# Heat transport and pressure buildup during carbon dioxide injection into depleted gas reservoirs Simon A. Mathias<sup>1</sup><sup>†</sup>, Jim N. McElwaine<sup>1</sup>, Jon G. Gluyas<sup>1</sup>

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In this article, a two-layer vertical equilibrium model for the injection of  $CO_2$  into a low 7 pressure porous reservoir containing methane and water is developed. The dependent 8 variables solved for include pressure, temperature and CO<sub>2</sub>-CH<sub>4</sub> interface height. In cong trast to previous two-layer vertical equilibrium models in this context, compressibility of 10 all material components is fully accounted for. Non-Darcy effects are also considered us-11 ing the Forchheimer equation. The results show that, for a given injection scenario, as the 12 initial pressure in the reservoir decreases, bpth the pressure buildup and the temperature 13 change increase. A comparison was conducted between a fully coupled non-isothermal 14 numerical model and a simplified model where fluid properties are held constant with 15 temperature. This simplified model was found to provide an excellent approximation 16 when using the injection fluid temperature for calculating fluid properties, even when 17 the injection fluid was as much as  $\pm 15^{\circ}$ C of the initial reservoir temperature. The impli-18 cations are that isothermal models can be expected to provide useful estimates of pressure 19 buildup in this context. Despite the low viscosity of  $CO_2$  at the low pressures studied, 20 21 non-Darcy effects were found to be of negligible concern throughout the sensitivity anal-† Email address for correspondence: s.a.mathias@durham.ac.uk

ysis undertaken. This is because the CO<sub>2</sub> density is also low in this context. Based on these findings, simplified analytic solutions are derived, which accurately calculate both the pressure buildup and temperature decline during the injection period.

# 25 1. Introduction

The potential for storing  $CO_2$  in geological reservoirs continues to attract the atten-26 tion of national greenhouse gas emission reduction strategies around the world. Reservoir 27 types under consideration include saline aquifers, depleted oil reservoirs and depleted gas 28 reservoirs. Saline aquifers have the advantage of being ubiquitous across the world (Ben-29 tham & Kirby 2005). However, depleted oil and gas reservoirs are often heralded due 30 to advantages associated with better levels of current characterization (due to previous 31 oil and gas production) and reduced uncertainty associated with the cap-rock integrity 32 (the trap mechanism has already been demonstrated through the presence of hydro-33 carbon product originally deposited millions of years earlier) (Loizzo et al. 2009). Many 34 depleted gas reservoirs have the added advantage of exceptionally low abandonment pres-35 sures along with highly compressible formation fluids (gas as opposed to oil and water). 36 Estimated  $CO_2$  storage capacities for depleted gas reservoirs have been found to be as 37 much as 13 times higher than those estimated for saline aquifers of equivalent geometries 38 (Barrufet *et al.* 2010). 39

Gas reservoirs within the UK continental-shelf are typically located between 700 m and 3600 m below sea level (Gluyas & Hichens 2003). Reservoir net-thicknesses range from 20 m to 300 m with gas saturations, fairly uniformly distributed within the reservoir units, representing between 50% and 85% of the available pore-space (Gluyas & Hichens 2003). The remainder of the pore-space is generally filled with residually trapped brine.

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<sup>45</sup> Reservoir geometries vary considerably, with the most common being domes or gently
<sup>46</sup> titled slabs, covering regions of up to 250 km<sup>2</sup> (Gluyas & Hichens 2003).

Prior to production, gas reservoirs typically exhibit pressures at or above hydrostatic 47 pressure (generally greater than 10 MPa). Many such reservoirs are highly compartmen-48 talized, exhibiting poor levels of aquifer influx. Consequently, at abandonment, reser-49 voir pressures are often found to be close to atmospheric conditions. Around the world, 50 gas reservoir abandonment pressures commonly range between 0.35 and 0.8 MPa (Mac-51 Roberts 1962; Okwananke et al. 2011). Note that in compartmentalized reservoirs, gas 52 saturations tend to change very little following reservoir depletion, due to the increase 53 in gas volume associated with the pressure decline. 54

A number of recent simulation studies have discussed the interesting thermal effects 55 that develop as a consequence of  $CO_2$  injection into geological reservoirs. These include cooling due to expansion, heating due to compression, heating and cooling due to disso-57 lution and vaporization, respectively, differences in temperature associated with injection 58 and reservoir fluids and heating due to viscous heat dissipation (Oldenburg 2007; Andre 59 et al. 2010; Han et al. 2010). Due to the Joule-Thomson coefficient of  $CO_2$  being larger at 60 lower pressures, such processes are likely to be of greater significance in low pressure de-61 pleted gas reservoirs as opposed to hydrostatic or over-pressured saline aquifers (Mathias 62 et al. 2010). 63

Most previous simulation work relating to  $CO_2$  storage has focused on pressures greater than 10 MPa (e.g. Andre *et al.* 2010; Mathias *et al.* 2013a). Exceptions to these include Han *et al.* (2012) who considered a minimum initial pressure of 6.89 MPa, Ziabaksh–Ganji & Kooi (2014) who assumed an initial pressure of 6 MPa, Afanasyev (2013) who assumed a minimum initial pressure of 4.5 MPa and Singh *et al.* (2011, 2012) who considered an initial pressure of 4 MPa. However, depleted gas reservoirs are often abandoned at

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<sup>70</sup> pressures lower than 1 MPa. Mukhopadhyay *et al.* (2012) presented numerical simulations <sup>71</sup> concerning  $CO_2$  injection into a depleted gas reservoir at 0.5 MPa. However, they ignored <sup>72</sup> thermal effects and considered the reservoir to be of infinite extent. This study seeks <sup>73</sup> to explore the importance of heat transport coupling on pressure buildup estimation <sup>74</sup> during  $CO_2$  injection in low pressure depleted gas reservoirs. Furthermore, non-Darcy <sup>75</sup> effects associated with high velocities around the injection well are incorporated using <sup>76</sup> the Forchheimer equation.

Significant temperature changes are most likely to occur when pressure gradients (in
time and space) are sharpest. This will mostly be the case during the injection period.
Consequently, although many previous CO<sub>2</sub> storage studies have studied the long periods
of time after CO<sub>2</sub> injection has ceased (e.g. Hesse *et al.* 2007, 2008; MacMinn *et al.* 2010,
2011), here it is pertinent only to consider the time prior to injection ceasing.

The outline of this article is as follows: Firstly, the governing equations concerning 82 mass conservation are presented for a system whereby pure  $CO_2$  is injected into a low 83 pressure closed reservoir containing  $CH_4$  and residually trapped water. Expressions for 84 vertically integrated fluxes are derived following the adoption of the Forchheimer equation 85 along with an assumption of vertical equilibrium. A corresponding energy conservation 86 statement is presented. Details of the solution procedure are provided followed by details 87 concerning the obtaining of relevant thermodynamic properties. Further insight is then 88 sought by the deriving of simplified analytic solutions for heat transport and pressure 89 buildup. A sensitivity analysis is then conducted to explore the role of initial pressure and 90 heat flow coupling on pressure buildup during CO<sub>2</sub> injection into low pressure depleted 91 gas reservoirs. Finally the article summarizes and concludes. 92

#### <sup>93</sup> 2. The mathematical model

<sup>94</sup> Consider a fully penetrating vertical injection well of radius,  $r_w$  [L], located at the cen-<sup>95</sup> ter of a horizontally oriented, homogeneous and isotropic, confined cylindrical reservoir <sup>96</sup> of thickness, H [L], and radial extent,  $r_e$  [L]. Four material components are considered <sup>97</sup> and referenced by the subscript, i, which takes the values c for CO<sub>2</sub>, m for CH<sub>4</sub>, w for <sup>98</sup> water and r for rock. A mixture theory is assumed such that all components are consid-<sup>99</sup> ered to exist at every point in space with some volume fraction,  $\theta_i$ . The four material <sup>100</sup> components must satisfy the volume constraint  $\sum_i \theta_i = 1$ .

