Modelling start-up injection of CO₂ into highly-depleted gas fields

Andrea Sacconi and Haroun Mahgerefteh*
Department of Chemical Engineering, University College London, London WC1E 7JE, UK

Abstract
The development and verification of a homogeneous relaxation model for simulating the highly transient flow phenomena taking place during the start-up injection of CO₂ into deep highly depleted gas fields is presented. The constituent mass, momentum, and energy conservation equations, incorporating a relaxation time to account for non-equilibrium effects, are solved numerically for single and two-phase flows along the steel lined injection well leading to the storage reservoir. Wall friction, gravitational field effects and heat transfer between the expanding fluid and the outer well layers are taken into account as source terms in the conservation equations. At the well inlet, the opening of the upstream flow regulator valve is modelled as an isenthalpic expansion process; whilst at the well outlet, a formation-specific pressure-mass flow rate correlation is adopted to characterise the storage site injectivity. The testing of the model is based on its application to CO₂ injection into the depleted Golden Eye Reservoir in the North Sea for which the required design and operational data are publically available. Three injection scenarios involving a rapid, medium and slow linear ramping up of the injected CO₂ flow rate to the peak nominal value of 33.5 kg/s are simulated. In each case, the predicted pressure and temperature transients at the top and bottom of the well are employed to ascertain the risks of well-bore thermal shocking, and interstitial ice or CO₂ hydrate formation leading to its blockage due to the rapid expansion cooling of the CO₂. The results demonstrate the efficacy of the proposed model as a tool for the development of optimal injection strategies and best-practice guidelines for the minimisation of the risks associated with the start-up injection of CO₂ into depleted gas fields.

Keywords: Global warming, Carbon Capture and Storage, CO2 injection, Transient flow modelling

*corresponding author h.mahgerefteh@ucl.ac.uk

1. Introduction
According to the IEA Energy Technology Perspective [1], Carbon Capture and Sequestration (CCS) is expected to play a key role in moving the CO₂ emitting energy intensive industries, such as iron and steel, cement and oil refineries onto a pathway consistent with limiting the increase in global average temperatures to well below 2°C above pre-industrial levels as agreed at the Paris Climate Conference in 2015. The safe and cost effective storage of the enormous amounts of CO₂ captured from these sources is an essential element of CCS and therefore of fundamental importance in ensuring its success. Highly-depleted gas fields offer excellent potential for the permanent storage of the captured CO₂ [2]. In the case of the UK for example, the Southern North Sea and the East Irish Sea depleted gas reservoirs provide almost 95% of the storage capacity required to meet UK’s CO₂ reduction commitments for the period 2020-2050 [3].

As compared to saline aquifers, depleted gas fields are better characterized given the availability of geological data, such as pressure, porosity and permeability, derived from years of gas production. They have seals that have successfully retained hydrocarbon gas for millions of years, and may offer a shorter route to practical implementation for early Carbon Capture and Storage (CCS) projects [4].

The UK has completed three large FEED study projects for offshore CO₂ storage at Hewett, Golden Eye and Endurance sites [5]. However, CO₂ storage at full industrial scale has only been demonstrated at a small number of sites around the world: Sleipner, In Salah & Snøvit [6], Ordos [7], and the Quest project [8].

In order to boost the confidence of both investors and the public and thus facilitate the full-scale deployment of CCS, it is of paramount importance to guarantee that the storage site will be of high quality and operate in a safe manner.
However, given the low reservoir pressures along with the unique thermodynamic properties of CO₂, the start-up injection of CO₂ into depleted low-pressure gas fields presents significant safety and operational challenges.

The most practical cost-effective option for transporting the captured CO₂ involves the use of sub-sea pipelines with the CO₂ in the dense or liquid phase, i.e. above 75 bar given the lower pressure drop along the pipeline as compared to the gas phase and the larger line pack [9–12]. As the sea temperature will be well below the CO₂ critical temperature (31.1 °C), the fluid will arrive in the liquid state. Given the much lower wellhead pressure, the uncontrolled injection of the CO₂ into the wellhead will lead to its rapid quasi adiabatic expansion (often referred to as Joule Thomson cooling) into a two-phase mixture leading to temperatures well below zero °C [13].

In practice, the rapid expansion cooling could pose several operational and safety risks, namely:

- CO₂ hydrate and ice formation following contact of the cold CO₂ with the interstitial water around the wellbore and the formation water in the perforations at the near well zone. The former poses the risk of well blockage, while the latter may severely reduce the reservoir injectivity and ultimately its storage capacity;
- thermal stress shocking of the wellbore casing steel leading to its fracture and the escape of CO₂;
- thermal stress shocking of the reservoir rocks leading to fracture thus changing the reservoir permeability and reducing its CO₂ locking’ effectiveness;
- superheating of the liquid CO₂ at the wellhead leading to its violent evaporation and over-pressurisation followed by CO₂ backflow into the injection system.

As such, developing appropriate start-up injection strategies where the rate of injection of CO₂ is gradually increased in a controlled manner is of paramount importance for avoiding the above risks. Key to this is the availability of reliable mathematical models for predicting the behaviour of the injected CO₂, in particular its variation of pressure and temperature along the well and ultimately at the point of entry into the depleted reservoir. The alternative is the heating of the CO₂ stream prior to injection, which is highly costly given the significant volumes involved.

Driven by the push to reduce CO₂ emissions along with the economic incentives associated with enhanced natural gas recovery involving CO₂ injection into depleted natural gas reservoirs, several, almost exclusively modelling studies focusing on the associated temperature and pressure transients with various degrees of sophistication have been reported in the open literature. The following is a critical review of the main models. The review does not cover the much simpler case of injection of CO₂ into aquifers [14]. Given the much higher aquifer pressures, the rapid fluid expansion transient phenomenon associated with the injection of CO₂ in depleted gas fields are not expected here and hence irrelevant to the scope of the present work.

