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Moslehi, S., Kahrobaei, S., Farajzadeh, R., & Voskov, D. (2026). DARTS-well: An open-source fully coupled well–reservoir numerical model using the Operator-based Linearization Approach. *Computer Methods in Applied Mechanics and Engineering*, 461, Article 119231. <https://doi.org/10.1016/j.cma.2026.119231>

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DARTS-well: An open-source fully coupled well–reservoir numerical model using the Operator-based Linearization Approach

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ARTICLE INFO

Keywords:

Coupled well–reservoir modeling

Multiphase flow

Thermal flow

Operator-Based Linearization

GCS

Depleted hydrocarbon reservoirs

ABSTRACT

During subsurface energy-transition operations, such as carbon dioxide sequestration, underground hydrogen storage, and geothermal energy extraction, fluid flow into the well and reservoir can induce strong hydraulic and thermal interactions between the well and the near-wellbore region. These interactions are particularly critical during high-pressure CO₂ injection into depleted reservoirs, where significant temperature reductions may occur along and around the well, leading to complex phase behavior and potentially reducing injectivity. Conventional standalone well or reservoir models, however, fail to resolve these well–reservoir interactions. A fully coupled well–reservoir model is therefore essential to ensure accurate, safe, and efficient subsurface energy-transition operations. To address this need, we develop an open-source, computationally efficient numerical model for transient, thermal, multiphase flow in a fully coupled well–reservoir system. A multiphase, transient wellbore model is developed using the Drift-Flux Model and fully coupled with the high-performance, open-source Delft Advanced Research Terra Simulator (open-DARTS). Open-DARTS uses Operator-Based Linearization (OBL), where state-dependent properties are grouped as operators and interpolated from multidimensional tables generated on the fly, reducing the cost of evaluating residuals and derivatives in Newton–Raphson iterations. The wellbore model is verified against an analytical solution and benchmarked against industry-standard well simulators for single- and two-phase, isothermal and thermal flow in vertical and inclined wells, and the coupling approach is also benchmarked against a commercial coupled simulator. We then simulate liquid CO₂ injection into a North Sea–representative depleted gas reservoir using grid and OBL resolutions selected by convergence analyses.

1. Introduction

Subsurface energy-transition technologies, such as Geological Carbon Sequestration (GCS), underground hydrogen storage (UHS), and geothermal energy extraction, play a critical role in reducing greenhouse gas emissions and enabling a sustainable energy future. Among these, GCS has been widely recognized by the Intergovernmental Panel on Climate Change (IPCC) as a key strategy for mitigating climate change. Depleted hydrocarbon reservoirs are among the most viable subsurface options for GCS, with an estimated global storage capacity of approximately 675 to 900 gigatons [1]. Depleted gas reservoirs are appealing targets for GCS because of

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<https://doi.org/10.1016/j.cma.2026.119231>

Received 9 April 2026; Received in revised form 23 June 2026; Accepted 8 July 2026

Available online 17 July 2026

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their proven seal, reservoir characterization knowledge, and existing infrastructure [1,2]. However, the injection of high-pressure CO₂ into a depleted hydrocarbon reservoir may introduce operational challenges in both the wellbore and the reservoir. During injection of compressed CO₂ into depleted reservoirs, pressure reduction across the surface choke and further possible pressure drop along the wellbore cause cooling due to the Joule-Thomson effect and the latent heat of vaporization, potentially compromising well integrity. Additionally, the influx of cold CO₂ at the sandface, and the further cooling it undergoes in the near-wellbore region, may lead to the formation of CO₂ hydrates and even ice under extreme conditions, which can potentially impair the wellbore injectivity [3–8]. To better understand the mass and energy flow and their dynamics inside a well–reservoir system, and thereby anticipate temperature transients that can induce cooling-related wellbore damage, numerical simulation plays a key role to predict the state of the system and prevent/mitigate risks associated with low-temperature conditions. However, simulating the wellbore and reservoir separately can lead to inaccurate predictions as these two connected media have mutual hydraulic and thermal effects.

The need for coupled well–reservoir modeling for CO₂ sequestration operations can be viewed from two perspectives: wellbore modeling and reservoir modeling. From a standalone wellbore modeling perspective, the reservoir is typically represented by a constant injectivity index. In reality, however, reservoir rock and fluid properties may change over time (e.g., due to salt precipitation, hydrate formation, etc.), causing well injectivity to change. In addition, the pressure of a finite-acting reservoir increases over time due to the accumulation of the injected CO₂. Such variations directly influence the pressure profile along the wellbore, which in turn alters the temperature profile and bottom-hole temperature, an important parameter for CO₂ disposal in depleted reservoirs. Consistent with this, Van Nimwegen et al. [9] coupled an in-house steady-state well simulator with CMG-STARS in a two-way manner to simulate liquid CO₂ injection into a depleted reservoir, showing that wellbore injectivity varies with reservoir pressure due to changes in the injected fluid properties and phase fractions.

From the reservoir modeling perspective, inflow is typically modeled with fixed temperature or enthalpy, or via lift tables, which fail to account for complex hydraulic and thermal changes within the wellbore. For instance, for injection of high-pressure CO₂ into depleted hydrocarbon reservoirs, using the tubing head temperature as the bottom-hole temperature for reservoir simulators can be misleading since CO₂ undergoes temperature changes along the wellbore due to a combination of potential energy loss, Joule-Thomson effects (heating for gravity-dominated pressure profiles and cooling for friction-dominated pressure profiles), phase-change enthalpy (latent heat of condensation or vaporization), and lateral heat exchange. Using conditions upstream of the choke is even more problematic since CO₂ may undergo substantial pressure and temperature changes across the choke. Such variations directly affect the temperature of CO₂ injected into the formation at the sandface, thereby influencing near-wellbore and reservoir conditions [10,11]. These limitations show that reservoir-only simulations are effectively blind to the hydraulic and thermal processes occurring inside the wellbore, motivating the need for coupled well–reservoir modeling.

Coupled well–reservoir modeling also enables detailed investigations of the extent of cooling in CO₂ injection scenarios involving transient periods such as well start-up, well shut-in, and intermittent CO₂ injection due to variable supply or ship-transport systems. A coupled well–reservoir model can also be beneficial for CO₂ injection into layered reservoirs or wells with multiple perforations. In these reservoirs, accurate calculation of the injection rate for each layer/perforation is challenging due to differences in fluid transmissibility in each layer/perforation (i.e., layer thickness and permeability) [12], differences in fluid mobility in each layer/perforation (i.e., phase relative permeability and viscosity), gravity override/underdrive inside the wellbore [13,14], the variability of the flow pattern and phase properties along the wellbore and preferential feeding of upper perforations [12]. This variable distribution of CO₂ influx into the reservoir interval can lead to different extents of salt precipitation and hydrate formation, indicating the importance of coupling and simultaneous simulation of the reservoir and wellbore.

The standard well model is the most commonly used approach for modeling wells in reservoir simulations. It treats the well as an internal boundary condition or a source/sink term within the perforated reservoir blocks [15]. While providing computational efficiency, this model has limitations. It is blind to the physics within the wellbore, including multiphase flow, thermal effects, and changes in CO₂ properties under varying thermodynamic conditions. Therefore, a multi-segment wellbore modeling approach is required to capture wellbore physics. To calculate phase velocities for multiphase fluid flow in multi-segment pipes (e.g., wells), various approaches are used in the literature. The Equivalent Porous Medium (EPM) model, also referred to as the Equivalent Permeability Model, is the simplest approach, which considers the pipe as a porous medium [16,17]. It uses Darcy's law as the momentum equation to calculate fluid velocity in the pipe, considering a porosity value of 1 and a very high permeability. This model has shown deviations when used to describe CO₂ leakage flow in the wellbore due to exclusion of inertial forces [18–20] and also in CO₂ injection scenarios [21].

