desaturation that accompany rapid gas desorption; this is an outcome of the static relationship between saturation and pressure that is employed by MF_{VG}. Upon cessation of pumping, MF_{VG} over-estimates desaturation as ECLIPSE simulates rapid gas re-adsorption whereby gas in coal cleats is quickly removed and replaced by water.

4.2.2. Sloping layers

Introduction of a sloping segment to the synthetic coal measure sequence leads to significant scatter of S_w vs. p. Fig. 11a (diamond markers) shows the ECLIPSE scatterplot at a simulation time of 20 years for layer 4 (which is similar to that for layer 6) where a north–south segment of slope 2% is introduced to the central part of the model domain between rows 153 and 215 (a distance of 3000 m); this slope is applied to all model layers so that the thickness of each remains uniform. Buoyant upslope migration of gas to the top of coal seams is visible in Fig. 10 which depicts the spatial disposition of saturation in the upper coal layer (layer 4) at the end of the production period (i.e. at a simulation time of 20 years).

Parameters for use of the modified van Genuchten function were obtained for MF_{VG} simulations conducted on the sloping-segment model by visually fitting this function to the ECLIPSE-generated S_w vs. p scatterplot of Fig. 11a. See the red line superimposed on the S_w vs. p scatterplot in this figure; parameters pertaining to this curve are listed in Table 6. Fig. 11c and d compare pressure and saturation profiles through the centre of the model domain computed by ECLIPSE with those computed by MF_{VG} when using these parameters (see red lines again). Drawdown profiles are in good agreement while saturation profiles (which, as stated

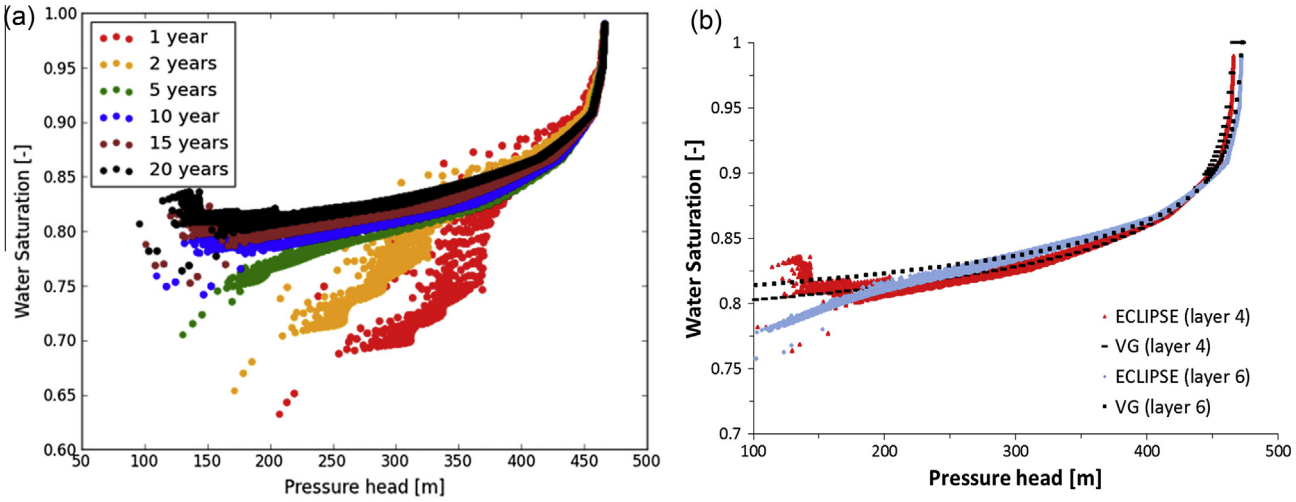

Fig. 8. (a) S_w vs. p at different times since commencement of extraction for coal seam layer 4; (b) Estimated modified van Genuchten-curves for layers 4 and 6; parameters are listed in Table 5.