Olenburg [15] employed the commercially available ToughTOUGH2 module to simulate the radial variation of the reservoir temperature at the bottom of the well for different natural gas reservoir permeabilities and constant injection CO₂ flow rates, reporting a cooling of approximately 20 °C. Goodarzi et al [16] employed a coupled flow, aeromechanical and heat transfer model for the injection and sequestration of CO₂ in Ohio Valley. However their model was limited to simulating the impact on the injection zone and the surrounding formations in order to evaluate the risk of induced fracturing of the storage formation following exposure to the incoming low temperature CO₂ stream.

Linga and Lund [17] developed a sophisticated two-fluid model applied to CO₂ injection wells incorporating the Span–Wagner equation-of-state [18]. However, much the same as Li et al [19], the application of their model was limited to predicting the resulting temperature and pressure profiles following well blowout and during shut in. Temperatures as low as −48 °C were predicted upon blowout concluding that this temperature was not necessarily low enough to cause damage to the steel pipe itself, but likely to pose a hazard due to mechanical stresses that arise due to thermal contraction.
Lund et al [28] employed a heat conduction model based on finite volume method for determining the heat transfer from the well to the casing, annular seal, and rock formation following the injection of CO\textsubscript{2} for EoR applications. Their predictions of the temperature variations at various locations in and around a given well during CO\textsubscript{2} injection
were found to be in relatively good agreement with those based on small scale laboratory experiments. The authors used their model to conclude, as expected, that by replacing cement with an annular sealant material with higher thermal conductivity, the temperature difference across the seal can be significantly reduced thus reducing the risk associated with the thermal shocking of the well.

In a report by Shell [29] (see Section 4), the transient variations of the well head and well bottom pressure and temperature were reported for the injection of CO\textsubscript{2} into the depleted Golden Eye reservoir using OLGA. However no information is publicly available describing the detailed development of the above flow model in pipes for the simulation of the more complex start-up injection of CO\textsubscript{2} through a vertical well discharging into the reservoir at different ramping up injection rates.

Based on the above review, it is clear that much of the reported models on CO\textsubscript{2} injection into well bores are based on steady-state flow assumption where the rapid pressure and temperature transients associated with the start-up injection process cannot be handled. The drift-flux flow models dealing with multi-phase flow behaviour usually contain several empirical parameters that must be determined experimentally. They are also notoriously prone to numerical stabilities or singularities at either flow regime transitions or when the liquid volume fraction approaches zero [30]. The use of the sophisticated commercial simulator OLGA, also incorporating drift-flux flow complicates the model validation since little information is publicly available regarding its details.

In this paper the development and verification of a mathematical model for simulating the transient flow phenomena taking place during the start-up injection of CO\textsubscript{2} into highly depleted gas fields is presented. The formulation is based on a Homogeneous Relaxation Model (HRM), where mass, momentum, and energy conservation equations are considered for single or two-phase flows. The model accounts for phase and flow dependent fluid/wall friction and heat transfer, variable well cross sectional area as well as deviation of the well from the vertical.

At the well inlet, the opening of the upstream flow regulator valve is modelled as an isenthalpic expansion process; whilst at the well outlet, a pre-defined site-characteristic pressure-mass flow rate correlation is used to simulate the migration of the CO\textsubscript{2} into the geological substrate. The developed model is next employed to perform a detailed sensitivity analysis of the most important parameters affecting the CO\textsubscript{2} flow behaviour, including the upstream temperature, pressure and time variant mass flow rate; the latter being representative of the feed pressure ramping up process. These investigations are intended to demonstrate the efficacy of the injection model presented as a practical tool for the development of optimal injection strategies and best-practice guidelines for minimising the risks associated with the start-up injection of CO\textsubscript{2} into depleted gas fields.

2. Model formulation

2.1 Wells and injection scenarios

Wells are an essential component of any CO\textsubscript{2} storage project. They are the only way by which CO\textsubscript{2} can be discharged into underground reservoirs in the timeframes required. It is important to recognise that the injected CO\textsubscript{2} is not stored in the wells. The well represents the transportation route through which the CO\textsubscript{2} will be released into reservoirs and then remain safely trapped. Wells are drilled for a range of purposes such as exploration, appraisal, production, injection or monitoring. Well objectives strongly influence its design, depth, size and cost. The information gathered from existing wells drilled and used by oil and gas operators proves to be very useful in characterising the subsurface geology of a site [5]. A schematic of typical well for the injection of CO\textsubscript{2} into a depleted gas field is represented in Figure 1. The well is composed of various layers and surrounded by a formation, whose composition varies from site to site. Wells have to be carefully analysed in order to assess their suitability for CO\textsubscript{2} injection in depleted oil and gas fields [31].

Before the steady injection of CO\textsubscript{2} into the reservoir can be started, it is necessary to perform time-dependent operations to estimate important reservoir properties, e.g. permeability and pressure. Such operations include start-up, shut-in and emergency shut-down, which prove to be critical in the overall design of the well [9]. Even after steady injection conditions are reached, the well may be shut in and started up for maintenance of the upstream transportation
system or other routine checks. It is therefore of paramount importance to be able to predict the behaviour of the CO₂, in terms of pressure and temperature, particularly at the top and bottom of the well in order to identify and quantify potential risks.