Unlike the EPM, the Multi-Fluid Model (MFM) considers the pipe as an actual void space and so uses the Navier–Stokes equation as the momentum equation to calculate phase velocities. In this model, a 1D momentum equation is written for each phase present in the pipe. The momentum equations contain terms describing momentum exchange between the phases, and closure relations for these terms are required, which have different forms for different flow patterns. This model can experience numerical problems specially when a fully implicit technique is used to solve the system of equations [22] and may display discontinuities in pressure drop and liquid hold-up at some flow-pattern transitions, which can give rise to convergence problems within the simulator [23]. Similar to MFM, the Drift-Flux Model (DFM) also considers the pipe as an actual void space, but instead of having multiple momentum equations, a single momentum equation is written for the mixture as a whole, and a slip relation is used to account for the relative motion of liquid and gaseous phases [23,24]. Therefore, the DFM is computationally more efficient due to using a single governing equation [25], but is an approximate formulation compared to the more rigorous MFM. However, it is more stable and robust because of providing a smooth and continuous slip relation for all flow patterns. The DFM is free from singularities at small values of volume fractions, while in the MFM, the disappearance of the phase may induce the growth of velocity to unrealistic values [25]. A simplified version of the DFM is the no-slip homogeneous model, which does not consider slip between phases. Therefore,

it is more suitable for downward-flow cases or the cases where the phases have close properties (near the critical point) [26]. The coupled well–reservoir simulator CALYSTO [27] and CO2Well-TOUGH2 [28] use the no-slip homogeneous approach to model two-phase flow of CO₂ in pipes.

Based on the discussion above, the DFM is used in this study to calculate phase velocities in CO₂ wells. To solve the system of conservation equations for the wellbore, however, different approaches are used in the literature. In the fully-implicit scheme, phase velocity is considered as a primary variable for which a momentum equation needs to be solved. This requires inclusion of the momentum equations of pipe segments in the Jacobian matrix and introducing specific linear solvers and preconditioners [29]. This approach is currently used in most commercial simulators. An alternative is a semi-implicit approach, in which phase velocities are not treated as primary unknowns in the Newton system. Instead, the conservation equations are solved implicitly for pressure, overall composition, and temperature (or enthalpy), while the phase velocities are updated directly using the DFM closure, rather than being introduced as additional primary variables. This approach was implemented and coupled in a semi-implicit manner in TOUGH2 simulator using numerical derivatives [30]. This semi-implicit approach is adopted in this study and will be described in more details below.

The developed well model, using the semi-implicit DFM specified above, is verified with the analytical solution and benchmarked against T2Well [30] and OLGA [31]. The verified well model is fully coupled with the open-source Delft Advanced Research Terra Simulator (open-DARTS) [32–34]. The coupling approach is also tested against that in the Shell in-house coupled well–reservoir model [4]. The reservoir model used in this study, open-DARTS, utilizes the Operator-Based Linearization (OBL) technique [35,36], which reduces the computational time for resolving the highly nonlinear physics stemming from large variations in fluid properties and their expensive evaluation during simulation. The fully coupled approach applied here, unlike two-way coupling approach, has higher solver stability, which also leads to a shorter total computational time. The computational and numerical performance of the developed model is investigated in the results. Using the developed coupled well–reservoir model, convergence analyses are performed for the OBL, wellbore, and reservoir grid resolutions. Lastly, to demonstrate the coupled well–reservoir model, a representative case study is considered involving the injection of liquid CO₂ into a highly depleted gas reservoir. Beyond the liquid CO₂ injection case demonstrated here, the fully coupled formulation can be used to investigate water-related near-wellbore processes, such as dry-out, salt precipitation, and hydrate or ice formation/dissociation, where the coupled evolution of pressure, temperature, phase behavior, and injectivity is essential. In addition, the implementation within open-DARTS provides a path for future computational extensions that exploit the GPU capabilities of the simulator, enabling more efficient simulations of large-scale and high-resolution coupled well–reservoir problems.

2. Methodology

To develop the coupled well–reservoir model, a multi-segment wellbore model is first developed using the two-phase DFM, described in Sections 2.1 and 2.2. The developed well model is then full coupled with the open-DARTS reservoir simulator, described in Section 2.3.

2.1. Wellbore model: Introduction to the two-phase drift-flux model (DFM)

Based on the discussion in the Introduction, the DFM is used to model two-phase fluid flow in wells in this study. The DFM formulation implemented in T2Well [30], which is a modified version of the original DFM proposed by Shi et al. [23], is adopted here. The model accounts for slip between gaseous and liquid phases using a combination of two mechanisms. One mechanism results from the non-uniform profiles of velocity and phase distribution over the pipe cross-section. The other mechanism results from the tendency of gas to rise vertically through the liquid due to buoyancy. In this approach, the gas velocity (v_g) and liquid velocity (v_l) are calculated from the mixture velocity (v_m) as

$$v_g = C_0 \frac{\rho_m}{\rho_m^*} v_m + \frac{\rho_l}{\rho_m^*} v_d, \quad (1)$$

$$v_l = \frac{(1 - s_g C_0) \rho_m}{(1 - s_g) \rho_m^*} v_m - \frac{s_g \rho_g}{(1 - s_g) \rho_m^*} v_d, \quad (2)$$

where C_0 is the profile parameter, ρ_m and ρ_m^* are the average density and the profile-adjusted average density, respectively, ρ_g and ρ_l are gas and liquid density, respectively, v_d is the drift velocity, and s_g is gas saturation. The closure relations used to evaluate these quantities are given in [Appendix A](#).

2.2. Wellbore model: Governing equations and their implementation

The mass- and energy-conservation equations are discretized in space using the finite-volume scheme and in time using a backward, first-order, Euler scheme. The scalar variables, such as pressure, overall mole fractions, and temperature (or specific enthalpy), are evaluated at segment centroids, while velocities are computed at segment interfaces, resulting in a staggered-grid arrangement. The momentum equation is discretized semi-implicitly, similar to the T2Well simulator [30]. As an example, the

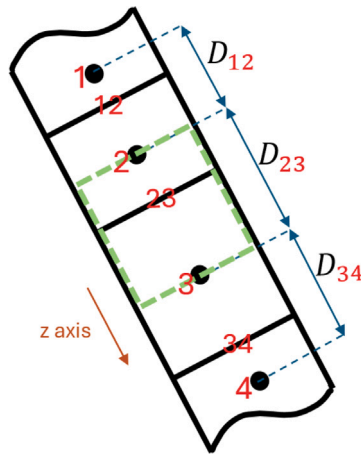


Fig. 1. Indexing of control volumes and their interfaces for a wellbore.

