# A Lambert W function solution for estimating sustainable injection rates for storage of $CO_2$ in brine aquifers

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## Abstract

It is often of interest to estimate the maximum possible $CO_2$ injection rate for a given maximum pressure buildup and injection duration scenario. Analytical solutions exist to estimate pressure buildup due to constant rate injection for a specified duration. In this article, it is shown that such solutions can be rearranged for injection rate by virtue of the Lambert W function. It is also shown that the Lambert W function argument is sufficiently small such that a simple asymptotic approximation of the Lambert W function is sufficient in this context.

*Key words:* $CO_2$ injection, Geologic carbon sequestration, Pressure buildup, Lambert W function

## 1. Introduction

In the context of geological carbon sequestration, it is often of interest to estimate the maximum possible $CO_2$ injection rate for a given maximum pressure buildup and injection duration scenario (e.g. Mathias et al., 2009a, 2013; Ehlig-Economides and Economides, 2010; Okwen et al., 2011a). Much development has been made concerning formulation of analytical solutions to estimate pressure buildup as a consequence of constant rate $CO_2$ injection (Burton et al., 2008; Vilarrasa et al., 2010; Mathias et al., 2009b, 2011a,b; Okwen et al., 2011b). Although for single phase flow Darcy law problems it is straightforward to rearrange analytical solutions for pressure buildup to solve for injection rate (consider Theis, 1935), for two-phase flow problems (such as $CO_2$ injection into a brine aquifer), pressure is not a linear function of injection rate. Therefore a simple rearrangement is not possible. More recently, Mathias et al. (2013) used the pressure buildup equation of Mathias et al. (2011b) in conjunction with an iterative approach to obtain a maximum sustainable injection rate for a given pressure and injection duration scenario. In the current article, the pressure buildup equation of Mathias et al. (2011b) is explicitly rearranged to solve for injection rate by exploitation of an asymptotic expansion of the Lambert W function.

The structure of the article is as follows. A large time approximation for the pressure buildup equation of Mathias et al. (2011b) is briefly described. The problem is then rearranged to yield a Lambert W function solution for injection rate. The appropriate branch of the Lambert W function is determined and the pertinence of an asymptotic expansion in this context is demonstrated. Finally, some comparisons are made with sustainable injection rates predicted using TOUGH2 (Pruess et al., 1999).

## 2. A large time approximation

Mathias et al. (2011b) derived an analytical solution for one-dimensional radial flow from a well during a constant rate injection of pure $CO_2$ into a homogenous and isotropic confined brine aquifer originally free of $CO_2$. Noting that the exponential integral function, $E_1(x)$, can be approximated using $E_1(x) \approx -0.5772 - \ln x + O(x)$, it can be shown that for large times of practical interest (> 1 year), Eq. (57) of Mathias et al. (2011b) reduces to

$$P - P_0 = \frac{\mu_c \alpha(\beta - \epsilon \ln \alpha)}{\mu_b(c_r + c_b)} \tag{1}$$

where $P$ [ML$^{-1}$T$^{-2}$] and $P_0$ [ML$^{-1}$T$^{-2}$] are the current and initial fluid pressures, $\mu_c$ [ML$^{-1}$T$^{-1}$] is the dynamic viscosity of pure $CO_2$, $\mu_b$ [ML$^{-1}$T$^{-1}$] is the dynamic viscosity of brine (free of $CO_2$), $c_r$ [M$^{-1}$LT$^2$] is the compressibility of the rock, $c_b$ [M$^{-1}$LT$^2$] is the compressibility of the brine and $\alpha$ [-] is a dimensionless injection rate defined by

$$\alpha = \frac{M_0 \mu_b(c_r + c_b)}{4\pi H \rho_c k} \tag{2}$$

where $M_0$ [MT$^{-1}$] is the mass injection rate of $CO_2$, $H$ [L] is the formation thickness, $\rho_c$ [ML$^{-3}$] is the density of pure $CO_2$, $k$ [L$^2$] is permeability and

$$\beta = P_{rpD} - \frac{\ln \zeta}{k_{rs}} - \frac{\mu_b q_{D3} \gamma}{\mu_c} \tag{3}$$

$$\epsilon = \frac{\mu_b q_{D3}}{\mu_c} - \frac{1}{k_{rs}} \tag{4}$$

where $P_{rpD}$ [-] is a dimensionless pressure contribution associated with relative permeability effects, found from Eq. (7) of Mathias et al. (2013), $k_{rs}$ [-] is the permeability reduction factor due to salt precipitation, $q_{D3}$ [-] is a volumetric flow rate reduction factor resulting from $CO_2$ dissolution in brine, found from Eq. (27) of Mathias et al. (2011b), and $\zeta$ is a similarity transform defined by

$$\zeta = \frac{\phi\mu_b(c_r + c_b)r^2}{4kt} \tag{5}$$

where $\phi$ [-] is porosity, $r$ [L] is radial distance from the origin of the well (set to the well radius when looking at well pressures), $t$ [T] is time, and $\gamma$ [-] is a term which provides the pressure response of the bulk of the brine aquifer, found from

$$\gamma = \begin{cases} 0.5772, & \zeta_E > 0.5615 \\ \\ \dfrac{3}{2} - \dfrac{1}{\zeta_E} - \ln\zeta_E, & \zeta_E < 0.5615 \end{cases} \tag{6}$$

where

$$\zeta_E = \frac{\phi\mu_b(c_r + c_b)r_E^2}{4kt} \tag{7}$$

and $r_E$ [L] is the radial distance from the origin of the injection well to an impermeable outer boundary of the reservoir.