2.2 Fluid dynamics

The following gives an account of the extension of our previously developed Homogeneous Relaxation Model ((HRM) [32,33]) employed for the simulation of the time-dependent flow of CO₂ injected into the well. The system of four partial differential equations for the CO₂ liquid/gas mixture, to be solved in the well tubing can be written in the well-known conservative form as follows:

\[
\frac{\partial}{\partial t} U + \frac{\partial}{\partial z} F(U) = S_1 + S_2
\]  

Where, we define;

\[
U = \begin{pmatrix} \rho A \\ \rho u A \\ \rho u A \\ A \end{pmatrix}, \quad F(U) = \begin{pmatrix} \rho u A \\ \rho u^2 A + \rho P \\ \rho u A + \rho P u H \end{pmatrix}, \quad S_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad S_2 = \begin{pmatrix} 0 \\ 0 \\ A(F + \rho u g) \\ A(Fu + \rho u^2 g + Q) \end{pmatrix}
\]  

In the above, the first three equations correspond to mass, momentum, and energy conservation respectively. The fourth equation accounts for the fact that the well bore cross-sectional area A at any location along the well does not change with time, but may vary along the well. u and \( \rho \) are the mixture velocity and density respectively. \( P \) is the mixture pressure, while \( E \) and \( H \) represent the specific total energy and total enthalpy of the fluid, respectively. These are in turn defined as:

\[
E = e + \frac{1}{2} u^2
\]

\[
H = E + \frac{P}{\rho}
\]

where, \( e \) is the specific internal energy. \( z \) denotes the axial coordinate, \( t \) the time, \( F \) the viscous friction force, \( Q \) the heat flux, and \( g \) the gravitational acceleration. Given the rapid transients during decompression, phase slip is ignored. However, non-equilibrium liquid-vapour transition is accounted for by a relaxation to thermodynamic equilibrium through the following equation [34]:

\[
\frac{\partial x}{\partial t} + u \frac{\partial x}{\partial z} = \frac{x_e - x}{\theta}
\]
where, $\alpha$ is the mixture vapour quality and $\theta$ is a relaxation time accounting for the delay in the phase change transition. The mixture density $\rho$ is defined as:

$$\frac{1}{\rho} = \frac{x}{\rho_{sv}(P)} + \frac{1-x}{\rho_{ml}(P, e_{ml})}$$

(6)

while the mixture internal energy is defined as:

$$e = xe_{sv}(P) + (1-x)e_{ml}$$

(7)

Where, the subscripts $sv$ and $ml$ refer to the saturated vapour and meta-saturated (super-heated) liquid phases respectively.

The various source terms appearing on the right-hand side of equation (2) are described next.

The frictional loss, $F$ can be expressed as:

$$F = -f_w \frac{\rho u^2}{D_p}$$

(8)

where, $f_w$ is the Fanning friction factor, calculated using Chen’s correlation [35], and $D_p$ is the internal diameter of the pipe.

The gravitational term is given by

$$\beta(z) = \rho g \sin \theta$$

(9)

where, $\theta$ is the well deviation from the vertical. In practice, a well is often not drilled in the perfectly vertical direction. Deviations may be caused by geological conditions, specifics of the drilling technology and the process conditions [36,37]. The well deviation and consequently the corresponding gravitational term in equation (9) is usually expressed through two different quantities: True Vertical Depth (TVD) and Measured Depth (MD). The former denotes the vertical distance from the wellhead to a point in the well path. Such quantity is calculated from directional survey data. MD on the other hand denotes the actual length of the well, and it is always greater than the corresponding TVD, given the wellbore deviation from the vertical.

In equation (2) the source term, $Q$ accounts for the heat exchange between the fluid and the well wall. The corresponding heat transfer coefficient, $\eta$ is calculated using the well-known Dittus-Boelter correlation [38]:

$$\eta = 0.023 Re^{0.8} Pr^{0.4} \frac{k}{D_p}$$

(10)

where, $k$, $Re$ and $Pr$ are the thermal conductivity, Reynolds number and Prandtl number for the fluid respectively. The heat exchange between the fluid and the well wall is given by:

$$Q = \frac{4}{D_p} \eta (T_w - T)$$

(11)

where, $T_w$ and $T$ are the fluid and wall temperatures respectively. Note that $T_w = T_w(z,t)$, i.e. $T_w$ is not assumed constant, but variable with time and space. The transient heat conduction in the coordinate $r$ (the radial direction from the axis of the well towards the well layers and the formation surrounding the well) is solved using the following equation [28]:

$$\rho(r)c_p(r) \frac{\partial}{\partial t} T(r,t) = \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa(r) \frac{\partial}{\partial r} T(r,t) \right)$$

(12)

where, $c_p$ and $\kappa$ respectively represent heat capacity and heat conductivity at the radial coordinate $r$. 
In order to close the Homogeneous Relaxation Model system of equations (Equation (1)&(2)), the pertinent thermodynamic properties for vapour and liquid phases are calculated with the aid of the Peng–Robinson Equation of State (EoS) [39]. It should be noted that while other more accurate EoS exist for pure CO\textsubscript{2} exist e.g. [18,40], the computational workload required to use them in conjunction with our Homogeneous Relaxation Model is currently prohibitive. The PR equation of state is given by

\[ P = \frac{R}{v - b} - \frac{c\delta}{v^2 + 2bv} + \frac{b^2}{v} \]  \hspace{1cm} (13)

where, \(c\), \(b\) and \(\delta\) are respectively given by:

\[ c = 0.45724 \frac{(RT_c)^2}{P_c} \]  \hspace{1cm} (14)

\[ b = 0.0778 \frac{RT_c}{P_c} \]  \hspace{1cm} (15)

\[ \delta = \left[ 1 + (0.37464 + 1.54226\omega - 0.2699\omega^2) \left( 1 - \frac{T}{T_c} \right) \right] \]  \hspace{1cm} (16)

where, \(P_c\), \(T_c\) and \(\omega\) are respectively the critical pressure, the critical temperature and the acentric factor for CO\textsubscript{2}.