The reservoir is initially filled with CH<sub>4</sub> alongside a uniform residual saturation of water with volume fraction,  $\theta_w$  [-]. The H<sub>2</sub>O is assumed to be residually trapped and immobile such that  $\theta_w \rho_w$  is constant (Singh *et al.* 2011, 2012). The volume fraction of the rock is  $\theta_r = 1 - \phi$ , where  $\phi$  [-] is the porosity, and the product  $\theta_r \rho_r$  is also constant. The compressibility of all components is allowed for although, as shown later, in the context of this study, the compressibility and thermal expansion of the water and rock are negligible due to the relatively small pressure and temperature changes involved.

The CO<sub>2</sub> is injected at the origin at a constant mass flow rate,  $M_0$  [MT<sup>-1</sup>]. Although 108 the  $CO_2$  and  $CH_4$  are miscible (Ren *et al.* 2000), for simplicity, dispersion and mixing of 109 the two components are ignored and a sharp interface is assumed, located at an elevation 110 of  $h_c$  [L] above the base of the reservoir (similar to Nordbotten & Celia 2006). At 35°C, 111 for pressures ranging between 0.7 MPa and 15 MPa, the densities of  $CO_2$  and  $CH_4$  range 112 between 12 kg/m<sup>3</sup> to 815 kg/m<sup>3</sup> and 4 kg/m<sup>3</sup> to 111 kg/m<sup>3</sup>, respectively (Lemmon et113 al. 2013). The ranges of corresponding dynamic viscosities for  $CO_2$  and  $CH_4$  are 15.5 114  $\mu$ Pa s to 73.6  $\mu$ Pa s and 11.6  $\mu$ Pa s to 16.2  $\mu$ Pa s, respectively (Lemmon *et al.* 2013). 115 Because the  $CO_2$  is denser than the  $CH_4$ ,  $h_c$  represents the thickness of the  $CO_2$  layer. 116 The thickness of the CH<sub>4</sub> layer is then  $h_m = H - h_c$ . 117

Let us denote P(r, t) [ML<sup>-1</sup>T<sup>-2</sup>] and T(r, t) [ $\Theta^{-1}$ ] as the pressure and temperature at the location of the CO<sub>2</sub>-CH<sub>4</sub> interface, respectively, where r [L] is the horizontal radial distance from the center of the injection well and t [T] is time after commencement of injection.

In most cases of physical interest,  $r_e \gg H$ , so it is convenient to make a shallowness 122 assumption (Nordbotten & Celia 2006; Hesse et al. 2007, 2008; MacMinn et al. 2010, 123 2011). This can be rigorously derived as an expansion in  $H/r_e \ll 1$ , but the result is 124 equivalent to assuming vertical equilibrium. It is therefore assumed that the temperature 125 is uniform vertically and identical in the rock,  $CO_2$ ,  $CH_4$  and water. The densities  $\rho_i$ 126  $[ML^{-3}]$  for each fluid species are also assumed to be constant vertically and given by 127 the equation of state evaluated at the interface, that is using P and T. The vertical 128 momentum equation is then simplified by assuming an equilibrium between gravity and 129 hydrostatic pressure such that (Hesse *et al.* 2007) 130

$$P(r, z, t) = \begin{cases} P(r, t) + \rho_c g(h_c - z), & 0 \le z \le h_c, \\ P(r, t) + \rho_m g(h_c - z), & h_c < z \le H, \end{cases}$$
(2.1)

where P [ML<sup>-1</sup>T<sup>-2</sup>] is the local pressure,  $\rho_c$  [ML<sup>-3</sup>] and  $\rho_m$  [ML<sup>-3</sup>] are the densities of CO<sub>2</sub> and CH<sub>4</sub>, respectively, g [LT<sup>-2</sup>] is gravitational acceleration and z [L] is the height above the base of the reservoir. After depth integrating, the primary dependent variables of our model then become P(r, t), T(r, t) and  $h_c(r, t)$ . Some general features of the conceptual model are illustrated further in Figure 1.

Note that assuming the fluids are incompressible, ignoring heat transport and temperature changes and ignoring the density difference between the different components, such a problem reduces to the classic Buckley & Leverett (1942) equation, where relative permeability is assumed to be a linear function of  $h_c$  and  $h_c$  is equivalent to fluid saturation.

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FIGURE 1. Schematic diagram of conceptual model.

#### 2.1. Mass conservation

 $_{142}$  The depth integrated mass conservation equation for the CO<sub>2</sub> and CH<sub>4</sub> can be written

$$\frac{\partial}{\partial t} \left( \theta_i \rho_i h_i \right) = -\frac{1}{r} \frac{\partial}{\partial r} (r \rho_i Q_i) \equiv R_i, \tag{2.2}$$

where  $R_i$  [ML<sup>-2</sup>T<sup>-1</sup>] denotes the right-hand-side of equation (2.2) and the vertically integrated volume fluxes,  $Q_i$  [L<sup>2</sup>T<sup>-1</sup>], are defined as

$$Q_c = \int_0^{h_c} q_c \, dz, \quad \text{and} \quad Q_m = \int_{h_c}^H q_m \, dz,$$
 (2.3)

and  $q_i$  [LT<sup>-1</sup>] are the respective volume fluxes.

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#### <sup>146</sup> 2.1.1. Determination of the vertically integrated volume fluxes

Volume fluxes, in the context of simulating  $CO_2$  storage problems, are generally calculated using Darcy's law. However, due to the lower dynamic viscosity of  $CO_2$  at the relevant pressures of concern, it is pertinent to consider Non-Darcian losses using the Forchheimer equation (Zeng & Grigg 2006). Therefore the fluxes  $q_i$  are defined by the <sup>151</sup> Forchheimer equation

$$\frac{\mu_i q_i}{kk_{rg}} + \rho_i b q_i |q_i| + \frac{\partial P}{\partial r} = 0, \qquad \begin{array}{l} 0 \le z \le h_c \quad \text{when } i = c \\ h_c < z \le H \quad \text{when } i = m \end{array}$$

$$(2.4)$$

where k [L<sup>2</sup>] is the reservoir permeability,  $k_{rg}$  [-] is the relative permeability of the gas, which is treated uniform and constant, b [L<sup>-1</sup>] is the Forchheimer coefficient and  $\mu_i$ [ML<sup>-1</sup>T<sup>-1</sup>] are the dynamic viscosities of CO<sub>2</sub> and CH<sub>4</sub>. Denoting  $J = \partial P / \partial r < 0$ , the appropriate positive real root can be written as

$$q_i = -\frac{kk_{rg}}{\mu_i} \left(\frac{2J}{1 + (1 - \epsilon_i J)^{1/2}}\right),$$
(2.5)

156 where

$$\epsilon_i = 4\rho_i b \left(\frac{kk_{rg}}{\mu_i}\right)^2. \tag{2.6}$$

<sup>157</sup> A Maclaurin series expansion about small  $\epsilon_i J$  leads to

$$q_i = -\left[1 + \epsilon_i J/4 + O(\epsilon_i^2 J^2)\right] \frac{k k_{rg} J}{\mu_i},\tag{2.7}$$

from which it can be seen that the accuracy of the Darcy approximation is given by the size of the non-dimensional group  $\epsilon_i J$ . The issue for radially divergent (and convergent) flow problems, J becomes very large as one approaches the origin (the injection well in this case). Therefore, it is not clear whether non-Darcy effects can be ignored from information about  $\epsilon_i$  alone.