## 3. Lambert W function solution for injection rate

Eq. (1) can be rearranged to get

$$-\frac{P_D}{\epsilon}\exp\left(-\frac{\beta}{\epsilon}\right) = -\frac{P_D}{\epsilon\alpha}\exp\left(-\frac{P_D}{\epsilon\alpha}\right) \tag{8}$$

where

$$P_D = \frac{\mu_b(c_r + c_b)(P - P_0)}{\mu_c} \tag{9}$$

From Eq. (8), it can be seen that an explicit solution for the dimensionless injection rate, $\alpha$, can be written as follows

$$\alpha = -\frac{P_D}{\epsilon W\left(-\frac{P_D}{\epsilon}\exp\left(-\frac{\beta}{\epsilon}\right)\right)} \tag{10}$$

where $W$ denotes the Lambert W function whereby $y = W(x)$ satisfies the equation $x = ye^y$ (Coreless et al., 1996).

The Lambert W function has two real branches, referred to as $W_0$ and $W_{-1}$, respectively, whereby (Coreless et al., 1996)

$$W(x) = \begin{cases} W_0(x), & W(x) \geq -1 \\ W_{-1}(x), & W(x) < -1 \end{cases} \tag{11}$$

From a practical viewpoint, it can be said that the maximum sustainable injection rate will increase with increasing maximum allowable pressure, i.e.

$$\frac{d\alpha}{dP_D} > 0 \tag{12}$$

Making the substitution

$$x = -\frac{P_D}{\epsilon}\exp\left(-\frac{\beta}{\epsilon}\right) \tag{13}$$

and noting that

$$\frac{dW}{dx} = \frac{W}{x[1 + W(x)]} \tag{14}$$

differentiation of Eq. (10) with respect to $P_D$ leads to

$$\frac{d\alpha}{dP_D} = \frac{-1}{\epsilon[1 + W(x)]} \tag{15}$$

from which it is observed that the constraint given in Eq. (12) is satisfied only when $W(x) < -1$. Therefore, considering Eq. (11), $W(x) = W_{-1}(x)$. Consequently it can be said that

$$\alpha = -\frac{P_D}{\epsilon W_{-1}\left(-\frac{P_D}{\epsilon}\exp\left(-\frac{\beta}{\epsilon}\right)\right)} \tag{16}$$

## 4. Evaluating the Lambert W function

The Lambert W function, $W(x)$, can be easily evaluated in MATLAB using the LAMBERTW function (Coreless et al., 1996). However, MATLAB's implementation is computationally quite expensive. Furthermore, the exponential argument in Eq. (13) is generally quite a large negative argument, often leading MATLAB to report zero for the exponential term. Therefore it is worth to consider the asymptotic expansion of $W(x)$ for $x < 0$ and $x \to 0^-$ (Chapeau-Blondeau and Monir, 2002)

$$\begin{aligned} W_{-1}(x) = \quad & L_1 - L_2 + \frac{L_2}{L_1} + \frac{(-2+L_2)L_2}{2L_1^2} + \\ & + \frac{(6-9L_2+2L_2^2)L_2}{6L_1^3} + O\left(\left\{\frac{L_2}{L_1}\right\}^4\right) \end{aligned} \tag{17}$$

where $L_1 = \ln(-x)$ and $L_2 = \ln(-L_1)$.

The exponential term in Eq. (13) is eliminated by substituting Eq. (13) directly into the definition of $L_1$ to obtain

$$L_1 = \ln\left(\frac{P_D}{\epsilon}\right) - \frac{\beta}{\epsilon} \tag{18}$$

## 5. Comparison with TOUGH2

Mathias et al. (2013) previously compared the pressure buildup equation, Eq. (57), of Mathias et al. (2011b) (i.e., Eq. (1) in the current article) with well pressures simulated using the numerical simulator, TOUGH2 (Pruess et al., 1999). The simulations involved injecting $CO_2$ at a constant rate of 15 kg/s for 40 years into three different reservoirs. The three reservoirs were identical except for the value of exponents, $m$ and $n$ (with $m$ set equal to $n$), used in the relative permeability functions. The higher the $m$ value, the more non-linear the relative permeability.

In the current article, the pressure data from the TOUGH2 simulations in Fig. 2 of Mathias et al. (2013) is used to demonstrate the effectiveness of Eq. (16) at calculating the optimal injection rate for a given pressure limit. The model parameters used, relevant to Eq. (16), are presented in Table 1. Note that the values of $P_{rpD}$ and $q_{D3}$ for the three relative permeability scenarios were previously calculated (although not reported) by Mathias et al. (2013). These are now presented in Table 2.