From equation (13), the internal energy may be calculated using the identity [41]:

\[ e - e_{ig} = \int_v^\nu \left[ T \left( \frac{\partial P}{\partial T} \right)_v - P \right] dv \]  \hspace{1cm} (17)

where, the subscript, \(ig\) refers to ideal gas. The mixture speed of sound, \(c\) is defined through the relation:

\[ \frac{1}{\rho c^2} = \frac{x}{\rho c_v^2} + \frac{1-x}{\rho c_l^2} \]  \hspace{1cm} (18)

3. Numerical solution method

As the HRM system of equations (2) cannot be solved analytically, a suitable numerical method has been employed within the Finite Volume framework. More specifically, in order to accurately capture the rich flow dynamics, the AUSM+ up Flux Vector Splitting scheme [42] has been applied to the fluid problem. The solution domain is first divided into \(N\) cells and integrated over the \(i\)-th computational cell \([z_{i-1/2}, z_{i+1/2}]\), \(i = 1, ..., N\), to yield the semi-discrete formulation:

\[ \frac{dU_i}{dt} = -\frac{1}{\Delta x} \left( F_{i+1/2} - F_{i-1/2} \right) + S_{1,i} + S_{2,i} \]  \hspace{1cm} (19)

where \(i + \frac{1}{2}\) denotes the interface between cells \(i\) and \(i + 1\), at which the inter-cell flux \(F_{i+1/2}\) has to be computed. Following the standard AUSM method [42], the conservative flux vector is split into convective and pressure fluxes:

\[ F_{i+1/2} = f_{c_{i+1/2}} + f_{p_{i+1/2}} \]  \hspace{1cm} (20)

where

\[ f_{c_{i+1/2}} = \begin{pmatrix} \rho uA \\ \rho u^2A \\ \rho uA \\ 0 \end{pmatrix}_{i+1/2}, \quad f_{p_{i+1/2}} = \begin{pmatrix} 0 \\ AP \\ 0 \\ 0 \end{pmatrix}_{i+1/2} \]  \hspace{1cm} (21)

3.1 Convective flux discretisation

From equation (21) the convective flux can be written explicitly as
\[ f^c = \dot{m} \left( \begin{bmatrix} 1 \\ u \\ H \\ 0 \end{bmatrix} \right) = \dot{m} \Psi \]

where, \( \dot{m} \) is the area-weighted mass flux:

\[ \dot{m} = \rho u A \]

The numerical flux at cell interface \( i + \frac{1}{2} \) is then defined as:

\[ f^c_{i+\frac{1}{2}} = \dot{m}^* \Psi^* = \dot{m}^* \frac{1}{2} (\Psi_i + \Psi_{i+1}) + \frac{1}{2} |\dot{m}^*| (\Psi_i - \Psi_{i+1}) \]  

(24)

In order to express \( \dot{m}^* \), the interface speed of sound \( a^+_{i+\frac{1}{2}} \) and the left and right Mach numbers are defined as follows:

\[ a^+_{i+\frac{1}{2}} = \frac{a_i + a_{i+1}}{2}, \quad M_i = \frac{u_i}{a^+_{i+\frac{1}{2}}}, \quad M_{i+1} = \frac{u_{i+1}}{a^+_{i+\frac{1}{2}}} \]  

(25)

The interface Mach number is next defined as:

\[ M^+_{i+\frac{1}{2}} = M^+_1(M_i) + M^-_1(M_{i+1}) \]  

(26)

where \( M^+ \) and \( M^- \) are the polynomials introduced by Liou [40] and the subscripts indicating the order of the polynomial used:

\[ M^+_1 = \frac{1}{2} (M \pm |M|) \]

(27)

\[ M^-_1 = \pm \frac{1}{4} (M \pm 1)^2 \]

(28)

\[ M^+_1 = \begin{cases} \frac{M^+_1}{M}, & \text{where } |M| \geq 1 \\ \pm M^+_1 (1 \mp 16B M^+_2) & \end{cases} \]  

(29)

with \( B = \frac{1}{8} \).

In order to approximate numerically the area-weighted mass flux introduced in equation (23), we define:

\[ \dot{m}^* = a^+_{i+\frac{1}{2}} \left[ \frac{\rho A}{2} \left( M_{i+1}^+ + M_{i+\frac{1}{2}}^+ \right) + \frac{\rho A}{2} \left( M_{i+\frac{1}{2}}^- + M_{i+1}^- \right) \right] \]

where, \( M_{i+\frac{1}{2}}^\pm = \bar{M}_{i+\frac{1}{2}}^\pm \). However, at low Mach numbers this approximation approaches a central difference scheme and can suffer from odd-even decoupling [43]. In order to avoid poor numerical solutions, a velocity-based dissipation is add to \( \bar{M}_{i+\frac{1}{2}}^\pm \):

\[ M_{i+\frac{1}{2}}^\pm = \frac{\bar{M}_{i+\frac{1}{2}}^\pm - K_p \max(1 - \bar{M}^2, 0) \frac{P_{i+1} - P_i}{\bar{\rho} \bar{a}^2}}{2} \]

(31)

where, \( \bar{M}, \bar{\rho} \) and \( \bar{a} \) represent the arithmetic averages of the values attained by Mach number, density and speed of sound in cells \( i \) and \( i + 1 \). \( K_p \) is a constant, which is set to unity in this study.

While the above scheme has proven to be remarkably robust, in order to avoid instabilities at discontinuities in the cross-sectional area, given its greater degree of dissipation at low Mach numbers, we follow [44] to replace \( \bar{M}_{i+\frac{1}{2}}^\pm \) in Eq. (26) with

\[ \bar{M}_{i+\frac{1}{2}} = M^+_1(M_i) + M^-_1(M_{i+1}) \]  

(32)

3.2 Pressure flux discretisation

In equation (21) pressure flux \( f^p_{i+\frac{1}{2}} \) was introduced. According to the AUSM+ splitting, its non-zero element is defined as:

\[ (AP)_{i+\frac{1}{2}} = A_{i+\frac{1}{2}} (P^+_5(M_i) \cdot P_i + P^-_5(M_{i+1}) \cdot P_{i+1}) \]  

(33)
where the polynomials \( P_5^{\pm} \) are those introduced in Liou [40] and the subscript indicates the order of the polynomial used:

\[
P_5^{\pm} = \begin{cases} \frac{M_1^{\pm}}{M}, & \text{where } |M| \geq 1 \\ \pm M_2^{\pm}(2 \mp M - 16CMM_2^{\pm}) \end{cases}
\]  

with \( C = \frac{3}{16} \).