discretized momentum equation at the interface 23 between two neighboring wellbore segments 2 and 3 in Fig. 1 can be written as

$$\frac{(\rho_m v_m - \rho_m^n v_m^n)_{23}}{\Delta t} + \frac{\delta_3^n - \delta_2^n}{A_{23}(z_3 - z_2)} = - \left(\frac{\Gamma f^n \rho_m v_m |v_m^n|}{2A} \right)_{23} - \frac{p_3 - p_2}{z_3 - z_2} + (\rho_m)_{23} g \cos(\theta_{23}), \quad (3)$$

where Δt is the time-step size, A is the wellbore cross-sectional area defined at interfaces, z is the along-wellbore coordinate defined at segment centroids, Γ is the internal perimeter of the wellbore, f is the Fanning friction factor (relations used for calculation of the Fanning friction factor are given in Appendix B), p is segment pressure, and θ is the wellbore inclination from vertical. In these discrete equations, superscript n denotes the previous time level, while terms without it denote the current time level. δ_2 and δ_3 are the momentum terms at the 2nd and 3rd segments, which is defined as the weighted-average of that at all neighboring interfaces. For example, δ_2 is

$$\delta_2 = \frac{(A_{12}\delta_{12})/D_{12} + (A_{23}\delta_{23})/D_{23}}{A_{12}/D_{12} + A_{23}/D_{23}}, \quad (4)$$

where δ_{12} and δ_{23} are momentum terms at interfaces 12 and 23. As an example, δ_{12} is defined as

$$\delta_{12} = A_{12} \sum_{j=1}^{n_p} (\rho_j s_j v_j^2)_{12} \quad (5)$$

If the wellbore has a constant radius and all the segments of the wellbore have the same size, Eq. (4) reduces to

$$\delta_2 = \frac{\delta_{12} + \delta_{23}}{2} \quad (6)$$

To calculate the momentum terms at the centroids of the boundary segments of the wellbore, we need to calculate the momentum terms at the external faces of the wellbore using the boundary conditions defined, but if the boundary is a perforation, since the fluid enters or exits the well perpendicular to the direction of flow and momentum is a vector quantity, there is no net transfer of momentum along the wellbore due to fluid flow at the perforation, meaning $\delta_{perf} = 0$ [37].

From Eq. (3), the product of mixture density and velocity at interface 23 at the current time step is calculated as

$$(\rho_m v_m)_{23} = - \frac{w}{z_3 - z_2} (p_3 - p_2) + w g \cos(\theta_{23}) (\rho_m)_{23} - w \left(\frac{\delta_3^n - \delta_2^n}{A_{23}(z_3 - z_2)} - \frac{(\rho_m^n v_m^n)_{23}}{\Delta t} \right), \quad (7)$$

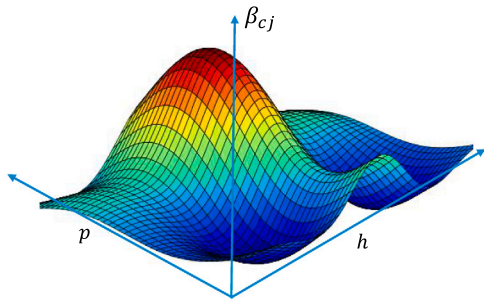
where

$$w = \frac{1}{1/\Delta t + (\Gamma f^n |v_m^n|)_{23}/(2A_{23})}. \quad (8)$$

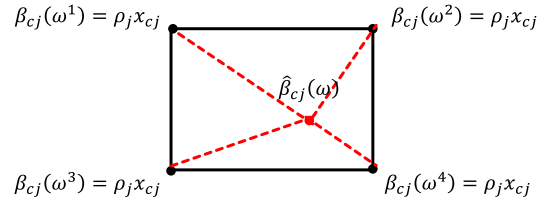
The phase velocities at interface 23 at the current time step, $(v_g)_{23}$ and $(v_l)_{23}$, are then calculated using the following equations with both the drift velocity and the profile parameter evaluated at the previous time level

$$(v_g)_{23} = \left(\frac{C_0^n}{\rho_m^*} (\rho_m v_m) + \frac{\rho_l}{\rho_m^*} v_d^n \right)_{23}, \quad (9)$$

$$(v_l)_{23} = \left(\frac{1 - C_0^n s_g}{(1 - s_g)\rho_m^{*n+1}} (\rho_m v_m) - \frac{s_g \rho_g}{(1 - s_g)\rho_m^*} v_d^n \right)_{23}. \quad (10)$$



(a) Parameterization of the operator β_{cj} in 2D (pressure and specific enthalpy) space with a predefined OBL resolution.



(b) Interpolation process for β_{cj} operator. ω^1 through ω^4 are four supporting points, and ω is the current physical state of a given control volume at a given timestep during simulation, where the operator is interpolated.

Fig. 2. Parameterization and interpolation of operators (here for β_{cj}) in open-DARTS.

The discretized mass conservation equation of the c th component for segment 3 is given below as

$$V_3 \left[\left(\sum_{j=1}^{n_p} s_j \rho_j x_{cj} \right) - \left(\sum_{j=1}^{n_p} s_j \rho_j x_{cj} \right)^n \right]_3 + \Delta t \sum_{l=23,34} \left(\sum_{j=1}^{n_p} v_j^l A^l s_j^{l,up} \rho_j^{l,up} x_{cj}^{l,up} \right) + \Delta t q_{c,3} = 0, \quad c = 1, \dots, n_c, \quad (11)$$

where V is the segment volume, x_{cj} is the mole fraction of component c in phase j , and q_c is the sink/source rate of component c . The superscript up denotes the upwinded value of the corresponding property, evaluated according to the flow direction at interface l .

The discretized energy conservation equation for segment 3 is as follows

$$V_3 \left[\left(\sum_{j=1}^{n_p} s_j \rho_j \left(h_j + \frac{(v_j^2)^n}{2} + gz \cos(\theta) \right) - p \right) - \left(\sum_{j=1}^{n_p} (s_j \rho_j)^n \left((h_j)^n + \frac{(v_j^2)^n}{2} + gz \cos(\theta) \right) - p^n \right) \right]_3 + \Delta t \sum_{l=23,34} \left[\sum_{j=1}^{n_p} A^l s_j^{l,up} \rho_j^{l,up} \left(v_j^l h_j^{l,up} + (v_j^l)^n \left(\frac{(v_j^l)^2}{2} \right)^{up} + (v_j^l)^n (gz^l \cos(\theta^l))^{up} \right) \right] + \Delta t q_{heat,3} = 0, \quad (12)$$

where h is specific enthalpy and q_{heat} is the energy source/sink rate.

2.3. Coupled well-reservoir model: Implementation of the mathematical formulation

Now that the wellbore model is presented, we need to couple it with a reservoir simulator. In this study, open-DARTS is used as the reservoir simulator and as the platform to solve the system of wellbore governing equations for the fully coupled well-reservoir model. Open-DARTS is a computationally-efficient simulator which can be used to model various subsurface-related energy transition problems [38–41]. In the framework of open-DARTS, the evaluation of the residuals and construction of the Jacobian matrix are done using the operator-based linearization (OBL) approach [35]. In this approach, appropriate state-dependent properties (e.g., overall composition, pressure, temperature, phase density, viscosity, relative-permeability, specific enthalpy, volume fraction, and thermal conductivity) are grouped together as state-dependent operators (e.g., operator β_{cj} in Fig. 2), and these operators are evaluated via interpolation from multidimensional tables dynamically generated during the simulation, which increases the speed of the simulator by faster evaluation of residuals and their corresponding derivatives. Evaluation of the operator β_{cj} for a specific state ω via parameterization and interpolation is shown in Fig. 2. The OBL approach also provides an opportunity to control the non-linearity of the physics of the model by changing the resolution of the parameter space to improve the performance and robustness of the simulation [42]. Further details related to the open-DARTS implementation can be found in Khait [43].