<sup>163</sup> Note that the uniform relative permeability values,  $k_{rg}$ , assumed for CO<sub>2</sub> and CH<sub>4</sub> are <sup>164</sup> equivalent to the end-point relative permeability for gas in a two-phase relative perme-<sup>165</sup> ability function,  $k_{rg0}$  [-] (e.g. Mathias *et al.* 2013a). In this article, for simplicity, CO<sub>2</sub> <sup>166</sup> and CH<sub>4</sub> are assumed to have the same relative permeabilities. In reality, they may have <sup>167</sup> different relative permeabilities due to differences in interfacial tension (IFT) and con-<sup>168</sup> tact angle associated with CO<sub>2</sub>-brine and CH<sub>4</sub>-brine mixtures. Bachu & Bennion (2008a) <sup>169</sup> observed a set of  $k_{rg0}$  values for the same sandstone core, ranging from 0.298 to 0.526,

for CO<sub>2</sub>-brine mixtures with IFT ranging from 56.2 mN/m to 19.8 mN/m, respectively (IFT was varied by increasing the fluid pressure from 1.378 MPa to 20 MPa). At 40°C and 1 MPa of pressure, the IFT for CO<sub>2</sub>-water and CH<sub>4</sub>-waters mixtures are around 90.95 mN/m (Bachu & Bennion 2008b) and 69.06 mN/m (Ren *et al.* 2000), respectively. Therefore, relative permeabilities for CO<sub>2</sub>-brine and CH<sub>4</sub>-brine mixtures can be expected to be quite different. However, ignoring this difference is unlikely to significantly affect the main findings discussed hereafter.

The system is assumed to be initially free of  $CO_2$ . Fluid pressure is assumed initially uniform in the radial direction, at a value of  $P_0$  at the base of the reservoir. The reservoir is confined on all sides by impermeable boundaries. Following, among others, Oldenburg (2007), Mathias *et al.* (2009), Han *et al.* (2010) and Mukhopadhyay *et al.* (2012), a constant mass flux of pure  $CO_2$  is applied at the injection well boundary. Such conditions are described mathematically as follows:

$$h_{c} = 0, r_{w} \leq r \leq r_{e}, t = 0,$$

$$P = P_{0}, r_{w} \leq r \leq r_{e}, t = 0,$$

$$Q_{c} = M_{0}/(2\pi r_{w}\rho_{c}), r = r_{w}, t > 0,$$

$$Q_{m} = 0, r = r_{w}, t > 0,$$

$$Q_{c} = 0, r = r_{e}, t > 0,$$

$$Q_{m} = 0, r = r_{e}, t > 0,$$

$$Q_{m} = 0, r = r_{e}, t > 0,$$

where  $P_0$  [ML<sup>-1</sup>T<sup>-2</sup>] is the initial pressure at the base of the reservoir.

Differentiating equation (2.1) with respect to r gives

$$J \equiv \frac{\partial P}{\partial r} = \begin{cases} \frac{\partial}{\partial r} (P + \rho_c g h_c) - g z \frac{\partial \rho_c}{\partial r}, & 0 \le z \le h_c \\ \\ \\ \frac{\partial}{\partial r} (P - \rho_m g h_m) - g z \frac{\partial \rho_m}{\partial r}, & h_c < z \le H \end{cases}$$
(2.9)

showing that J is a linear function of z given the shallowness assumption that the fluid

densities are uniform with depth. The flux equation (2.5) can then be substituted into

 $_{187}$  equation (2.3) and integrated to give

$$Q_i = -\frac{h_i k k_{rg}}{\mu_i} \left[ \frac{(1 - \epsilon_i J_{i2})^{3/2} - (1 - \epsilon_i J_{i1})^{3/2}}{3\epsilon_i^2 (J_{i2} - J_{i1})/4} + \frac{2}{\epsilon_i} \right]$$
(2.10)

188 where

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$$J_{c1} = \frac{\partial}{\partial r} (P + \rho_c g h_c), \ J_{c2} = J_{c1} - g h_c \frac{\partial \rho_c}{\partial r},$$
$$J_{m1} = \frac{\partial}{\partial r} (P - \rho_m g h_m) - g h_c \frac{\partial \rho_m}{\partial r}, \ J_{m2} = J_{m1} - g h_m \frac{\partial \rho_m}{\partial r}.$$
(2.11)

As written in equation (2.10), these fluxes appear singular for  $\epsilon_i = 0$ . However, further rearranging reveals that

$$Q_i = -\frac{h_i k k_{rg}}{\mu_i} \left( \frac{X_{i2} - X_{i1}}{J_{i2} - J_{i1}} \right), \quad X_{ij} = \frac{J_{ij}^2 (1 - 4\epsilon_i J_{ij}/3)}{(1 - \epsilon_i J_{ij})^{3/2} + 1 - 3\epsilon_i J_{ij}/2}, \quad j = 1, 2.$$
(2.12)

<sup>191</sup> Also note that for slightly compressible fluids (i.e., where fluid properties do not change <sup>192</sup> much with space and time)  $J_{i2} - J_{i1} \rightarrow 0$ , and equation (2.12) can be expanded to obtain

$$Q_{i} = -\frac{h_{i}kk_{rg}}{\mu_{i}} \left\{ \frac{2J_{iA}}{1 + (1 - \epsilon_{i}J_{iA})^{1/2}} + \frac{J_{iB}}{(1 - \epsilon_{i}J_{iA})^{1/2}} \left[ \frac{\Upsilon_{i}}{12} + \frac{\Upsilon_{i}^{3}}{64} + O(\Upsilon_{i}^{5}) \right] \right\}$$
(2.13)

193 where

$$J_{iA} = \frac{J_{i2} + J_{i1}}{2}, \quad J_{iB} = \frac{J_{i2} - J_{i1}}{2} \quad \text{and} \quad \Upsilon_i = \frac{\epsilon_i J_{iB}}{1 - \epsilon_i J_{iA}}.$$
 (2.14)

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# 2.2. Re-casting in terms of the primary dependent variables

The left-hand-side of equation (2.2) can be expanded in terms of the primary dependent variables of our model, P, T and  $h_c$ , such that:

$$\theta_i \rho_i h_i \left[ \left( \frac{1}{\theta_i} \frac{\partial \theta_i}{\partial P} + \frac{1}{\rho_i} \frac{\partial \rho_i}{\partial P} \right) \frac{\partial P}{\partial t} + \left( \frac{1}{\theta_i} \frac{\partial \theta_i}{\partial T} + \frac{1}{\rho_i} \frac{\partial \rho_i}{\partial T} \right) \frac{\partial T}{\partial t} + \frac{1}{h_i} \frac{\partial h_i}{\partial h_c} \frac{\partial h_c}{\partial t} \right] = R_i \quad (2.15)$$

197 where

$$\frac{\partial h_i}{\partial h_c} = \begin{cases} 1, & i = c \\ -1, & i = m \end{cases}$$
(2.16)