In equation (33) \( A_{i+\frac{1}{2}} \) can attain two different values in the two cells separated by the interface \( i + \frac{1}{2} \). Specifically, for the \( i \)-th cell, \( A_{i+\frac{1}{2}} \) takes the value of the area on the left of the interface, i.e. \( A_{i+\frac{1}{2}i} \), while in the case of the \( (i+1) \)-th cell, \( A_{i+\frac{1}{2}} \) is set to the value on the right of the interface, i.e. \( A_{i+\frac{1}{2}i+1} \). This strategy allows discontinuous variations in the area at the interface \( i + \frac{1}{2} \).

Finally, a dissipation term is added to \( P_{i+\frac{1}{2}} \). The form of the dissipation term developed by Liou [40] has been widely used for both single and two-phase flows [45,46] and is given by:

\[
P_{i+\frac{1}{2}} = P_5^+(M_i)(P)_i + P_5^-(M_{i+1})(P)_{i+1} - K_u P_5^+(M_i) P_5^-(M_{i+1})(\rho_i + \rho_{i+1})\alpha_{i+\frac{1}{2}}(u_{i+1} - u_i)
\]  

where, \( K_u \) is constant and set to unity. However, in order to maintain stability at discontinuities in the cross-sectional area, equation (35) is modified to incorporate a dependency on the cross-sectional area:

\[
P_{i+\frac{1}{2}} = P_5^+(M_i)(P)_i + P_5^-(M_{i+1})(P)_{i+1} - K_u P_5^+(M_i) P_5^-(M_{i+1})(\rho_i + \rho_{i+1})\alpha_{i+\frac{1}{2}} \frac{A_{i+\frac{1}{2}i+1} u_{i+1} - A_{i+\frac{1}{2}i} u_i}{\max(A_{i+\frac{1}{2}i+1}, A_{i+\frac{1}{2}i})}
\]  

3.3 Non-conservative fluxes

The discretisation of the source term, \( S_1 \) containing the non-conservative derivative requires special attention to ensure numerical stability. In particular we take:

\[
S_{1,i} = \frac{P_i}{\Delta z} \begin{pmatrix} 0 \\ \Delta_i A \end{pmatrix}
\]  

By analogy with the non-conservative terms in the multi-fluid equations studied by [47], the non-zero term in equation (37) is discretised as follows:

\[
\Delta_i A = A_{i+\frac{1}{2}i} - A_{i-\frac{1}{2}i}
\]  

where the areas at the interfaces are taken from within the cell. Analogously, it is easy to show that the non-disturbance relation discussed by [47] holds also here, i.e. under steady conditions with \( u = 0 \) and \( P = \text{const} \) the discretisation preserves the relation:

\[
\frac{\partial (AP)}{\partial z} = P \frac{\partial A}{\partial z}
\]  

3.4 Temporal discretisation

Equation (19) is integrated over the time interval, \( \Delta t \) using an Explicit Euler method. The vapour quality relaxation equation (5) is then solved as shown in [32].

3.5 Boundary conditions
So far the methodology for updating the cell value $U_i$ has been presented assuming that the neighbouring cell values $U_{i-1}$ and $U_{i+1}$ in order to compute the inter-cell fluxes $F_{i+\frac{1}{2}}$ and $F_{i-\frac{1}{2}}$ are available. Given that in practice a finite set of grid cells covering the computational domain exists, the first and last cells will not have the required neighbouring information. In order to close the flow equations, the relevant boundary conditions are imposed by adding a ghost cell at either end of the well [48]. All the thermodynamic properties in the ghost cells are set at the beginning of each time step according to the appropriate boundary condition. It is noted that the boundary conditions explicitly depend on time, given the unsteady nature of the start-up injection of CO$_2$.

The following gives a detailed account of both inflow and outflow boundary conditions.

The mass flow rate at the well injector is determined by the well operator according to the upstream conditions of the transportation system that supplies CO$_2$ to the storage site. The CO$_2$ arrives at a certain pressure and temperature and undergoes an isenthalpic process through a choke valve. The implementation of the inflow boundary condition is represented in Figure 2, where the temporal evolution of the thermodynamic variables in the ghost cell at the top of the computational domain is analysed. At every time step, $t$, a system of three nonlinear equations represented by the following three conditions using the Matlab DASSL solver are resolved:

1. the pressure in the ghost cell will equate the pressure in the first computational cell at time $t - \Delta t$;
2. the CO$_2$ feed stream, arriving with predefined upstream pressure and temperature, undergoes an isenthalpic process. The enthalpy in the ghost cell will therefore equate the enthalpy of the feed stream;
3. the mass flow rate, as imposed by the well operator, is preserved.

![Figure 2: Schematic representation of the isenthalpic inflow condition in the ghost cell at the top of the computational domain.](image)

Note that two of the above conditions carry information coming from outside the domain (namely, the conservation of enthalpy and the mass flow rate prescribed by the well operator), while only one piece of information is provided from the interior of the domain. This is in line with the analysis of time-dependent boundary conditions for subsonic inflows [49,50].

The outflow boundary condition has been modelled according to an empirical pressure-flow relationship derived from reservoir properties [19,29]:

$$\bar{A} + \bar{B} \times M + \bar{C} \times M^2 = P_{\text{BHF}}^2 - P_{\text{res}}^2 \quad (40)$$

where, $\bar{A}$ (Pa) is the minimum pressure required for the flow to start from the well into the reservoir, $\bar{B}$ (Pa s/kg) and $\bar{C}$ (Pa s/kg$^2$) are site-specific dimensional constants, $M$ (kg/s) is the instantaneous mass flow rate at the bottom hole, $P_{\text{BHF}}$ (bar) and $P_{\text{res}}$ (bar) are the instantaneous bottom hole pressure, and the reservoir static pressure respectively.