To incorporate and solve the wellbore governing equations in open-DARTS in a fully coupled manner, the discretized mass conservation equation in open-DARTS is reformulated in the operator general form as follows [44]

$$V_i \phi_{0i} [\alpha_c(\omega) - \alpha_c(\omega^n)]_i - \Delta t \sum_{l \in L(i)} \sum_{j=1}^{n_p} q_j \beta_{cj}(\omega^{l,up}) - \Delta t q_{c,i} = 0, \quad c = 1, \dots, n_c, \quad (13)$$

where V_i is the void volume of grid cell i , ϕ_{0i} is its porosity, and Δt is the time-step size. q_j is the phase volumetric rate, while $q_{c,i}$ represents the component c source/sink term for grid block i . n_p and n_c are the number of phases and components, respectively. ω and ω^n denote the primary variables at the current and previous time steps, respectively, and here we defined the state-dependent

operators α and β as

$$\alpha_c(\omega) = \sum_{j=1}^{n_p} s_j \rho_j x_{cj}, \quad \beta_{cj}(\omega) = \rho_j x_{cj}, \quad c = 1, \dots, n_c, \quad j = 1, \dots, n_p, \quad (14)$$

where s_j denotes phase saturation, ρ_j is phase molar density, and x_{cj} is mole fraction of component c in phase j .

Eq. (13) is a generic mass conservation equation for both reservoir and wellbore with only the difference in porosity, ϕ , in the accumulation term (ϕ is 1 in the wellbore) and the phase volumetric rate, q_j , in the flux term. Depending on the connection type, the phase volumetric rate is calculated differently. If the interface connects two reservoir grid cells, Darcy's law is used to calculate the phase volumetric rate as follows

$$q_j = -\Gamma^l \lambda_j(\omega) \Delta \psi_j^l, \quad j = 1, \dots, n_p, \quad (15)$$

where Γ^l is the geometric part of transmissibility for interface l , λ_j is the phase mobility, and $\Delta \psi_j^l$ is the phase pressure potential based on Darcy's law. If the interface connects two wellbore segments, the phase volumetric rate is calculated as follows

$$q_j = A s_j v_j, \quad j = 1, \dots, n_p, \quad (16)$$

where v_j are the phase velocities in the wellbore from the DFM given in Eqs. (9) and (10). If the interface connects a wellbore segment and a reservoir cell (i.e., perforation) and the reservoir block connected to the well is small enough, the radial form of Darcy's law can be used, given in Eq. (17). However, the nodal distance to the interface on the wellbore side is set to zero, which makes the resistance to flow inside the wellbore negligible, reflecting the open-pipe nature of the wellbore domain [30].

$$q_j = -\Gamma^w \lambda_j(\omega) \Delta \psi_j^l, \quad j = 1, \dots, n_p, \quad (17)$$

where Γ^w is the geometric part of the perforation transmissibility, given by $\Gamma^w = 2\pi K h / \ln(r_e/r_w)$, with r_e denoting the radius to the centroid of the reservoir cell and r_w the well radius.

To take thermal effects into account, the discretized energy conservation equation in open-DARTS is also reformulated and extended in the operator general form as follows [45]

$$\begin{aligned} & V_i \phi_{0i} [\alpha(\omega) - \alpha(\omega^n)]_i + V_i E_{p,i} \left[\sum_{j=1}^{n_p} \hat{\alpha}_j(\omega) - \sum_{j=1}^{n_p} \hat{\alpha}_j(\omega^n) \right]_i + V_i \sum_{j=1}^{n_p} E_{k,i,j}^n [\hat{\alpha}_j(\omega) - \hat{\alpha}_j(\omega^n)]_i \\ & - \Delta t \sum_{l \in L(i)} \sum_{j=1}^{n_p} \left[q_j \beta_j(\omega^{l,up}) + q_j \hat{\rho}_j(\omega^{l,up}) E_p^{l,up} + q_j \hat{\rho}_j(\omega^{l,up}) E_{k,j}^{l,up,n} \right] - \Delta t q_{E,i} = 0, \end{aligned} \quad (18)$$

where

$$\alpha(\omega) = \sum_{j=1}^{n_p} s_j \rho_j U_j, \quad \hat{\alpha}_j(\omega) = s_j \hat{\rho}_j, \quad \beta_j(\omega) = \rho_j h_j, \quad j = 1, \dots, n_p. \quad (19)$$

Here, $\hat{\rho}_j$ is the phase mass density, h_j denotes phase molar enthalpy, U_j is phase molar internal energy and $q_{E,i}$ represents the energy source/sink term for grid block i . Besides, we defined the specific potential energy evaluated at cell-centers (i) as

$$E_{p,i} = -g \times 10^{-3} (z_i - z_{ref}) \cos(\theta_i), \quad (20)$$

where z_i and z_{ref} are the measured depth of the grid cell i and reference grid cell, respectively. The specific kinetic energy of phase j is defined as

$$E_{k,j} = \frac{v_j^2}{2}. \quad (21)$$

In the coupled well–reservoir model, the nonlinear system of governing equations is solved iteratively using the Newton–Raphson method. The energy equation can be solved using either temperature or enthalpy as the primary variable, as appropriate for the scenario. To construct the Jacobian matrix, the reservoir and perforation phase volumetric rates (Eqs. (15) and (17)) are differentiated using the OBL approach, while the wellbore phase volumetric rates (Eq. (16)) are differentiated using both perturbation-based and OBL-based derivative evaluation, and their performance is compared in Section 3.3.5 for the presented representative case study. Perturbation-based numerical differentiation is motivated by the limit definition of the derivative

$$R'(x) = \lim_{h \rightarrow 0} \frac{R(x+h) - R(x)}{h}, \quad (22)$$

where x denotes a primary variable, h is an increment in x that approaches zero, and $R(x)$ and $R'(x)$ are the residual equation and its derivative with respect to x , respectively, but perturbation-based numerical differentiation replaces the limiting process $h \rightarrow 0$ with a small, finite perturbation h to obtain a practical approximation. Accordingly, each primary variable is perturbed by a prescribed increment and the resulting change in the residual equations is used to estimate the required derivatives. In this study, the developed coupled well–reservoir model is also used as a standalone wellbore model by excluding the reservoir domain and using appropriate flow boundary at perforation points.

Table 1

Spatial L_2^{RMS} errors against the analytical solution for the steady isothermal two-phase verification cases, computed using Equations (23) and (24). The absolute error has the same units as the corresponding quantity.

Scenario	Quantity	DARTS-well		T2Well	
		L_2^{RMS}	$E_{\text{rel}} [\%]$	L_2^{RMS}	$E_{\text{rel}} [\%]$
CO ₂ -water, 40 °C	Pressure profile [bar]	0.2071	2.3471	0.0658	0.7461
	Gas saturation profile [-]	0.0114	1.4117	0.0044	0.5403
Air-water, 20 °C	Pressure profile [bar]	0.0296	0.8768	0.0778	2.3011
	Gas saturation profile [-]	0.0015	0.1610	0.0017	0.1793

3. Results and discussion

This section first presents the verification and benchmarking of the developed multi-segment wellbore model and the well-reservoir coupling approach. Next, convergence analyses are performed for the OBL resolution and the wellbore and reservoir grid resolutions in the coupled model. Using the optimum parameters from the convergence analyses, a demonstration case of liquid CO₂ injection into a highly depleted hydrocarbon reservoir is presented. This section concludes with investigation of the computational and numerical performance of the developed model.