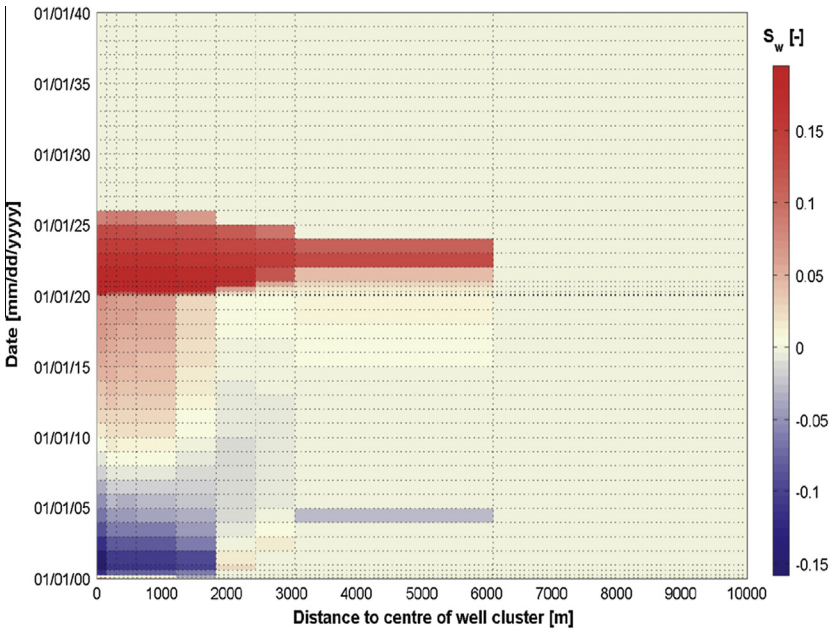

Fig. 9. Spatial and temporal differences in simulated water saturation between ECLIPSE and MF_{VG} in model layer 4. Blue colours indicate where MF_{VG} overestimates water saturation while red colours indicate where it calculates saturation values which are too low. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

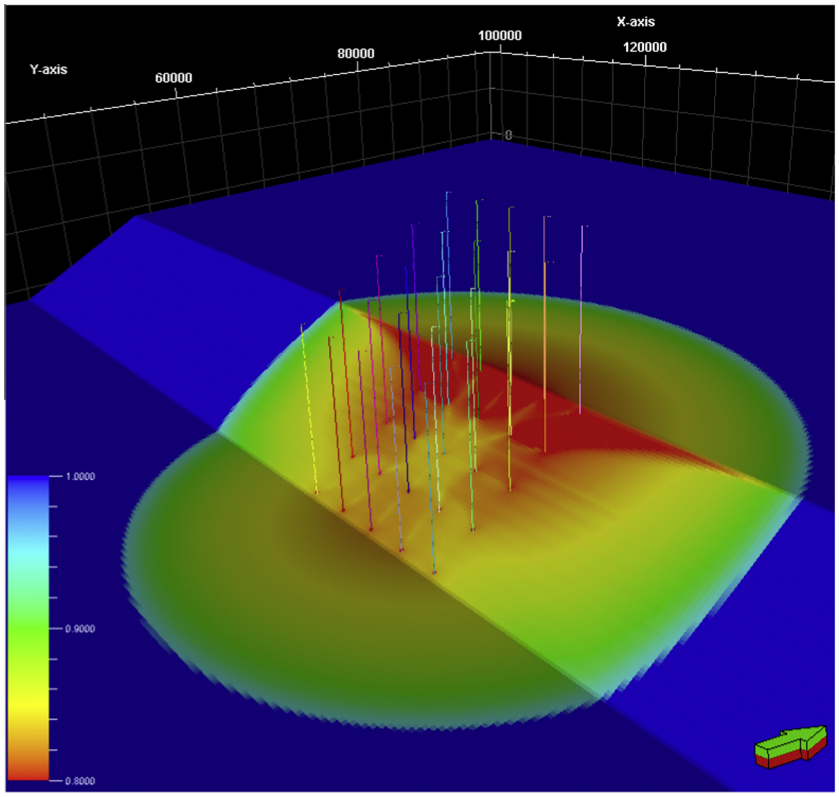

Fig. 10. Water saturation in layer 4 of the six layer model when a 2% slope is introduced to part of the model domain. Blue colours represent a water saturation of 1 where red colours pertain to lower water saturations. The vertical line segments represent the cluster of 25 CBM production wells located in the centre of the model domain. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

previously are of lesser importance to CBM impact assessment) do not agree as well. A poor fit with saturation profiles is not unexpected due to the role played by gas buoyancy in this simulation. Note the irregular shape of the ECLIPSE water saturation profile in Fig. 11d.