### 3.6 Heat exchange with the well layers

To reflect reality, eleven outer well layers are taken into account for the 1D radial heat transfer calculations (equations (10) to (12)). These include the tubing, A-annulus water, production casing, oil-based mud, surface casing, B-annulus water, cement, conductor casing, mudstone, sandstone, and chalk. The various layers are discretised into a number of
points in the radial direction from the well axis, and at every point the numerical finite volume heat transfer model computes the instantaneous temperature. Two boundary conditions, namely at the wall where the first well layer is in contact with the CO$_2$ mixture, and that for the outer layer in contact with the surrounding formation are employed. For the inner wall, the heat flux presented by equation (11) is prescribed for the outer wall. The formation temperature is assumed to be known from geological surveys.

4. Results and discussion

Given the availability of pertinent data for modelling purposes, the abandoned Peterhead CCS project [29] is used as a case study in this work. The project would have involved capturing one million tonnes of CO$_2$ per annum for 15 years from an existing combined cycle gas turbine located at Peterhead power station in Aberdeenshire, Scotland followed by pipeline transportation and injection into the depleted Golden Eye Reservoir. However, given the decision of the UK Government to withdraw the capital budget for the Carbon Capture and Storage Competition [51], the project was cancelled.

The data used for the case study include the well depth and geometry, pressure and temperature profiles, along with the surrounding formation characteristics as presented in [19,29] and summarised in Table 1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Well length</td>
<td>2582 m</td>
</tr>
<tr>
<td>Well internal diameter</td>
<td>0 – 800m depth: 0.125m</td>
</tr>
<tr>
<td></td>
<td>800 – 2582m depth: 0.0625m</td>
</tr>
<tr>
<td>Upstream pressure</td>
<td>115 bar</td>
</tr>
<tr>
<td>Inlet mass flow rate</td>
<td>Case 1: linearly ramped-up to 33.5 kg/s in 5 min</td>
</tr>
<tr>
<td></td>
<td>Case 2: linearly ramped-up to 33.5 kg/s in 30 min</td>
</tr>
<tr>
<td></td>
<td>Case 3: linearly ramped-up to 33.5 kg/s in 2 h</td>
</tr>
<tr>
<td>Upstream temperature</td>
<td>Case A: 278.15 K</td>
</tr>
<tr>
<td></td>
<td>Case B: 283.15 K</td>
</tr>
<tr>
<td>Formation temperature</td>
<td>Varying linearly with depth from 277.15 K to 353.15 K along the well</td>
</tr>
</tbody>
</table>

4.1 Case studies

Six CO$_2$ injection scenarios are considered in this part of the study and the resulting transient pressure and temperature profiles along the well are simulated using the above model. The injection scenarios include linear ramping up to a maximum injection flow rate of 33.5 kg/s in 5 min (case 1), 30 min (case 2) and 2 h (case 3) each at two starting injection temperatures of 278.15 K (case A) and 283.15 K (case B) for the vertical well. For reference purposes, each of the six scenarios will be named after the corresponding ramping up scenario and temperature given in Table 1. For example, case 1-A refers to linear ramp-up from 0 to 33.5 kg/s in 5 min at a feed temperature of 278.15 K and so on.

To ensure numerical stability and convergence, a Courant–Friedrichs–Lewy condition of 0.3 [52] a relaxation time of $10^{-4}$s and 300 computational cells are employed for conducting the injection simulations. For the numerical approximation of the heat exchanges with the well layers, the discretisation parameters given by [19] are employed. The above corresponds to ca ± 0.1% convergence error in the predicted temperatures and pressures.

For the heat transfer analysis, thickness, heat capacity, heat conductivity, and density for the eleven well layers are taken from [19]. To achieve converged solution of the heat conduction equation (12), the eight layers of well tubing and casing (overall thickness of ca 716 mm) have been discretised into 716 points, while 60 m of rock surrounding the well has been discretised into 1000 nodes.
The injection model was coded in FORTRAN, compiled using Intel compiler on Linux platform, and run on a desktop Intel® Xeon® W-2123 computer with 3.6 GHz CPU and 5Gb RAM.

The initial pressure and temperature profiles along the tapered well are given in Figures 3 and 4 respectively. The relatively low pressure at the bottom of the well (ca. 38 bar) means that the CO₂ remains in the gaseous phase in the first 400 m along the well, following which transition to the dense or liquid phase takes place (as indicated by the vertical dashed lines).

Figure 3: The initial pressure profile along the well (origin corresponds to the top of the well).

Figure 4: The initial temperature profile along the well (origin corresponds to the top of the well).

Figure 5 shows the variations of the CO₂ pressure and temperature at the top of the well as a function of time during the linear ramping up injection from 0 to 33.5 kg/s over min 300 s (case 1A). The feed CO₂ stream pressure and temperature are 115 bar and 278.15 K respectively. Figure 6 shows the same transient profiles but for the higher feed temperature of 283.15 K (case 1B) representing its prior heating. For both of the above initial conditions, the injected CO₂ is in the dense phase and remains so for the entire time frame (500 s) under consideration.
Figure 5: Transient pressure and temperature profiles at the top of the well for the fast injection ramping rate, case 1A (feed temperature 278.15 K). The vertical dashed line indicates the time (300 s) at which the injection flow rate reaches its peak value of 33.5 kg/s.

Figure 6: Transient pressure and temperature profiles at the wellhead for the fast injection ramping rate; case 1B (feed temperature 283.15 K). The vertical dashed line indicates the time (300 s) at which the injection flow rate reaches its peak value of 33.5 kg/s.

As it may be observed, in both cases an initial rapid depressurisation and cooling is followed by more rapid recoveries with the maximum values occurring at or shortly after the time (300 s) at which the injection rate reaches its peak value (33.5 kg/s). Also, whilst the temperature remains relatively constant thereafter, a secondary modest (ca. 5 bar) drop in the fluid pressure is obtained. As expected, the lower the feed temperature, the lower the minimum temperature attained. In the case of the feed temperature of 278.15 K, the lowest temperature reached at the top of the well is 265 K (case 1A). This compares with the slightly higher minimum temperature of 267.5 K for the feed temperature of 283.15 K (case 1B). Given that both of these minimum temperatures are below the freezing point for water, the presence of an appreciable amount of water in either the CO₂ stream or the well would pose the risk of blockage due to ice formation at the wellhead some 180 s after the injection process has commenced.