3.1. Verification and benchmarking of the wellbore model

This subsection verifies and benchmarks the developed wellbore model through comparisons with an analytical solution, T2Well, and OLGA-2022. The comparisons with the analytical solution and T2Well are presented for steady upward flow of gas and water in a water well. This verifies the numerical implementation and benchmarks it against the simulator T2Well whose drift-flux formulation served as the basis for the present model. Additional benchmarking is performed against OLGA-2022, a commercial wellbore simulator [31], using several transient wellbore-flow cases. The quantitative differences between DARTS-well and the reference solutions are evaluated using the integrated L_2^{RMS} error,

$$L_2^{\text{RMS}} = \left[\frac{1}{\xi_b - \xi_a} \int_{\xi_a}^{\xi_b} (q(\xi) - q_{\text{ref}}(\xi))^2 d\xi \right]^{1/2}, \quad (23)$$

and the corresponding relative error,

$$E_{\text{rel}} = \left[\frac{\int_{\xi_a}^{\xi_b} (q(\xi) - q_{\text{ref}}(\xi))^2 d\xi}{\int_{\xi_a}^{\xi_b} q_{\text{ref}}(\xi)^2 d\xi} \right]^{1/2} \times 100\%. \quad (24)$$

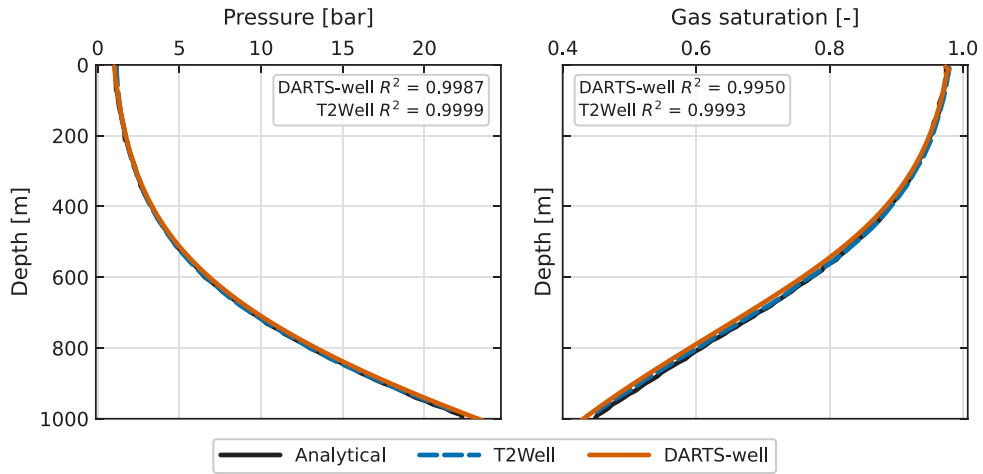
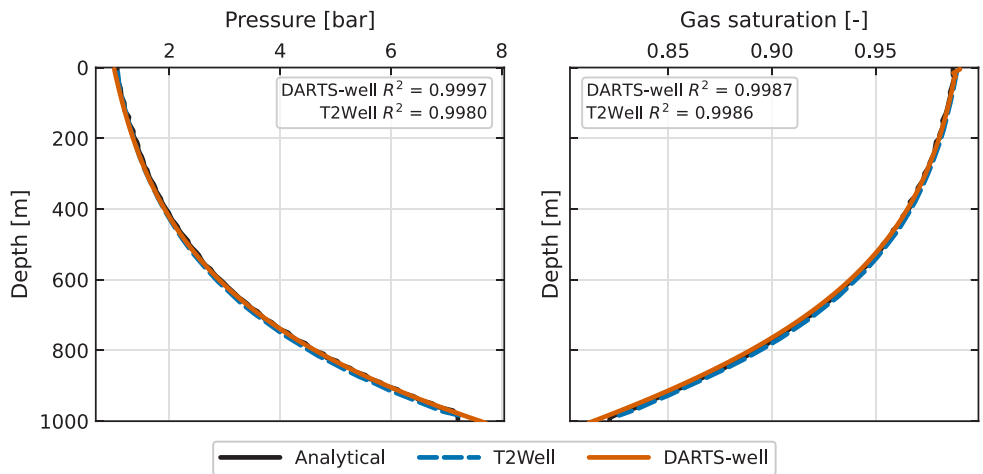
Here, q_{ref} denotes the reference solution. For time series, $\xi = t$; for well profiles, ξ is the measured depth. The integrals are approximated using the trapezoidal rule. For time-series comparisons with OLGA, DARTS-well results are linearly interpolated onto the OLGA output times over the common time interval.

3.1.1. Analytical verification and T2Well benchmarking for steady isothermal two-phase flow

Pan et al. [24,46] verified T2Well against analytical solutions for steady, isothermal, upward two-phase flow in a vertical 1000-m wellbore open to atmospheric pressure. The two cases considered are CO₂-water flow at 40 °C and air-water flow at 20 °C, respectively. The analytical solutions assume immiscible gas-water flow and no profile effects ($C_0 = 1$). Here, the same air-water and CO₂-water cases are simulated using DARTS-well as a standalone wellbore model, and the results are compared with the analytical and T2Well solutions in Fig. 3. The comparison shows good agreement between DARTS-well, T2Well, and the analytical solutions, with small differences that may be attributed to differences in the fluid-property models used in the simulators and analytical solution. The corresponding spatial L_2^{RMS} errors are summarized in Table 1.

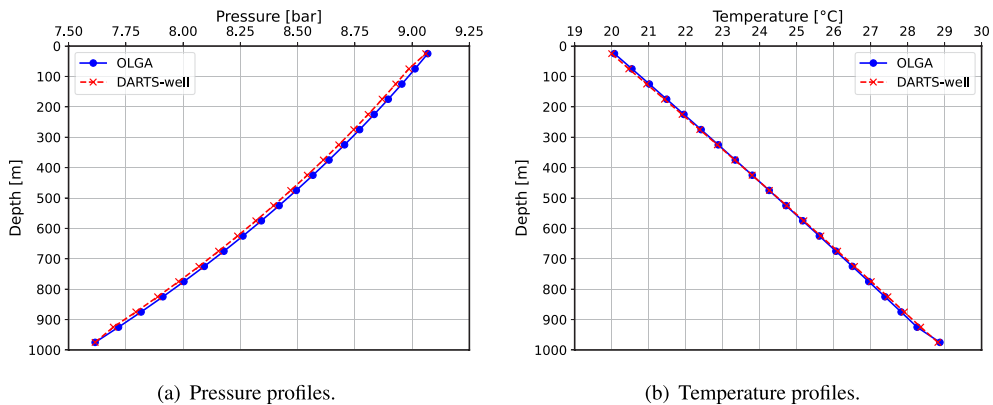
3.1.2. OLGA benchmarking for transient thermal single-phase (gas) single-component (CO₂) flow in a vertical wellbore

In this scenario, the injection of pure CO₂ into a vertical wellbore containing pure CO₂ is simulated. The input parameters of the simulation are given in Table 2. The final pressure and temperature profiles and BHP and BHT time series obtained from the well model are compared with those from OLGA, shown in Figs. 4 and 5, respectively. The final pressure and temperature profiles agree closely with OLGA. In the BHP and BHT time series, small differences occur during the unsteady-state period, while the two simulators converge to essentially the same steady state later in the simulation.

(a) CO₂-water flow.

(b) Air-water flow.

Fig. 3. Comparing DARTS-well and T2Well solutions with their analytical solution for upward flow of CO₂-water at 40 °C and air-water at 20 °C in a water well.



(a) Pressure profiles.

(b) Temperature profiles.

Fig. 4. Comparison of pressure and temperature profiles of the standalone well model with OLGA for the thermal single-phase single-component model.

Table 2

Information for the thermal single-phase (gas), single-component (CO_2) fluid flow in a vertical wellbore.