4.2.3. Sensitivity analysis

In order to test the sensitivity of MF_{VG} predictions to parameters of the modified van Genuchten function used to represent the dependence of S_w on p, random values for these parameters were generated. These were approximately centred on those used

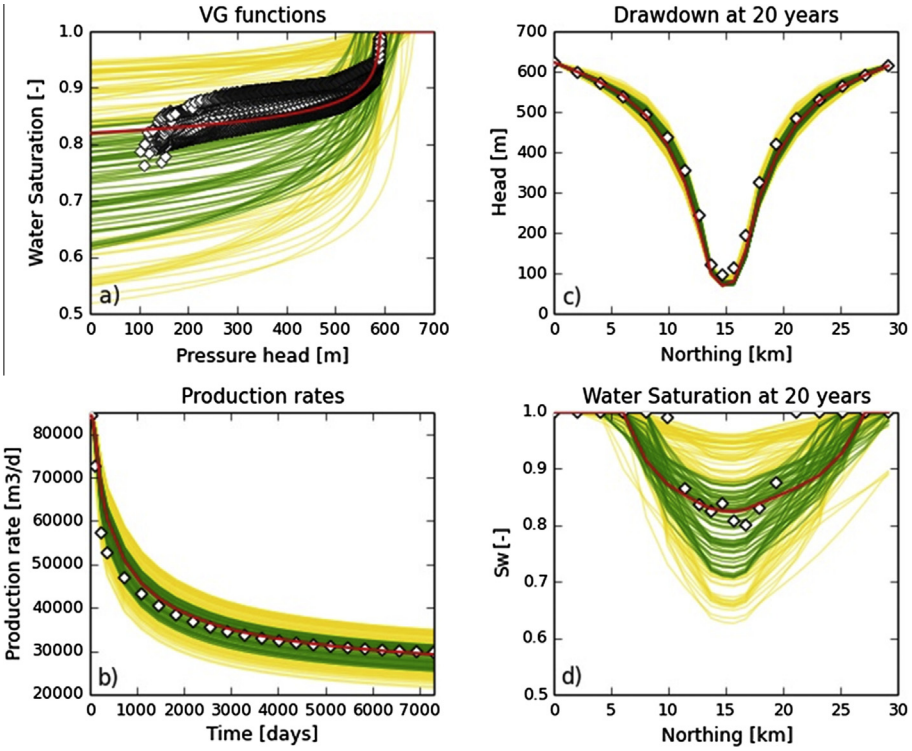

Fig. 11. (a) Modified van Genuchten functions superimposed on ECLIPSE-calculated S_w vs. p scatterplot. (b) Water extraction rates. (c) Drawdown profile through centre of the model domain at a simulation time of 20 years. (d) Water saturation profile through centre of the model domain at a simulation time of 20 years. ECLIPSE outputs are plotted using black diamond markers; red lines pertain to a MF_{VG} simulation using a modified van Genuchten function that was "fitted by eye" to the ECLIPSE-generated S_w vs. p scatterplot. Green and yellow lines pertain to randomly-generated modified van Genuchten parameters. See text for further details. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 6
The first column of values represents the modified van Genuchten parameters that were used to fit the S_w vs. p scatter plot obtained with ECLIPSE. The last two columns show the parameter bounds used in randomly generating modified van Genuchten functions that are tested as part of the sensitivity analysis conducted for the sloping six layer model.

Parameter	Initial value (fitted by eye)	Lower bound	Upper bound
S_r (–)	0.2	0.2	0.2
α (m^{-1})	0.15	0.01	0.60
β (–)	1.045	1.01	1.20
n (–)	2	2	2
h_b (m)	600	540	660

to generate the modified van Genuchten curve depicted in Fig. 11a. For all parameters a uniform probability distribution was employed spanning the interval between the upper and lower bounds listed in Table 6. Note that the bounds for h_b are narrow, reflecting the fact that this parameter can be derived from reservoir Langmuir properties with reasonable precision.

Fig. 11a shows the range of modified van Genuchten functions calculated from these random parameters together with the ECLIPSE scatterplot of S_w vs. p. These are coloured yellow, but with a subset coloured green; the basis for selection of the green subset is explained below. Fig. 11c shows layer 4 drawdowns computed using MF_{VG} along a profile through the centre of the model domain at a simulation time of 20 years. Drawdowns at simulation times of 2 and 10 years show similar patterns, but are not presented here. Saturations along this same profile are depicted in Fig. 11d. Water extraction rates are plotted against time in Fig. 11b. Yellow and green curve colouring in all of these figures corresponds to that in Fig. 11a. In all cases the pertinent ECLIPSE-calculated quantity is shown with black diamond markers. These figures demonstrate relatively small sensitivity of MF_{VG}-computed drawdowns to parameters employed by the modified van Genuchten function. Pumping rates are more sensitive to these parameters however; water saturations are the most sensitive.