Imposing the constraints that the products  $\theta_w \rho_w$  and  $\theta_r \rho_r$  are constant and that  $\sum_i \theta_i = 1$ , it can be shown that for i = c or m:

$$\frac{\partial \theta_i}{\partial P} = \frac{\theta_w}{\rho_w} \frac{\partial \rho_w}{\partial P} + \frac{\theta_r}{\rho_r} \frac{\partial \rho_r}{\partial P} \quad \text{and} \quad \frac{\partial \theta_i}{\partial T} = \frac{\theta_w}{\rho_w} \frac{\partial \rho_w}{\partial T} + \frac{\theta_r}{\rho_r} \frac{\partial \rho_r}{\partial T}$$
(2.17)

Now consider an isothermal compressibility,  $\alpha_i$  [M<sup>-1</sup>LT<sup>2</sup>], and an isobaric expansivity  $\beta_i$  [ $\Theta^{-1}$ ], for each of the four material components, defined as:

$$\alpha_i = \frac{1}{\rho_i} \left( \frac{\partial \rho_i}{\partial P} \right)_T \quad \text{and} \quad \beta_i = -\frac{1}{\rho_i} \left( \frac{\partial \rho_i}{\partial T} \right)_P \tag{2.18}$$

 $_{202}$  such that substitution of equation (2.17) into equation (2.15) leads to

$$\rho_i \left[ h_i \left( \alpha_{Ei} \frac{\partial P}{\partial t} - \beta_{Ei} \frac{\partial T}{\partial t} \right) + \theta_i \frac{\partial h_i}{\partial h_c} \frac{\partial h_c}{\partial t} \right] = R_i$$
(2.19)

203 where

$$\alpha_{Ei} = \theta_i \alpha_i + \theta_w \alpha_w + \theta_r \alpha_r \quad \text{and} \quad \beta_{Ei} = \theta_i \beta_i + \theta_w \beta_w + \theta_r \beta_r. \tag{2.20}$$

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# 2.3. Energy conservation

As mentioned above, pressure is assumed to be in a vertical equilibrium whilst the temperature and fluid properties are assumed to be vertically uniform. Consequently, heat transport is a one-dimensional process. An appropriate statement of energy conservation can therefore be written as (consider Chapter 2 of Nield & Bejan 2006):

$$\rho_E c_{pE} \frac{\partial T}{\partial t} - \beta_E T \frac{\partial P}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa_E \frac{\partial T}{\partial r} \right) - \left( \frac{\rho_c c_{pc} Q_c + \rho_m c_{pm} Q_m}{H} \right) \frac{\partial T}{\partial r} + \left[ \frac{(T \beta_c - 1) Q_c + (T \beta_m - 1) Q_m}{H} \right] \frac{\partial P}{\partial r} \equiv R_e$$
(2.21)

where  $R_e [ML^{-1}T^{-3}]$  is used to denote the right-hand-side of equation (2.21) and

$$\rho_E c_{pE} = \theta'_c \rho_c c_{pc} + \theta'_m \rho_m c_{pm} + \theta_w \rho_w c_{pw} + \theta_r \rho_r c_{pr},$$
  

$$\beta_E = \theta'_c \beta_c + \theta'_m \beta_m + \theta_w \beta_w + \theta_r \beta_r,$$
(2.22)  

$$\kappa_E = \theta'_c \kappa_c + \theta'_m \kappa_m + \theta_w \kappa_w + \theta_r \kappa_r,$$

with  $c_{pi}$  [L<sup>2</sup>T<sup>-2</sup> $\Theta^{-1}$ ],  $\beta_i$  [ $\Theta^{-1}$ ],  $\kappa_i$  [MLT<sup>-3</sup> $\Theta^{-1}$ ] being constant-pressure-specific-heatcapacity, thermal expansivity and thermal conductivity for the four material components, respectively and  $\theta'_c = \theta_c h_c / H$  and  $\theta'_m = \theta_m h_m / H$  are the depth weighted volume fractions for the CO<sub>2</sub> and CH<sub>4</sub>, respectively.

Note that the -1 in the  $(T\beta_i - 1)Q_i$  terms in equation (2.21) comes about due to shear heating associated with fluid movement. See Chapter 2 of Nield & Bejan (2006) for further discussion on this matter.

Also note that the expression for  $\kappa_E$  represents a significant overestimate of the conductivity for this composite medium. For further discussion concerning effective conductivity estimation, the reader is directed to the work of Zimmerman (1989). However, even with this upper bound estimate, conduction has been found to be of negligible effect in this context.

# <sup>222</sup> The initial and boundary conditions are:

$$T = T_0, \qquad r_w \le r \le r_e, \quad t = 0$$
  

$$T = T_w, \qquad r = r_w, \qquad t > 0$$
  

$$\partial T/\partial r = 0, \quad r = r_e, \qquad t > 0,$$
  
(2.23)

where  $T_0 \ [\Theta]$  is the vertically averaged initial temperature of the reservoir and  $T_w \ [\Theta]$  is the temperature of the injection fluid.

# 2.4. Solution by method of lines

Equations (2.19) and (2.21) now form a set of three, first order, quasi-linear, parabolic partial differential equations that can be written as:

$$\begin{pmatrix} \rho_c h_c \alpha_{Ec} & -\rho_c h_c \beta_{Ec} & \theta_c \rho_c \\ \rho_m h_m \alpha_{Em} & -\rho_m h_m \beta_{Em} & -\theta_m \rho_m \\ -\beta_E T & \rho_E c_{pE} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial P}{\partial t} \\ \frac{\partial T}{\partial t} \\ \frac{\partial h_c}{\partial t} \end{pmatrix} = \begin{pmatrix} R_c \\ R_m \\ R_e \end{pmatrix}$$
(2.24)

Equation (2.24) represents a set of three linear equations in the time derivative of the primary variables P, T, and  $h_c$ , which can be solved to give an equation for each time derivative separately provided that the Jacobian does not vanish, which does not occur for  $0 < h_c < H$ . A method of lines approach is adopted, using a first-order backward difference spatial discretisation and integrating the resulting set of ordinary differential equations with respect to time using the MATLAB ODE solver, ODE15s. A similar approach was previously adopted by Mathias *et al.* (2008, 2009).

## 2.5. Fluid and rock properties

Because interactions between the CO<sub>2</sub> and CH<sub>4</sub>, H<sub>2</sub>O are ignored, only pure component fluid properties are required. These can be obtained using the online NIST web-book developed by Lemmon *et al.* (2013). Parameters available from the web-book include  $\rho_i, c_{pi}, \mu_i, \kappa_i$  in addition to the constant-volume-specific-heat-capacity,  $c_{Vi}$  [L<sup>2</sup>T<sup>-2</sup> $\Theta^{-1}$ ], and the Joule-Thomson coefficient,  $\mu_{JTi}$  [M<sup>-1</sup>LT<sup>2</sup> $\Theta$ ]. Invoking the Maxwell relations, compressibility,  $\alpha_i$ , and thermal expansivity,  $\beta_i$ , can be obtained from (Cengel & Boles 2002, p. 627)

$$\alpha_i = \frac{T\beta_i^2}{\rho_i(c_{pi} - c_{vi})} \quad \text{and} \quad \beta_i = \frac{\rho_i c_{pi} \mu_{JTi} + 1}{T}$$
(2.25)

Intensive lookup tables can be developed for the three fluids for a wide range of temperatures and pressures, prior to running the numerical model. These can then be linearly

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interpolated within the ODE solver during simultaneous solution of the aforementionedPDEs.