Wellbore Geometry	Inclination angle: 0° (vertical wellbore) Total length: 1 km (20 segments, each segment 50 m) Diameter: 0.1 m Wall absolute roughness: 2.5×10^{-5} m
Fluid Properties	Wellbore initial fluid composition: Pure CO_2 Density: Peng–Robinson EoS Enthalpy: Peng–Robinson EoS Viscosity: Fenghour et al. [47] correlation
Initial Conditions	Wellhead pressure: 5 bar Wellhead temperature: 25°C Geothermal gradient: 25°C km^{-1} Fluid at rest (i.e., $v_{\text{fluid}} = 0 \text{ m s}^{-1}$)
Boundary Conditions	At wellhead: Injection rate: 2 kg s^{-1} Injection temperature: 20°C (constant) Injected fluid composition: Pure CO_2 At bottom-hole (perforation): Reservoir pressure: 5.89 bar Well injectivity: $1 \times 10^5 \text{ kg bar}^{-1} \text{ d}^{-1}$
Simulation Schedule	Duration: 10 min

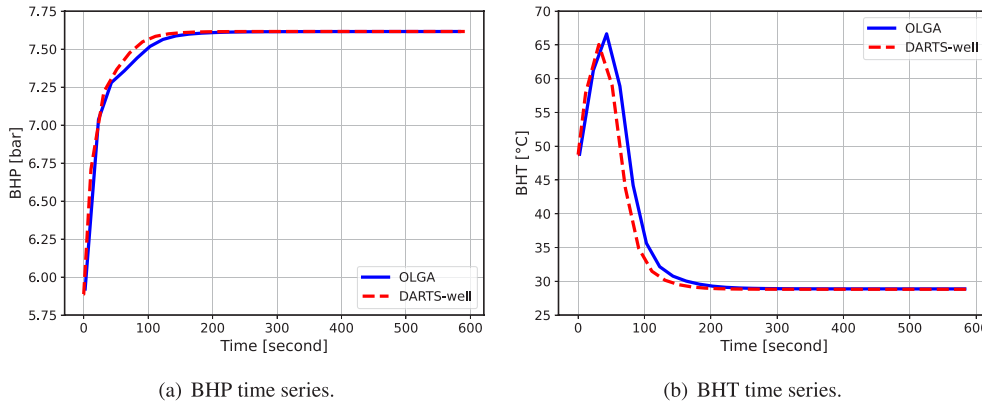


Fig. 5. Comparison of BHP and BHT time series of the standalone well model with OLGA for the thermal single-phase single-component model.

3.1.3. OLGA benchmarking for transient isothermal two-phase (gas and liquid) two-component (CO_2 and H_2O) flow in a vertical wellbore

In this scenario, the injection of pure CO_2 into a vertical wellbore containing a column of water is simulated. The information of the simulation case is given in Table 4, and a uniform injectivity index is used (further details on injectivity index in Appendix C). The final pressure and liquid hold-up profiles and BHP and bottom-hole liquid hold-up time series obtained from the standalone well model are compared with those from OLGA, as shown in Figs. 6 and 7, respectively. The pressure profiles and BHP time series agree closely with OLGA. The differences in liquid hold-up in Fig. 6-b arise from the distinct mathematical formulations and closure relations used by the developed well model (DFM) and OLGA (MFM). Specifically, the DFM simplifies the system by solving a single momentum equation for the mixture and relies on empirical correlations to describe phase interactions, such as slip velocity. In contrast, the MFM solves separate momentum equations for each phase, explicitly accounting for interphase momentum transfer and relative motion. These differences result in varying predictions of phase distribution, particularly liquid hold-up, under multiphase flow conditions. This scenario is also simulated using an inclined wellbore and the benchmark results are presented in Appendix D. The corresponding quantitative OLGA benchmarking errors are summarized in Table 3.

3.2. Benchmarking of the coupling approach

In this subsection, the coupling approach in the coupled well–reservoir model DARTS-well is tested against that in the Shell in-house coupled well–reservoir (lift-table–MoReS) model [8]. To this end, injection of liquid CO_2 in a depleted hydrocarbon reservoir is simulated using DARTS-well. The input data are the same as those used in the representative case study, given in Table 5, with the following differences: reservoir thickness: 100 m, compressibility: $1 \times 10^{-6} \text{ bar}^{-1}$, rock specific heat capacity: $0.9 \text{ kJ kg}^{-1} \text{ }^\circ\text{C}^{-1}$, rock density: 2100 kg m^{-3} , rock thermal conductivity: $2.5 \text{ W m}^{-1} \text{ }^\circ\text{C}^{-1}$, relative permeability Corey exponents: $n_{\text{vapor}} = 1$, $n_{\text{liquid}} = 1$, fluid

Table 3

Integrated L_2^{RMS} errors between DARTS-well and OLGA for the standalone wellbore benchmarks, computed using Equations (23) and (24). The absolute error has the same units as the corresponding quantity.

Scenario	Comparison	Quantity	L_2^{RMS}	E_{rel} [%]
Non-isothermal single-phase	Well profile	Pressure [bar]	0.0240	0.2843
		Temperature [$^{\circ}\text{C}$]	0.0570	0.2319
	Time series	Pressure [bar]	0.0285	0.3783
		Temperature [$^{\circ}\text{C}$]	2.2624	6.4120
Isothermal two-phase, vertical	Well profile	Pressure [bar]	0.2852	0.3860
		Liquid saturation [-]	0.0684	9.6844
	Time series	Pressure [bar]	0.4688	0.4440
		Liquid saturation [-]	0.0115	1.9058
Isothermal two-phase, inclined	Well profile	Pressure [bar]	0.3287	0.5386
		Liquid saturation [-]	0.0884	13.4832
	Time series	Pressure [bar]	0.4445	0.5645
		Liquid saturation [-]	0.0454	9.6152

Table 4

Information for the isothermal two-phase (gas and liquid), two-component (CO_2 and H_2O) fluid flow in a vertical wellbore.

Wellbore Geometry	Inclination angle: 0° (vertical wellbore) Total length: 1 km (20 segments, each segment 50 m) Diameter: 0.1 m Wall absolute roughness: 2.5×10^{-5} m
Fluid Properties	CO_2 -rich phase density: Peng–Robinson EoS Aqueous phase density: Garcia [48] correlation CO_2 -rich phase viscosity: Fenghour et al. [47] correlation Aqueous phase viscosity: Islam and Carlson [49] correlation Gas–liquid IFT: Macleod–Sugden surface tension model
Initial Conditions	Wellhead pressure: 10 bar System temperature: 40°C (constant) Wellbore initial fluid composition: Water Fluid at rest (i.e., $v_{\text{fluid}} = 0 \text{ m s}^{-1}$)
Boundary Conditions	At wellhead: Injection rate: 2 kg s^{-1} Injection temperature: System temperature Injected fluid composition: Pure CO_2 At bottom-hole (perforation): Reservoir pressure: 102.66 bar Wellbore injectivity: $1 \times 10^5 \text{ kg d}^{-1} \text{ bar}^{-1}$ (constant)
Simulation Schedule	Duration: 5 min for well profiles and 1 h for time series

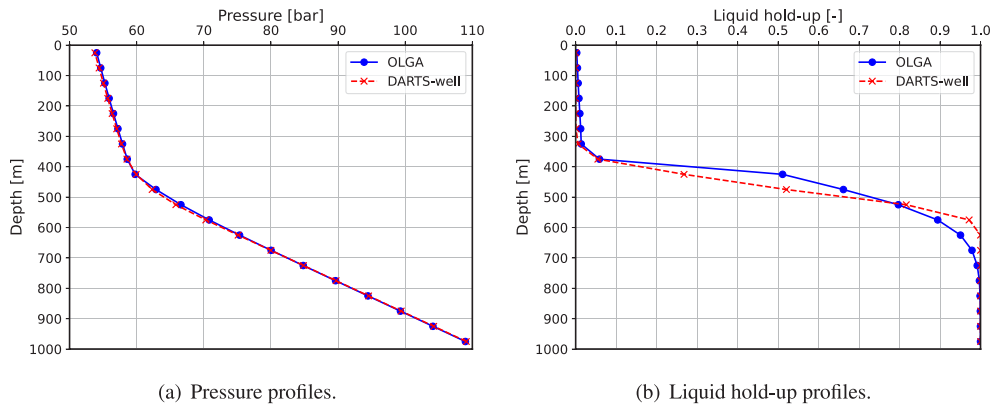


Fig. 6. Comparison of pressure and liquid hold-up profiles in the standalone well model and OLGA for the isothermal two-phase two-component fluid flow in a vertical wellbore.