From Fig. 2 of Mathias et al. (2013), it is shown that the well pressures in the reservoirs after 2 and 40 years were 14.0 MPa, 14.4 MPa, 15.1 MPa and 16.5 MPa, 16.9 MPa, 17.5 MPa, respectively for the three different relative permeability functions, respectively (as listed in Table 2). The last column of Table 2 contains estimates of sustainable injection rates, along with associated auxiliary variables, for these pressure and duration scenarios (treating the TOUGH2 pressures and times as maximum sustainable pressure and durations of injection, respectively) according to Eq. (16). It can be seen that for the six scenarios studied, estimated injection rate is within 1.3% of the rate determined using TOUGH2. This error is due to the simplifying assumptions made by Mathias et al. (2011b) in the derivation of the pressure buildup equation and numerical error associated with the solvers used within TOUGH2. Note that when pressures calculated using Eq. (57) of Mathias et al. (2011b) are used instead, the error is found to be zero, because Eq. (16) has been mathematically derived directly from Eq. (57).

## 6. Summary and conclusion

The focus of this article was to provide an explicit means of estimating a maximum sustainable $CO_2$ injection rate for a given maximum pressure buildup and temperature scenario. For single-phase flow Darcy law problems this is straightforward because injection rate is a linear function of pressure. However, for two-phase flow problems, the relationship between pressure and injection rate becomes non-linear. Nevertheless, it was shown that, for the two-phase flow pressure buildup equation of Mathias et al. (2011b), an explicit solution for injection rate can be derived (i.e., Eq. (16)) by virtue of the Lambert W function. Although the Lambert W function has two real

Table 1: Parameters used for the TOUGH2 comparison.

| Parameter | Symbol | Value |
|---|---|---|
| Injection rate, | $M_0$ | = 15 kg/s |
| Well radius, | $r_W$ | = 0.2 m |
| Radial extent, | $r_E$ | = 20 km |
| Porosity, | $\phi$ | = 0.2 |
| Rock compressibility, | $c_r$ | = $4.5 \times 10^{-10}$ Pa$^{-1}$ |
| Initial pressure, | $P_0$ | = 10 MPa |
| Permeability reduction factor due to salt precipitation, | $k_{rs}$ | = 1 |
| Formation thickness, | $H$ | = 30 m |
| Permeability, | $k$ | = 100 mD |
| $CO_2$ density, | $\rho_c$ | = 797 kg/m$^3$ |
| $CO_2$ viscosity, | $\mu_c$ | = $7.10 \times 10^{-5}$ Pa s |
| Brine viscosity, | $\mu_b$ | = $9.63 \times 10^{-4}$ Pa s |
| Brine compressibility, | $c_b$ | = $3.54 \times 10^{-10}$ Pa$^{-1}$ |

Table 2: Injection rate estimation based on TOUGH2 pressures.

| $t$ (yrs) | $m, n$ | $P$ (MPa) | $P_{rpD}$ | $q_{D3}$ | $\ln \zeta$ | $\zeta_E$ | $\gamma$ | $\beta$ | $\epsilon$ | $P_D$ | $\ln(-x)$ | $W_{-1}(x)$ | $\alpha$ | $M_0$ (kg/s) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | 14.0 | 5.3 | 0.955 | -22.1 | 2.45 | 0.58 | 20.0 | 12.0 | 0.044 | -7.3 | -9.5 | 0.000384 | 14.9 |
| 2 | 2 | 14.4 | 13.5 | 0.971 | -22.1 | 2.45 | 0.58 | 28.1 | 12.2 | 0.048 | -7.8 | -10.2 | 0.000389 | 15.1 |
| 2 | 3 | 15.1 | 31.1 | 0.970 | -22.1 | 2.45 | 0.58 | 45.7 | 12.2 | 0.055 | -9.1 | -11.6 | 0.000392 | 15.2 |
| 40 | 1 | 16.5 | 5.3 | 0.955 | -25.1 | 0.12 | -4.55 | 89.4 | 12.0 | 0.071 | -12.6 | -15.3 | 0.000385 | 14.9 |
| 40 | 2 | 16.9 | 13.5 | 0.971 | -25.1 | 0.12 | -4.55 | 98.6 | 12.2 | 0.075 | -13.2 | -16.0 | 0.000386 | 15.0 |
| 40 | 3 | 17.5 | 31.1 | 0.970 | -25.1 | 0.12 | -4.55 | 116.2 | 12.2 | 0.082 | -14.6 | -17.4 | 0.000387 | 15.0 |

branches, it was further shown that solution to practical problems will always involve the $W_{-1}$ branch. Furthermore, the Lambert function argument is generally likely to be very small, which means that a simple asymptotic approximation for the Lambert W function is sufficient in this context. A comparison of estimated injection rates for six scenarios with those predicted using the TOUGH2 results, previously presented by Mathias et al. (2013), shows the new equation to be an accurate approximation of the complete dynamic problem.

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