Thermal properties of the reservoir formation are taken from Oldenburg (2007) where available. These include density,  $\rho_r = 2600 \text{ kg m}^{-3}$ , constant-pressure-specific-heat-capacity,  $c_{pr} = 1000 \text{ J kg}^{-1}\text{K}^{-1}$ , thermal conductivity,  $\kappa_r = 2.51 \text{ W m}^{-1}\text{ K}^{-1}$ . A volumetric thermal expansivity of  $\beta_r = 39 \times 10^{-6} \text{ K}^{-1}$  is assumed, based on the linear thermal expansion coefficient (TEC) value provided for a water saturated Berea sandstone in Table IV-2 of Somerton (1992) (also see Somerton *et al.* 1981) (note that the volumetric TEC is three times the linear TEC, see for example Zimmerman (2000)).

Typically, rock compressibility is parameterized by a coefficient,  $c_r = (\theta_r - 1)^{-1} (d\theta_r/dP)_T$ (e.g. Chen *et al.* 2006). But in the current situation, the rock compressibility is defined as  $\alpha_r = \rho_r^{-1} (d\rho_r/dP)_T$ . Given that the rock is static, the product  $\theta_r \rho_r$  must be a constant. Therefore it can be shown that  $\alpha_r = (1 - \theta_r)\theta_r^{-1}c_r$ . Mathias *et al.* (2011b) previously assumed  $\theta_r = 0.8$  and  $\alpha_r = 4.5 \times 10^{-10}$  Pa<sup>-1</sup>. This corresponds to a value of  $\alpha_r = 1.125 \times 10^{-10}$  Pa<sup>-1</sup>.

# 260 3. Analytic Solutions

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# 3.1. Heat transport

The above problem refers to a system whereby  $CO_2$  displaces  $CH_4$ . However, the thermal front resulting from  $CO_2$  injection is generally behind the  $CO_2$ - $CH_4$  interface due to heat retardation associated with the specific capacity of the host rock and residually trapped water. Furthermore, although there are large changes in pressure resulting from the injection process, for constant mass injection rates, these mostly occur at the beginning of injection (consider Mathias *et al.* 2011b). Consequently, when considering the development of analytical solutions for heat transport in this context, Mathias *et al.* (2010)

argues one can additionally assume that (1) the presence of the  $CH_4$  can be ignored and (2) the pressure distribution is steady state. For mathematical tractability, Mathias *et al.* (2010) further assumes the fluid properties to be constant and uniform, and that heat conduction is negligible. In this way, equation (2.21) reduces to

$$\left(\theta_c \rho_c c_{pc} + \theta_w \rho_w c_{pw} + \theta_r c_{pr}\right) \frac{\partial T}{\partial t} = \rho_c q_c c_{pc} \left(\mu_{JTc} \frac{\partial P}{\partial r} - \frac{\partial T}{\partial r}\right)$$
(3.1)

 $_{273}$  and the profile for  $q_c$  becomes

$$q_c = \frac{M_0}{2\pi H \rho_c r}.$$
(3.2)

Substituting equation (2.4) into equation (3.1) then leads to

$$\frac{\partial T_D}{\partial \tau} + \frac{\partial T_D}{\partial \xi} = -\frac{1}{2\xi} - \frac{b_D}{(2\xi)^{3/2}} \tag{3.3}$$

<sup>275</sup> subject to the initial and boundary conditions:

$$T_D = 0, \qquad \xi > 1/2, \quad t_D = 0,$$
  

$$T_D = T_{wD}, \quad \xi = 1/2, \quad t_D > 0,$$
(3.4)

276 where

$$\tau = \frac{M_0 c_{pc} t}{2\pi H r_w^2 (\theta_c \rho_c c_{pc} + \theta_w \rho_w c_{pw} + \theta_r c_{pr})},\tag{3.5}$$

$$\xi = \frac{1}{2} \left(\frac{r}{r_w}\right)^2, \quad T_D = \frac{2\pi H \rho_c k k_{rg} (T - T_0)}{\mu_c \mu_{JTc} M_0}, \quad T_{wD} = \frac{2\pi H \rho_c k k_{rg} (T_w - T_0)}{\mu_c \mu_{JTc} M_0}, \quad (3.6)$$

$$b_D = \frac{kk_{rg}M_0b}{2\pi H\mu_c r_w}.$$
(3.7)

$$\frac{dT_D}{d\tau} = \frac{\partial T_D}{\partial \tau} + \frac{d\xi}{d\tau} \frac{\partial T_D}{\partial \xi}.$$
(3.8)

Consider  $d\xi/d\tau = 1$  such that  $\xi = \tau + \xi_0$ , where  $\xi_0 = \xi(\tau = 0)$ . By setting  $d\xi/d\tau = 1$ and comparing to equation (3.3) it can then be said that

$$\frac{dT_D}{d\tau} = -\frac{1}{2(\tau + \xi_0)} - \frac{b_D}{(2(\tau + \xi_0))^{3/2}}.$$
(3.9)

Integrating equation (3.9) with respect to  $\tau$ , applying applying the initial condition in Equation (3.4) and then substituting  $\xi_0 = \xi - \tau$  yields

$$T_D(\xi(\tau),\tau) = -\frac{1}{2}\ln\left(\frac{\xi}{\xi-\tau}\right) + \frac{b_D}{2^{1/2}}\left[\frac{1}{\xi^{1/2}} - \frac{1}{(\xi-\tau)^{1/2}}\right].$$
 (3.10)

In a similar way, the complete derivative with respect to  $\xi$  can be written

$$\frac{dT_D}{d\xi} = \frac{d\tau}{d\xi}\frac{\partial T_D}{\partial \tau} + \frac{\partial T_D}{\partial \xi} = -\frac{1}{2\xi} - \frac{b_D}{(2\xi)^{3/2}}.$$
(3.11)

Integrating equation (3.11) with respect to  $\xi$  and applying the boundary condition in equation (3.4) yields

$$T_D(\xi, \tau(\xi)) = T_{wD} - \frac{1}{2}\ln(2\xi) + b_D \left[\frac{1}{(2\xi)^{1/2}} - 1\right].$$
(3.12)

The two solutions are separated in the  $\xi\tau$ -plane by the characteristic line,  $\tau = \xi - 1/2$ . It follows that the solution for the domain defined in equation (3.4) is fully described by  $CO_2$  injection in depleted gas reservoirs

$$T_{D} = \begin{cases} -\frac{1}{2} \ln\left(\frac{\xi}{\xi - \tau}\right) + \frac{b_{D}}{2^{1/2}} \left[\frac{1}{\xi^{1/2}} - \frac{1}{(\xi - \tau)^{1/2}}\right], & \xi - \tau > \frac{1}{2} \\ T_{wD} - \frac{1}{2} \ln(2\xi) + b_{D} \left[\frac{1}{(2\xi)^{1/2}} - 1\right], & \xi - \tau \le \frac{1}{2} \end{cases}$$
(3.13)  
en  $h_{D} = 0$  equation (3.13) is identical to the result previously presented by Mathias

When  $b_D = 0$ , equation (3.13) is identical to the result previously presented by Mathias et al. (2010), obtained by Laplace transform and assuming Darcy's law.