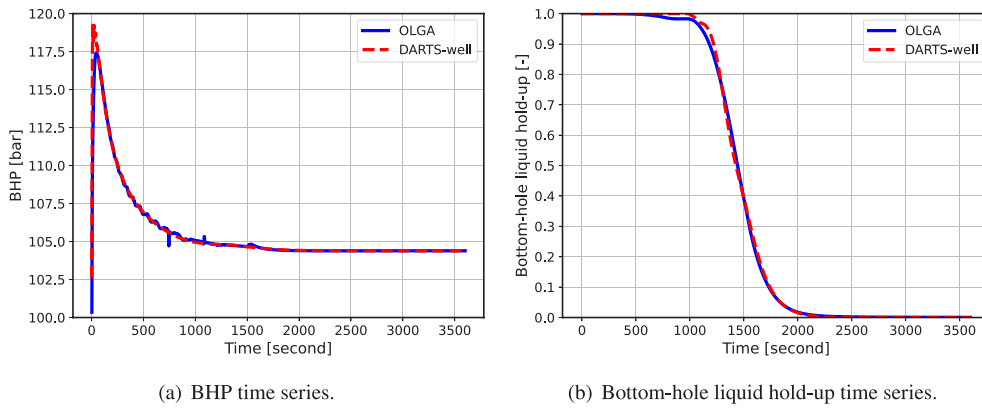


Fig. 7. Comparison of the time series of bottom-hole pressure and liquid holdup in the standalone well model and OLGA for the isothermal two-phase, two-component flow in a vertical wellbore.

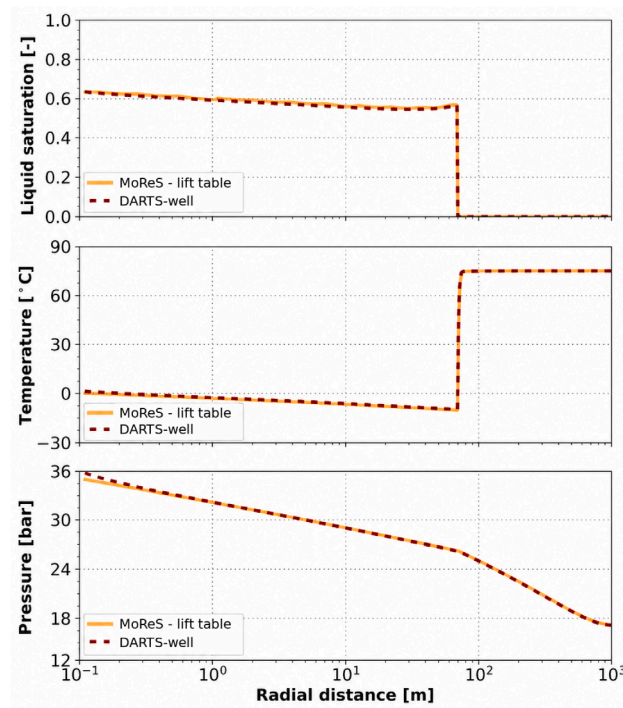


Fig. 8. Comparison of reservoir results using the DARTS-well and lift-table-MoReS coupling approaches.

thermal conductivity: $0 \text{ W m}^{-1} \text{ }^{\circ}\text{C}^{-1}$, injection rate: 31.69 kg s^{-1} , and injected fluid conditions: $P = 80 \text{ bar}$, $T = 20 \text{ }^{\circ}\text{C}$. Using DARTS-well as a standalone well model, a lift table is also generated, which provides the bottom-hole temperature and CO_2 gas/liquid mass fractions under a range of BHPs. Since in DARTS-well, fluid flow at perforation is treated in the same way as fluid flow in porous media, the results of the segment above the perforation is used to generate the lift table. This lift table is then coupled with the reservoir simulator MoReS. The reservoir results of the two coupled models are in good agreement as shown in Fig. 8.

3.3. Representative case study

In our previous studies, the developed coupled well-reservoir model was used for isothermal and thermal injection of gaseous CO_2 into a depleted hydrocarbon reservoir [44,45]. In this study, the coupled model is used to simulate liquid CO_2 injection into a highly-depleted gas reservoir using parameters representative of a North Sea GCS project, the properties of which are summarized in Table 5. To this end, firstly, the convergence analyses of the OBL, wellbore, and reservoir grid resolution are investigated. Afterwards, using the optimum grid resolutions, the simulation is implemented for one year of injection time.

Table 5

Well and reservoir data used for the representative case study.

Wellbore Geometry	Inclination angle: 0° (vertical wellbore) Total length: 2 km Diameter: 0.1016 m Wall absolute roughness: 2.032×10^{-5} m
Reservoir Geometry	Grid type: 1D cylindrical grid Thickness: 50 m Radius: 1000 m
Reservoir Rock Properties	Porosity: 0.21 Horizontal/vertical permeability: 100/100 mD Density: 2100 kg m^{-3} Compressibility: 0 bar^{-1} Specific heat capacity: $2.5 \text{ kJ kg}^{-1} \text{ }^{\circ}\text{C}^{-1}$ Thermal conductivity: $3 \text{ W m}^{-1} \text{ }^{\circ}\text{C}^{-1}$
Fluid Properties	Density: Peng–Robinson equation of state (PR EoS) Enthalpy: PR EoS Viscosity: Fenghour et al. [47] correlation Relative permeability: Brooks–Corey model ($n_{\text{vapor}} = 1.5$, $n_{\text{liquid}} = 1.5$) Thermal conductivity: $0.04 \text{ W m}^{-1} \text{ }^{\circ}\text{C}^{-1}$ (gaseous CO_2) and $0.08 \text{ W m}^{-1} \text{ }^{\circ}\text{C}^{-1}$ (liquid CO_2)
Initial Conditions	Wellhead pressure: 7.81 bar Reservoir pressure: 11 bar Wellhead temperature: $15 \text{ }^{\circ}\text{C}$ Geothermal gradient: $30 \text{ }^{\circ}\text{C km}^{-1}$ Reservoir temperature: $75 \text{ }^{\circ}\text{C}$ Reservoir and well initial fluid composition: Pure CO_2 ($s_w = 0$) Fluid at rest (i.e., $v_{\text{fluid}} = 0 \text{ m s}^{-1}$)
Boundary Conditions	At wellhead: Injection rate: 30 kg s^{-1} (ramp-up time: 3 min) Injected fluid enthalpy: $-12414 \text{ kJ kmol}^{-1}$ (@ $P = 60 \text{ bar}$, $T = 10 \text{ }^{\circ}\text{C}$) Injected fluid composition: Pure CO_2 At reservoir boundaries: No flow (closed boundary).

Table 6Convergence of BHP and BHT with OBL resolution. Integrated time-domain L_2^{RMS} and relative errors are computed with respect to the 5000-point OBL reference solution.