Figure 7 shows the CO₂ hydrate phase diagram [53]. The dark grey region (V-I-H) represents the conditions at which CO₂ hydrate is stable together with gaseous CO₂ and water ice (below 273.15 K). Table 2 shows the minimum CO₂ temperatures at the wellhead and the corresponding pressures for the six test scenarios (see Table 1).
Reference to Figure 7 along with the data presented in Table 2 indicates that hydrate formation is unlikely at the prevailing injection conditions.

Figure 8 and 9 respectively present the wellhead pressure and temperature transient profiles for the longer injection ramping up durations of 30 min (1800 s) and 2 h (7200 s). The feed temperature in both cases is 278.15 K (cases 2A and 3A). The observed trends in pressure and temperature are similar to those for the shorter ramping-up period with the exception of being more in concert with one another as compared to the faster pressure ramping scenarios. The latter is consistent with the longer opportunity for CO\(_2\) to attain thermal and pressure equilibration along the injection well. For the medium injection rate (Figure 8), the termination of the temperature recoveries closely coincides with the time at which the peak injection rate is reached. In the case of the long injection rate however, thermal stabilisation occurs some 1800 s later. Most importantly, the longer the injection ramping up period, the lower is the minimum CO\(_2\) temperature reached at the wellhead thus increasing the risk of wellhead blockage due to ice formation. The minimum temperature of ca. 252 K (21°C below the freezing point for water) is observed for case 3-A (Figure 9) corresponding to an injection ramping-up period and temperature of 7200 s and 278.15 K respectively.
Figure 8: Transient pressure and temperature profiles at the top of the well for the medium injection ramping rate, case 2-A (feed temperature = 278.15 K). The vertical dashed line indicates the time (1800 s) at which the injection flow rate reaches its peak value of 33.5 kg/s.

Figure 9: Transient pressure and temperature profiles at the top of the well for the slow injection ramping rate, case 3-A (feed temperature = 278.15 K). The vertical dashed line indicates the time (7200 s) at which the injection flow rate reaches its peak value of 33.5 kg/s.

Interestingly, as well as being more pronounced in the magnitude of their drops, the pressure and temperature profiles of cases 2-A (Figure 8) and 3-A (Figure 9) are in better concert with one another as compared to the faster pressure ramping scenarios (Figures 5 and 6). Also, for case 3-A (Figure 9) at 7200 s, where the linear ramp-up injection reaches the peak flow rate, neither the pressure nor the temperature immediately stabilise.

Figures 10 to Figure 12 respectively represent the variations of pressure and temperature at the bottom of the well as a function of time for the fast (Figure 10; case 1-A), medium (Figure 11: case 2-A) and slow (Figure 12: case 3-A) injection ramping strategies. The lower feed temperature of 278.15 K is assumed in all cases. As expected, the bottom well pressure increases as the CO₂ injection proceeds reaching a maximum value ca. 197 bar. Interestingly, for the medium (Figure 11) and the slow-injection ramping rates (Figure 12), the well bottom pressure reaches its maximum constant value at or soon after the time at which the peak injection rates are attained (1800 s and 7200 s). However in the case of the fast injection ramping up (Figure 10), the pressure at the bottom of the well keeps increasing, albeit by a modest amount, well after the maximum injection rate has been reached.
Figure 10: Transient pressure and temperature profiles at the bottom of the well for the fast injection ramping rate, case 1A (feed temperature 278.15 K; see Table 1). The vertical dashed line indicates the time (300 s) at which the injection flow rate reaches its peak value of 33.5 kg/s.

Referring to the temperature profiles, in all three cases, the bottom well temperature decreases with time as the ‘cooled’ injected CO$_2$ at the top of the well travels towards it. Moreover, the magnitude of the drop in the temperature at the bottom of the well increases with increase in the injection ramping up period with the minimum temperature corresponding to 284.5 K. Given that this temperature is well above the freezing point for water, for the conditions simulated, there is no risk of ice or hydrate formation at the bottom of the well.

Figure 11: Transient pressure and temperature profiles at the bottom of the well for the medium injection ramping rate, case 2-A (feed temperature = 278.15 K). The vertical dashed line indicates the time (1800 s) at which the injection flow rate reaches its peak value of 33.5 kg/s.
Finally Figure 13 shows a comparison of the simulated wellhead transient temperature profiles at the three injection ramping up durations of 5 min (300 s), 30 min (1800 s) and 2 h (7200 s). The injection temperature and pressure are 276 K and 115 bar respectively. The solid lines represent the simulated data generated using the present model. The dotted lines on the other hand show the predicted data reproduced from the Peterhead CCS project report [29] for CO$_2$ injection into the depleted Golden Eye Reservoir using the commercial software, OLGA [26].

As it may be observed, both sets of simulations produce very similar trends; the initial rapid drop in temperature upon the injection of CO$_2$ is followed by a rapid recovery. The magnitude and the duration of the drop in temperature both increase with increase in the injection ramping up duration. Also, the slower the injection ramping up rate, the longer it takes for the fluid temperature to recover. Remarkably all three injection ramping up rates indicate minimum temperatures falling well below zero °C indicating the risk of well blockage due to ice formation in the event of the presence of appreciable amounts of water as well as the possibility of well bore fracture due to thermal shocking. This risk increases as the injection ramping up rate increases. As for the finite disagreement between the predictions between the two sets of simulations, it is difficult to draw any plausible conclusions given the absence of the detailed pertaining theory, in particular the formulation of the boundary conditions at the wellhead and the reservoir along with their implementation into the flow model capable of handling a time variant feed rate in the OLGA software.

5. Conclusion
As part of the challenge in combating global warming, depleted gas fields present ideal locations for storing the huge quantities of CO$_2$ captured from fossil fuel power plants and various energy intensive industrial emitters.