#### 3.2. Pressure buildup

Disregarding statements made in the previous section, following Mukhopadhyay *et al.* (2012), consider the additional assumptions: (1) the difference between the  $CH_4$  and  $CO_2$  properties is negligible, (2) temperature changes are negligible and (3) the water and rock are incompressible. The mass conservation equations reduces to

$$\theta_c \rho_c \alpha_c \frac{\partial P}{\partial t} = -\frac{1}{r} \frac{\partial}{\partial r} \left( r \rho_c q_c \right) \tag{3.14}$$

<sup>295</sup> subject to the initial and boundary conditions:

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$$P_{I} = P_{0}, \qquad r_{w} \leq r \leq r_{e}, \quad t = 0,$$
  

$$\rho_{c}q_{c} = M_{0}/(2\pi H r_{w}), \quad r = r_{w}, \qquad t > 0,$$
  

$$\rho_{c}q_{c} = 0, \qquad r = r_{e}, \qquad t > 0.$$
  
(3.15)

The above PDE is non-linear due to the dependence of  $\rho_c$ ,  $\alpha_c$  and  $\mu_c$  on P. Mukhopadhyay *et al.* (2012) linearize the above the equation by imposing a Pitzer correlation for the relationship between  $\rho_c$  and P. The linearized PDE is then solved in Laplace transform space and inverted back to the time-domain to obtain an analytical solution for Pin the form of an integral equation, which is evaluated numerically.

An arguably more simple route to solution of equation (3.14) is to invoke the pseudo-

pressure concept of Al–Hussainy *et al.* (1996), whereby a pseudo-pressure,  $\psi$  [ML<sup>-3</sup>T<sup>-1</sup>], is defined by the derivative

$$\frac{d\psi}{dP} = \frac{\rho_c}{\mu_c} \tag{3.16}$$

 $_{304}$  such that the Forchheimer equation, equation (2.4), along with equation (3.14) transform  $_{305}$  to

$$\frac{(\rho_c q_c)}{kk_{rg}} + \frac{b}{\mu_c} (\rho_c q_c)^2 + \frac{\partial \psi}{\partial r} = 0, \qquad (3.17)$$

$$\theta_c \alpha_c \mu_c \frac{\partial \psi}{\partial t} = -\frac{1}{r} \frac{\partial}{\partial r} \left( r \rho_c q_c \right). \tag{3.18}$$

Al-Hussainy *et al.* (1996) propose that the  $\alpha_c \mu_c$  term in equation (3.18) can be approximated as a constant based on fluid properties obtained at a pressure half way between the minimum and maximum pressures being considered. Mukhopadhyay *et al.* (2012) identify this feature as a disadvantage. However, application of the pseudo-pressure concept in conjunction with the pseudo-time concept of Agarwal (1979) leads to a significant improvement.

Agarwal (1979) provides a pseudo-time,  $\eta$  [-], defined by the derivative

$$\frac{d\eta}{dt} = \frac{1}{\alpha_c \mu_c} \tag{3.19}$$

 $_{313}$  such that equation (3.18) reduces to

$$\theta_c \frac{\partial \psi}{\partial \eta} = -\frac{1}{r} \frac{\partial}{\partial r} \left( r \rho_c q_c \right). \tag{3.20}$$

The relationship between  $\psi$  and P is obtained by numerically evaluating the integral

$$\psi = \int_{P_0}^{P} \frac{\rho_c}{\mu_c} dP. \tag{3.21}$$

The relationship between  $\eta$  and t requires more creativity. The difficulty is that  $\mu_c$  and  $\alpha_c$  vary in both time and space. However, a good approximation for  $\eta$  can be obtained by assuming P is uniform in space, such that

$$\pi H r_e^2 \theta_c \frac{d\rho_c}{dt} \approx M_0, \qquad (3.22)$$

318 which on integration yields

$$\pi H r_e^2 \theta_c (\rho_c - \rho_{c0}) \approx M_0 t, \qquad (3.23)$$

thus providing an approximate relationship between  $\rho_c$  and t. Note that  $\rho_{c0} = \rho_c (P = \rho_c)$ <sub>320</sub>  $P_0$ .

Dividing equation (3.19) by (3.22) leads to

$$\frac{d\eta}{d\rho_c} \approx \frac{\pi H r_e^2 \theta_c}{M_0 \alpha_c \mu_c},\tag{3.24}$$

which on integration yields an approximate relationship between  $\eta$  and  $\rho_c$ .

$$\eta \approx \frac{\pi H r_e^2 \theta_c}{M_0} \int_{\rho_{c0}}^{\rho_c} \frac{1}{\alpha_c \mu_c} d\rho_c.$$
(3.25)

Considering an identical problem but with slightly compressible fluids (e.g. Mathias *et al.* 2008; Mijic *et al.* 2013), the analytical solution for the problem defined by above the system of equations can be written as

$$\psi - \psi_0 = \frac{M_0}{2\pi H k k_r} \left[ W + \bar{b}_D r_w \left( \frac{1}{r} - \frac{16}{5r_e} + \frac{2r}{r_e^2} - \frac{r^3}{3r_e^4} \right) \right]$$
(3.26)

326 where

$$W = \begin{cases} \frac{1}{2} E_1 \left( \frac{\eta_e r^2}{4\eta r_e^2} \right), & \eta_0 < \eta < 0.2423 \eta_e \\ \\ \frac{2\eta}{\eta_e} + \frac{r^2}{2r_e^2} - \ln\left(\frac{r}{r_e}\right) - \frac{3}{4}, & \eta \ge 0.2423 \eta_e \end{cases}$$

$$\eta_e = \frac{\theta_c r_e^2}{kk_{rg}}$$
(3.28)

327 and

$$\bar{b}_D = \frac{kk_{rg}M_0b}{2\pi H\bar{\mu}_c r_w} \tag{3.29}$$

where  $\bar{\mu}_c$  is an estimate of an equivalent constant CO<sub>2</sub> viscosity and (Mathias & Todman 229 2010)

$$\eta_0 \approx \eta_e \left(\frac{r_w}{r_e}\right)^2 \left[\frac{(2\pi/\bar{b}_D)^2}{7 \times 10^3} + \frac{(2\pi/\bar{b}_D)^{1/2}}{3 \times 10^7}\right]^{-1}.$$
(3.30)

# **330 4.** Numerical Solutions

Numerical solutions for the full equation were performed to explore and compare the 331 pressure and temperature response. Sensitivity analysis was undertaken around a base 332 case described by the parameters given in Table 1. These parameter are considered to be 333 typical of many depleted gas reservoirs around the UK continental shelf. The constant 334  $CO_2$  injection rate of 0.3 Mt/year is based on a recommendation made by Mathias *et al.* 335 (2013b), following a statistical analysis of historical oil and gas production rates in the 336 UK continental shelf. The numerical models employ a radial grid, discretised using 200 337 equal intervals in  $\log_{10}$  space, from  $r_w$  to  $r_e$ . The Forchheimer parameter, b, is calculated 338 using the correlation of Geertsma (1974)339

$$b = 0.005 \,\theta_g^{-5.5} (kk_{rg})^{-0.5} \tag{4.1}$$

	Formation thickness,	$H=150~{\rm m}$
	Permeability,	$k=100~{\rm mD}$
	Relative permeability,	$k_{rg} = 0.6$
	$\mathrm{CO}_2$ injection rate,	$M_0 = 0.3 \text{ Mt/year}$
	Initial pressure,	$P_0 = 0.7 \text{ MPa}$
	Radial extent of reservoir,	$r_e=3000~{\rm m}$
	Well radius,	$r_w = 0.1 \text{ m}$
	Residual water content,	$\theta_w = 0.05$
	Initial temperature,	$T_0 = 35^{\circ}\mathrm{C}$
	Injection temperature,	$T_w = 35^{\circ}\mathrm{C}$
	Volume fraction of rock,	$\theta_r = 0.8$
TABLE 1. Parameter values assumed for base case		

Simulation output for the aforementioned base case are presented in Fig. 2. The constant injection of  $CO_2$  leads to an increase in fluid pressure. The  $CO_2$  front pushes the methane radially outward. Fluid pressure is greatest at the injection well. Consequently, the  $CO_2$  expands as it moves away from the injection well and experiences lower pressures. This leads to Joule-Thomson cooling, which cools both the fluid and rock behind the front. These changing temperatures and pressures lead to increases/decreases in relevant fluid properties, which feedback to the fluid dynamics of the system.