The set of curves coloured green in Fig. 11 afford a better fit with ECLIPSE-calculated pumping rates than those coloured yellow. Fit was measured using a weighted least squares objective function calculated on the basis of differences between ECLIPSE and MF_{VG} pumping rates; weights were calculated as the inverse of ECLIPSE pumping rates. A green colouration threshold was set at an objective function value that indicates a root-mean-square misfit of 5% of ECLIPSE-calculated pumping rates. It is apparent from Fig. 11 that parameters employed by the modified van Genuchten function which endow MF_{VG} with the ability to fit water extraction rates well, are also those which result in a good fit with the ECLIPSE-generated S_w vs. p scatterplot, and a moderate fit with ECLIPSE-calculated saturations.

The above analysis suggests that model outputs of most interest to CBM regional impact assessment are relatively insensitive to the exact choice of modified van Genuchten function parameters. If a S_w vs. p curve described by this function passes roughly through an ECLIPSE-generated S_w vs. p scatterplot, then drawdowns and pumping rates computed by MF_{VG} will approximate those computed by ECLIPSE.

5. Discussion

The outcomes of a series of numerical experiments have been presented. These experiments were conducted in order to examine whether use of a modified single-phase groundwater simulator, configured to allow desaturation to occur in coal layers, is justifiable when assessing the effects of CBM production on regional groundwater systems.

Use of a modified Richards equation approach in place of a dual-phase flow approach rests on the assumption that water saturation (and with it relative permeability of water) is a function only of water pressure. Simulations undertaken using the ECLIPSE reservoir simulator demonstrate that such a functional relationship between S_w and p is approached with increasing simulation times and with increasing distances from pumping centres. The asymptotic monotonic relationship between S_w and p appears to become exact where dual-phase flow is horizontal, and takes place through a homogeneous medium.

Where coal seams are not horizontal an asymptotic relationship between S_w and p becomes more difficult to define. This is an outcome of gas buoyancy, a feature of multiphase flow that cannot be captured using a single phase model supplied with a pre-calculated S_w vs. p relationship. In spite of this, modelling results reported herein show that a set of parameters employed by a modified van Genuchten function can nevertheless be found that allows a groundwater simulator to account for the presence of a near-well gas phase reasonably well. Furthermore, the ability of a single-phase model to reproduce CBM-extraction-induced drawdowns appears to be relatively insensitive to the values of individual parameters assigned to this function; so too, but to a slightly lesser extent, is its ability to reproduce water extraction rates. It is important to note that no alterations to any of the hydraulic properties used by the dual-phase reservoir simulator are required when providing these to the single-phase groundwater model employing the modified Richards equation methodology described herein. Thus permeabilities, relative permeabilities, porosities and elastic properties remain unchanged and are therefore consistent between the single and dual-phase models. Therefore (if up-scaling issues are ignored) properties employed by the single-phase model represent the true physical properties of the subsurface media from which CBM extraction takes place.

Implementation of the presented methodology in real-world CBM impact assessment settings relies on the assumption that a modeller can obtain a pre-calculated S_w vs. p relationship. In many cases this will not be a problem, as extensive reservoir modelling will have been carried out by gas companies whose activities require that impact be calculated. S_w vs. p scatterplots such as those depicted in the present paper can be readily obtained from standard output files produced by these models. A modified van Genuchten curve can be easily fitted to these scatterplots. However if reservoir modelling outcomes are unavailable, or if gas companies are unwilling to share such information, useable estimates of parameters required by this modified van Genuchten function can still be made. A residual water saturation of 0.1–0.2 is reasonable in most circumstances (note that this parameter is also required by multi-phase models). The gas bubble point pressure can be readily equated to the pressure at which the Langmuir isotherm releases gas from coal. α and β parameters used by the modified van Genuchten equation (which define the curve characteristics between the residual and full water saturation extremes) can be selected to achieve a water desaturation of 0.3–0.5 at a pressure head somewhat greater than the bottom hole pressure constraint on extraction wells. "Somewhat greater" takes account of the pressure differential between wells and model cells as expressed by Eq. (12). Simulation results presented herein indicate that reasonable impact predictions can be made even with only approximate representations of these values.

In spite of their apparent low sensitivity, uncertainties in parameters used by the modified van Genuchten equation can and should be taken into account when assessing the uncertainties of model predictions of management interest, wherever regional drawdown predictions are made using a model which employs the modified Richards equation approach described herein, as should the uncertainties of all other model parameters. Through undertaking sensitivity analyses such as those documented herein, and/or by employing linear analysis to determine the contributions that different model parameters make to the overall uncertainties of particular model predictions (see, for example, Gallagher and Doherty, 2007), the impact of uncertainties associated with selection of a suitable desaturation curve can be compared with those associated with other error-prone aspects of model construction, particularly those associated with up-scaling.