A significant expansion induced cooling of the high pressure CO$_2$ arriving at the top of the low pressure wellhead leading to the storage reservoir poses a number of potential hazards, including; well blockage, thermal shocking of the well bore steel lining and a reduction in the effective storage capacity. As such, the controlled gradual expansion of the CO$_2$ at the point of injection into the well balancing the requirement to minimise the temperature trop whilst ensuring maximum injection rate during the start-up injection is fundamentally important.

In this paper, we presented the development, testing and verification of a rigorous mathematical model for simulating the highly transient flow and heat transfer effects taking place throughout the well bore during the start-up injection of CO$_2$ into highly depleted gas reservoirs.

Through the development and integration of the appropriate boundary conditions at the wellhead, the well bottom (reservoir permeability) and taking into account the detailed well bore properties such as its heat transfer characteristics and the surrounding core, well tapering and deviation from the horizontal, our model can be used as a useful practical engineering tool for determining the optimum injection ramping up rates.

Based on the application of the injection model simulating the injection of CO$_2$ in a real offshore depleted gas field in the North Sea, we make the following important observations for three selected nominal injection ramping up rates representing slow, medium and slow injection scenarios:

i) in all cases tested, the temperature of expanded CO$_2$ at the wellhead drops well below zero °C representing the risk of well blockage due to ice formation in the event of the presence of an appreciable amount of water and well bore fracture due to thermal shocking. However, well blockage due to hydrate formation proved unlikely;

ii) remarkably, the magnitude of the temperature drop increases with decrease in the injection ramping up rate. This means that slower injection ramping up rate gives rise to a higher risk of well blockage. The above observation is consistent with the published literature;

iii) as expected the preheating of the CO$_2$ prior to its injection reduces the risk of ice formation. However, the corresponding energy and hence cost implications will most likely not make this a viable option especially given the significant quantities of CO$_2$ being injected in practice (typically, millions of tonnes to reach full reservoir capacity);

iv) in none of the three test cases examined does the well bottom temperature drops below zero °C indicating minimal risk of the blockage of the well bore bottom perforations.

In conclusion, it is important to point out that the above observations are based on the application of the model developed to the particular, albeit realistic test case examined in the present study. As such the findings should not be considered as universally applicable to all cases involving injection of CO$_2$ into depleted gas reservoirs. Each injection scenario should be investigated based on the prevailing conditions. Certainly, this study shows that the choice of the injection ramping up rate has a profound impact on the highly transient temperature and pressure profiles incurring during the start-up injection process and the subsequent risks. The mathematical model presented in this work, once translated into a robust computational software, can be used as a valuable tool by engineers to determine the optimum injection ramping up rates into depleted gas reservoirs. This will contribute to accelerating the role out of CCS in transitioning the CO$_2$ emitting energy intensive industries onto a pathway consistent with the quest to limit the increase in the global average temperatures.

6. Acknowledgement
The authors are grateful to the UK Carbon Capture and Storage Research Centre for the funding of this work through the Flexible funding Call 2 C2-183.

7. **Nomenclature**

\( A \) = well bore cross sectional Area \((m^2)\)

\( \tilde{A} \) = minimum pressure required for the flow to start from the well into the reservoir \((Pa)\)

\( \tilde{B} \) = site-specific dimensional constant \((Pa \ s \ Kg^{-1})\)

\( \tilde{C} \) = site-specific dimensional constant \((Pa \ s \ Kg^{-2})\)

\( c_p \) = heat capacity at constant pressure \((J \ K^{-1})\)

\( D_p \) = internal diameter of the pipe \((m)\)

\( E \) = specific total energy \((J \ Kg^{-1})\)

\( e \) = specific internal energy \((J \ Kg^{-1})\)

\( F \) = viscous friction force

\( f_w \) = Fanning friction factor

\( g \) = gravitational acceleration \((m \ s^{-2})\)

\( H \) = total enthalpy of the fluid \((kJ \ kg^{-1})\)

\( k \) = fluid thermal conductivity \((W \ m^{-1} \ K^{-1})\)

\( \kappa \) = heat conductivity \((W \ m^{-1} \ K^{-1})\)

\( M \) = instantaneous mass flow rate at the bottom hole \((kg \ s^{-1})\)

\( ml \) = meta-stable(super-heated) liquid phase

\( \dot{m} \) = area-weighted mass flux \((kg \ s^{-1} \ m^{-2})\)

\( \mathcal{M} \) = Mach number

\( \tilde{M} \) = arithmetic averages of the values attained by Mach number

\( P \) = Mixture pressure \((bar)\)

\( P_{BHF} \) = instantaneous bottom hole pressure \((bar)\)

\( P_c \) = critical pressure \((bar)\)

\( Pr \) = Fluid Prandtl number

\( P_{res} \) = reservoir static pressure \((bar)\)

\( Re \) = Reynolds number

\( Q \) = heat flux \((W \ m^{-2})\)

\( sv \) = saturated vapour phase
\( T \) = fluid temperature (K)
\( t \) = time (s)
\( T_c \) = critical temperature (K)
\( T_w \) = wall temperature (K)
\( u \) = mixture velocity (m s\(^{-1}\))
\( x \) = mixture vapour quality
\( z \) = space coordinate

**Greek Symbols**

\( \rho \) = mixture density (Kg m\(^{-3}\))
\( \theta \) = relaxation time (s)
\( \theta \) = well deviation from the vertical (°)
\( \eta \) = Corresponding heat transfer coefficient (W m\(^{-2}\) K\(^{-1}\))
\( \omega \) = acentric factor for CO\(_2\).
\( \bar{\rho} \) = density of sound in cells \( i \) and \( i + 1 \) (Kg m\(^{-3}\))
\( \bar{a} \) = Speed of sound in cells \( i \) and \( i + 1 \) (m s\(^{-1}\))

8. References

[1] Energy Technology Perspectives 2017
   https://webstore.iea.org/energy-technology-perspectives-2017


[38] Dittus FW, Boelter LMK. Heat Transfer in Automobile Radiators 1930;2:443.


kgkg