Fig. 2a shows the pressure distribution (measured at the base of the reservoir, *i.e.*,  $P + \rho_c g h_c$ ) at different times. Pressure conforms to a logarithmic relationship, consistent with radially symmetric problems associated with single-phase and slightly compressible fluids (e.g. Mijic *et al.* 2013). The pressure wave meets the outer boundary of the reservoir, at  $r = r_e$ , just after one year, the pressure is then seen to increase across the reservoir. Fig. 2b shows temperature distributions for different times. Near to the well, temper-



FIGURE 2. Results from the base case simulation (see Table 1) including plots of: a) pressure at the base of the reservoir, b) temperature and c) the  $CO_2$ -CH<sub>4</sub> interface height against radial distance for various times, as indicated in the legends.

ature declines with increasing distance according to a logarithmic relationship, similar to the analytical solution previously derived by Mathias *et al.* (2010). Finally, some distance away from the well, temperature recovers back to the initial temperature. The temperature decline occurs due to the expansion of the  $CO_2$  as it migrates away from the injection well and experiences continuously decreasing pressures.

Fig. 2c shows the geometry of the  $CO_2$ -CH<sub>4</sub> interface at different times, which takes the form of a moderately dispersed front. The dispersion is partly due to the gravity effects associated with the diffusive-like derivative of  $h_c$  in equation (2.11). Dispersion is also brought about due to the mobility difference between the CO<sub>2</sub> and CH<sub>4</sub> (consider Nordbotten & Celia 2006). As discussed in Section 3.1, all the changes in temperature induced by CO<sub>2</sub> injection reside far behind the CO<sub>2</sub>-CH<sub>4</sub> interface due to the retarding effect of the combined heat capacity of the rock, water and CO<sub>2</sub>.

Fig. 3 presents results from a sensitivity analysis around the base case described para-365 metrically in Table 1. Subplots a, c, e and g show plots of change in bottom hole pressure 366 in the injection well (*i.e.*,  $P(r = r_w) + \rho_c g h_c - P_0$ ). Subplots b, d, f and h show plots of 367 temperature against distance after 20 years of injection. The solid lines are from the fully 368 coupled numerical model (hereafter referred to as non-isothermal). The circular dots are 369 from a simplified form of the numerical model whereby all fluid properties are held con-370 stant with temperature according to the injection fluid temperature (hereafter referred 371 to as isothermal). The dashed lines are results from the analytical solutions presented in 372 Sections 3.1 and 3.2. 373

Figs. 3a and b show results looking at sensitivity to permeability. Note that an increase in permeability has a similar effect to an increase in formation thickness and/or a decrease in injection rate. Decreasing permeability leads to increased well pressures and spatial pressure gradients. Consequently decreasing permeability leads to increased



FIGURE 3. Presentation of the sensitivity analysis around the base case described in Table 1 for: a) and b) permeability, c) and d) injection fluid temperature, e) and f) non-Darcy effects, and g) and h) initial pressure, as indicated in the legends. Plots a), c), e) and g) show plots of change in bottom hole pressure against time. Plots b), d), f) and h) show plots of temperature against radial distance after 20 years of injection. The solid lines, circular dots and dashed lines are from the fully coupled model, a simplified isothermal model and the analytical solutions, respectively.

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temperature loss away from the well. Interestingly, the difference between the isothermal 378 and non-isothermal simulation results is virtually unnoticeable, except for the estimated 379 temperature decline associated with the 30 mD model. The difference between the mod-380 els is small because the fluid properties change very little over the temperature range of 381 30 and 35 °C at these pressures. A more significant difference is observed for the 30 mD 382 models, because the temperature decline is more severe. 383

Recall, the dashed lines are results from the analytical solutions. It is clear from Fig. 3a. 384 that the pseudo-pressure and pseudo-time approach is very effective at predicting the 385 well pressures in this context, despite its ignoring of the  $CH_4$  fluid properties. The heat 386 transport analytical solution is also seen to be effective here (see Fig. 3b). 387

Note that previously, Mathias et al. (2010) observed discrepancies between numerical 388 simulation and the analytical solution (assuming Darcian flow) for temperature changes 389 greater than  $5^{\circ}$ C. It was argued that this was due to the applying of the initial pressure 390 for calculating the constant fluid properties used. Here an estimate of the well pres-391 sure half-way through the injection period (i.e., at 10 years) is used, obtained from the 392 aforementioned analytical solution for pressure buildup, in conjunction with the injection 393 fluid temperature. This is found to be very effective for all the analytical solution results 394 presented in Figs. 3b, d, f and h. 395

Recently, Ziabaksh–Ganji & Kooi (2014) argued that a notable deficiency in the an-396 alytical solution of Mathias et al. (2010) (and therefore also the new solution presented 397 in Section 3.1, which uses the Forchheimer equation) was the ignoring of heating due to 398 compression. Considering Fig. 3a, it can be seen that there are initially large changes in 399 pressure with time. But after less than a small fraction of a year, the change in pressure 400 with time is dramatically reduced. In contrast, the large pressure changes with radial 401 distance persist throughout the injection period (consider again Fig. 2a). Consequently, 402

 $_{403}$  cooling due to expansion as the CO<sub>2</sub> moves away from the injection well has a significantly  $_{404}$  more dominant effect in this context.

Figs. 3c and d show results from similar simulations to those used for Fig. 3a and b 405 except looking at sensitivity to injection fluid temperature. All model parameters were 406 set to the values stated in Table 1, except for the injection fluid temperature,  $T_w$ , which 407 was set to values shown in the legend. Note that the initial reservoir temperature was 408 fixed at 35 °C for all the simulations. It is apparent from Fig. 3c, that injection fluid 409 temperature, ranging from 20 to 50 °C, has very little impact on well pressure develop-410 ment. Furthermore, it is noted that again there is very little difference between results 411 from the non-isothermal and isothermal models, and the analytical solutions are found 412 to provide a good approximation to the well-pressure and temperature response of the 413 system. 414

Figs. 3e and f explore the importance of non-Darcy effects. Results are presented, 415 again using the base case described by Table 1, using (1) Darcy's law (*i.e.*, b = 0), (2) 416 the Forchheimer equation with the Geertsma (1974) correlation (the base case), and (3)417 a simulation with enhanced non-Darcy effects, obtained by multiplying the b parameter 418 obtained from the Geertsma (1974) correlation by a factor of 10. There is no noticeable 419 difference between Darcian and Forchhimer equation models using Geertsma (1974) cor-420 relation, for both heat transport and pressure. When the non-Darcy effects are enhanced 421 by a factor of 10, a small increase in pressure is apparent along with a corresponding 422  $1.5^{\circ}$ C temperature decline. The analytical solutions for pressure and heat transport are 423 found to continue to provide good approximations in this context. 424

The Geertsma (1974) correlation has been found to correspond to large quantities of empirical data (Mathias & Todman 2010). Multiplying the correlation by 10 represents an upper bound on likely non-Darcy effects in this porosity range. Therefore, it can be

concluded that non-Darcy effects are unlikely to be a particular issue in this context. Their importance can be determined in future studies by considering the dimensionless group,  $b_D$ , defined in equation (3.7). For all the simulations presented in this paper, with the exception of the Darcian and the enhanced non-Darcy simulations,  $b_D$  was found to range from 0.07 to 0.46. The enhanced non-Darcy simulation corresponded to a  $b_D = 2.61$ .