In spite of the good performance of the modified Richards equation formulation in replicating water-phase pressures computed by a dual-phase reservoir simulator, some problems still remain. One of these is the tendency of the former methodology to over-predict drawdown at early simulation times close to extraction wells. This error is caused by the high levels of desaturation that temporarily exist close to extraction wells; removal of water from pore storage required to achieve this desaturation provides a buffer against rapidly increasing drawdown. This condition is not replicated by the single-phase simulator employed in our study because close to wells, at small simulation times, the pseudo-equilibrium condition which underpins use of a static S_w vs. p relationship is not attained. It may simply need to remain a recognized disadvantage of employing this modelling approach when assessing regional CBM impact at early times close to extraction wells.

Another remaining problem is that of simulating pressures during recovery. The present study suggests that use of the modified Richards equation approach incurs far smaller errors in recovery pressure predictions than those incurred by a standard groundwater flow simulator which does not include such functionality. Nevertheless, simulation of recovery still appears to be somewhat problematical. Fig. 5b demonstrates that the relationship between S_w and p during this time is anything but static. The theoretical basis for use of the methodology described herein is therefore degraded. However this must be seen in perspective. Gas-related processes that accompany CBM drawdown recovery have been studied very little, if at all. Undocumented ECLIPSE runs carried out by the authors suggest that the rate of drawdown recovery is sensitive to (1) the properties of coal measure interburden material and adjacent stratigraphic units, (2) the nature and proximity of boundary conditions, and (3) the rate at which gas diffuses back into the coal matrix once pressure starts to rise. The last of these is a subject of which little is known.

Finally we include a note on run times. Model runs undertaken during the study documented herein demonstrate that MODFLOW-USG and ECLIPSE run times are comparable where the former allows desaturation. Conceptually, an advantage of using a modified Richards equation approach in place of multiphase reservoir simulation is that one would expect the former to run faster, as only one system of equations (for pressure) must be solved rather than two coupled systems of equations (for pressure and saturation). For the six-layer model described herein, ECLIPSE simulation times range between 15 min and 1 h, while MODFLOW-USG simulation times range between 20 min and 1 h. (An Intel I7-2600 CPU running at 3.4 Ghz with a 64-bit operating system was employed.) However simulation times for both MODFLOW-USG and ECLIPSE varied widely. ECLIPSE simulation times tend to increase if larger inter-layer permeability contrasts are introduced, if sloping model layers are introduced, and when high initial gas concentrations are assigned to the coal matrix. MODFLOW-USG simulation times tend to increase if water saturation falls to a low level and if pumping becomes bottom-hole pressure constrained in layers of low (relative) permeability. It is important to note, however, that simulation time comparisons for synthetic models with uniform properties, a small number of extraction wells, and simple boundary conditions may not necessarily be valid in a regional simulation context involving multi-layered models with heterogeneous properties and complex boundary

conditions which include explicit or implicit interaction with surface water systems.

6. Conclusions

CBM impact assessment occupies a unique position in the modelling landscape. It is situated at the boundary between two very different modelling contexts, namely reservoir modelling on the one hand and regional groundwater modelling on the other hand. At the present point in time, it is not served well by software and techniques that have been developed for either of these contexts. State-of-the-art reservoir modelling software is expensive, closed source, requires a specialized skillset to use, and is not well adapted to representation of boundary conditions to which regional groundwater systems are commonly subject. On the other hand, groundwater models cannot simulate processes that are integral to gas extraction, this resulting in a tendency to over-predict impact of this extraction on regional groundwater systems.

The present paper presents a methodology that allows outcomes of reservoir modelling studies to be used by a groundwater model modified to account for the presence of a gas phase. Of importance is the definition of an appropriate relationship between water saturation and reservoir pressure that can be derived from such studies. The latter can be approximated with a modified van Genuchten relationship that enables a groundwater flow model to characterize desaturation. Use of this function allows the groundwater model to predict drawdowns and water extraction rates incurred by CBM extraction reasonably well.

The methodology presented herein allows a groundwater model to be used for regional CBM impact assessment, leaving reservoir modelling to do what it does best, namely perform detailed simulation of flow of gas and water near wells. Saturation vs. pressure relationships emerging from reservoir modelling can be used by a regional groundwater over those parts of its model domain where gas extraction takes place, while it assesses impact over an area that is far larger than the domain of any reservoir model. The impacts of gas extraction on broad scale coal measure sequences, on stratigraphic horizons that overlie and underlie coal measure sequences, and over areas where any of these horizons abut surficial alluvial systems, or interact directly with surface water systems, can thereby be assessed by a model that is primarily constructed for this task.

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