Originally it was hypothesized that non-Darcy effects would be important because of the low viscosity of  $CO_2$  at the low pressures of interest. However, equation (2.6) shows that the significance of non-Darcy effects is also dependent on fluid density. The density of  $CO_2$  must also therefore be sufficiently low in this context, such that non-Darcy effects are not significant here.

The final subplots, Figs. 3g and h, show sensitivity due to initial pressure, as indicated 439 by the values in the legend. The change in pressure in the well is found to decrease 440 with increasing initial pressure. This is due to the fluid density increasing with pressure, 441 which leads to a reduction in volumetric injection rate. The temperature change is close 442 to zero for the 10 MPa example. The temperature decline increases with decreasing initial 443 pressure. This is due to the increased pressure gradients that occur due to the increased 444 volumetric injection rate, combined with the increased Joule-Thomson coefficient of the 445  $CO_2$  (associated with lower pressures). 446

The performance of the analytical solution for pressure buildup is found to reduce with increasing initial pressure. The main reason is that higher initial pressures correspond to a larger mass of residing CH<sub>4</sub>. Consequently, the effect of ignoring of CH<sub>4</sub> fluid properties (in the analytical solution) becomes more important. This is less of an issue with regards to the analytical solution for heat transport because temperature changes are significantly reduced at higher pressures.

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<sup>453</sup> Zeidouni *et al.* (2013) previously used the analytical solution of Mathias *et al.* (2010) <sup>454</sup> to verify their non-isothermal simulations obtained using CMG-GEM. They noted that <sup>455</sup> the analytical solution underestimated cooling and heating due to the neglection of brine <sup>456</sup> vaporisation and  $CO_2$  dissolution, respectively. The neglection of partial miscibility (va-<sup>457</sup> porisation and dissolution) between the  $CO_2$  and the residual brine represents a limitation <sup>458</sup> of the numerical simulations conducted in the current study as well.

Andre et al. (2010) studied effects associated with partial miscibility in this context 459 at a reservoir pressure of 15 MPa and an injection temperature of  $40^{\circ}$ C. They found 460 temperature variation due to vaporisation and dissolution to be around  $1^{\circ}$ C to  $3^{\circ}$ C, 461 respectively. Inspection of the empirical equation for solubility limit of  $CO_2$  in water 462 proposed by Spycher et al. (2003) suggests that dissolution is likely to be an order of 463 magnitude less in the context of the low pressure environments considered in this article. 464 Conversely, the work of Spycher *et al.* (2003) suggests that the reduction in pressure from 465 15 MPa to 0.7 MPa would lead to a doubling in the amount of water evaporated. However, 466 evaporation of residual water around the injection well would lead to an increase in gas 467 relative permeability. This in turn would give rise to lower pressure gradients (consider 468 Mathias et al. 2011b) and hence less Joule-Thomson cooling. 469

At this stage it is interesting to compare some of the above features with those as-470 sociated with  $CO_2$  injection into brine aquifers. For brine aquifers, the pore space is 471 predominantly filled with brine, which has a larger viscosity and lower compressibility 472 than the injected  $CO_2$ . For compartmentalized aquifers, this gives rise to a significant 473 restriction on the amount of  $CO_2$  that can be injected, if pressures are to be constrained 474 below fracture pressure limits (Mathias et al. 2013a). Consequently, throughout the in-475 jection duration, the vast majority of the reservoir pore-space continues to be occupied 476 by brine. Therefore, in contrast to depleted gas reservoirs, the compressibility of the 477

<sup>478</sup> injection fluid is found to have very little impact on pressure buildup (Mathias *et al.* <sup>479</sup> 2011a). Furthermore, because of the much larger viscosity difference between the  $CO_2$ <sup>480</sup> and the brine, along with the interfacial tension that develops between the  $CO_2$ -rich and <sup>481</sup> aqueous fluid phases, the mobility difference between the injection and reservoir fluid has <sup>482</sup> a much more significant impact on the pressure buildup process (Mathias *et al.* 2009, <sup>483</sup> 2013a).

# 484 5. Summary and conclusions

In this article, a two-layer vertical equilibrium model for the injection of  $CO_2$  into a 485 porous reservoir containing methane and water is developed. The dependent variables 486 solved for include pressure, temperature and  $CO_2$ - $CH_4$  interface height. In contrast to 487 previous two-layer vertical equilibrium models in this context, compressibility of all mate-488 rial components is fully accounted for. Non-Darcy effects are also considered, which may 489 become important for low viscosity fluids. With some approximations, analytic solutions 490 for both the pressure buildup and heat transport are derived and shown to capture the 491 main dynamics and agree well with the numerical solutions. 492

The results show that, for a given injection scenario, as the initial pressure in the reservoir decreases, both pressure buildup and temperature change increase. A comparison was conducted between a fully coupled non-isothermal numerical model and a simplified model where fluid properties are held constant with temperature. This simplified model was found to provide an excellent approximation when using the injection fluid temperature for calculating fluid properties, even when the injection fluid was as much as  $\pm 15^{\circ}$ C of the initial reservoir temperature. The implications are that isothermal models can be expected to provide useful estimates of pressure buildup in this context.

<sup>501</sup> Non-Darcy effects were incorporated using the Forchheimer equation with the Forch-

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<sup>502</sup> heimer parameter, b, calculated using the Geertsma (1974) correlation. An expression <sup>503</sup> for a dimensionless Forchheimer parameter,  $b_D$ , was provided (recall equation (3.7)), <sup>504</sup> which can be used to assess the importance of non-Darcy effects. Non-Darcy effects are <sup>505</sup> likely to be negligible providing bD < 1. Despite the low viscosity of CO<sub>2</sub> at the low <sup>506</sup> pressures studied, non-Darcy effects were found to be of negligible concern throughout <sup>507</sup> the sensitivity analysis undertaken. This is because the CO<sub>2</sub> density is also low in this <sup>508</sup> context.

The analytical solution for pressure buildup, using the pseudo-pressure and pseudo-509 time concepts of Al-Hussainy et al. (1996) and Agarwal (1979), respectively, was found 510 to provide a good approximation of the fully coupled numerical model for initial pressures 511  $\leq$  3 MPa. However, for higher pressures, the approximation was less accurate. The main 512 reason for this is that the analytical solution ignores the presence of the reservoir gas, 513  $CH_4$ . Larger initial reservoir pressure corresponds (for a fixed volume saturation) to a 514 larger mass of residing  $CH_4$ , leading the  $CH_4$  to play a more important role concerning 515 pressure buildup. 516

The analytical solution for heat transport was found to be a good approximation throughout the sensitivity analysis. However, it was found to be important to apply a sensible reference pressure and temperature for calculating the  $CO_2$  properties. Fluid properties for this purpose were calculated using the injection fluid temperature with an estimate of well-pressure half-way through the injection period, obtained using the analytical solution for pressure buildup with pseudo-pressure and pseudo-time.

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