OBL nodes	$L_2^{\text{RMS}}(\text{BHP})$ [bar]	$E_{\text{rel}}(\text{BHP})$ [%]	$L_2^{\text{RMS}}(\text{BHT})$ [$^{\circ}\text{C}$]	$E_{\text{rel}}(\text{BHT})$ [%]
100	0.3058	0.7880	0.3032	6.5127
200	0.1196	0.3082	0.1176	2.5257
500	0.0190	0.0489	0.0186	0.4001
1000	0.0046	0.0118	0.0045	0.0966

3.3.1. Convergence analysis of the OBL grid resolution

In this subsection, the convergence analysis of the OBL grid resolution is investigated. Here, an N -point OBL resolution denotes N nodes in each parameter-space dimension; for the present pressure-enthalpy parameterization, this corresponds to an $N \times N$ OBL table. The convergence is evaluated by comparing the lower-resolution OBL results against the 5000-point OBL reference solution. As shown in Table 6, the OBL approximation converges toward the 5000-point reference solution as the OBL resolution is refined. Coarser OBL tables produce larger BHP and BHT errors, while refinement from the 100–200 point range to 500 points reduces the relative errors by approximately one order of magnitude. Based on this convergence behavior, the 500-point OBL resolution is considered as an acceptable resolution as a practical compromise between accuracy and runtime for similar simulations. It is also worth noting that the 100-point case, despite using a coarser table than the 500-point case, required more runtime because the coarse OBL representation degraded nonlinear convergence by insufficiently resolving the thermodynamic behavior.

3.3.2. Convergence analysis of the wellbore grid resolution

The objective of this subsection is to determine the optimal wellbore grid resolution that ensures sufficient accuracy while maintaining computational efficiency for the simulations in this study. Although the wellbore contains far fewer cells than a reservoir grid, each additional well segment requires DFM phase-velocity calculations and closure evaluations, which are more expensive than Darcy flux calculations in the reservoir. To this end, five uniformly distributed segment sizes are tested: 5-m, 10-m, 50-m, 100-m, and 200-m segments, corresponding to 401, 201, 41, 21, and 11 segments. The convergence of the wellbore-grid resolution is evaluated by comparing the BHP and BHT time series against the 5-m segment-length reference solution. As shown in Table 7, the errors decrease as the wellbore segment length is refined. Refining the segment length to 50 m reduces the relative BHP and BHT errors to 0.008% and 0.585%, respectively, small enough to be adopted as an optimum well resolution to balance computational efficiency and solution accuracy for similar simulations.

Table 7

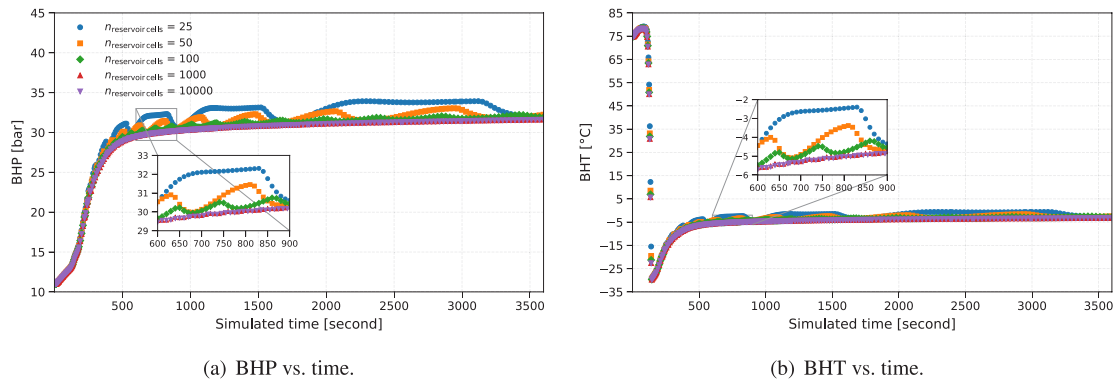
Convergence of BHP and BHT with wellbore-grid resolution. Integrated time-domain L_2^{RMS} and relative errors are computed with respect to the 401-segment reference solution.

Well resolution	L_2^{RMS} (BHP) [bar]	E_{rel} (BHP) [%]	L_2^{RMS} (BHT) [°C]	E_{rel} (BHT) [%]
11	0.0065	0.0166	0.0681	1.4636
21	0.0039	0.0101	0.0453	0.9734
41	0.0031	0.0080	0.0272	0.5850
201	0.0020	0.0053	0.0053	0.1146

Table 8

Convergence of BHP and BHT with reservoir-grid resolution. Integrated time-domain L_2^{RMS} and relative errors are computed with respect to the 10000-cell reservoir-grid reference solution.

Reservoir resolution	L_2^{RMS} (BHP) [bar]	E_{rel} (BHP) [%]	L_2^{RMS} (BHT) [°C]	E_{rel} (BHT) [%]
25	1.9109	6.4077	2.2398	14.1280
50	0.8807	2.9531	1.0391	6.5544
100	0.3928	1.3171	0.4677	2.9501
1000	0.0312	0.1046	0.0383	0.2417

**Fig. 9.** Convergence of BHP and BHT time series with respect to reservoir grid resolution.

3.3.3. Convergence analysis of the reservoir grid resolution

In addition to wellbore discretization, reservoir grid resolution also plays an important role in the accuracy and efficiency of coupled well–reservoir simulations. To investigate this, five reservoir grid resolutions ($n_{\text{reservoir cells}}$) are tested: 25, 50, 100, 1000, and 10000 cells. Reservoir cell sizes are distributed logarithmically in the radial direction away from the well, and the simulated time in this subsection is 1 h since reservoir grids with large grid cells encounter convergence failure for longer simulated times. The convergence of the reservoir-grid resolution is evaluated by comparing the BHP and BHT time series against the 10000-cell reservoir-grid reference solution. As shown in Table 8, the errors decrease systematically as the reservoir grid is refined. The coarse grids with 25, 50, and 100 reservoir cells produce relatively large deviations from the reference solution. Refining the grid to 1000 reservoir cells reduces the relative BHP and BHT errors to 0.105% and 0.242%, respectively, indicating that this resolution provides a sufficiently accurate approximation for the quantities of interest.

Fig. 9 shows the corresponding BHP and BHT time series. As shown, if the number of the reservoir blocks is not sufficiently large, i.e., if the reservoir blocks are not refined enough, oscillations appear in the BHP and BHT time series, which are originally a result of oscillations inside the reservoir domain. Each oscillation in BHP and BHT corresponds to the formation of liquid CO_2 in a new reservoir block. If the reservoir grid is not fine enough, these oscillations lead to solver failure for longer simulated times. Based on these results, 1000 reservoir cells can be used as an optimum reservoir-grid resolution since it provides the converged solution, with smaller reservoir grid cells overlapping with these results.

3.3.4. Long-term simulation results

Based on the parameters chosen from the convergence analyses conducted previously, a simulation is run for one year. The profiles of pressure, temperature, and liquid volume fraction (hold-up for wellbore and saturation for reservoir) along the wellbore and 1D horizontal reservoir at certain report times are shown in Fig. 10. As shown in Fig. 10-a, the controlling mechanism on the wellbore pressure profile shifts during injection: it is initially gravity-dominated (initial pressure profile is solely driven by gravity), then becomes friction-dominated, later exhibits a mixed regime (gravity-dominated in the upper interval and friction-dominated in the lower interval), and finally returns to a fully gravity-dominated profile. The dominant mechanism controlling the pressure profile is crucial, because it determines whether pressure drops from the top to the bottom of the wellbore. This, in turn, governs

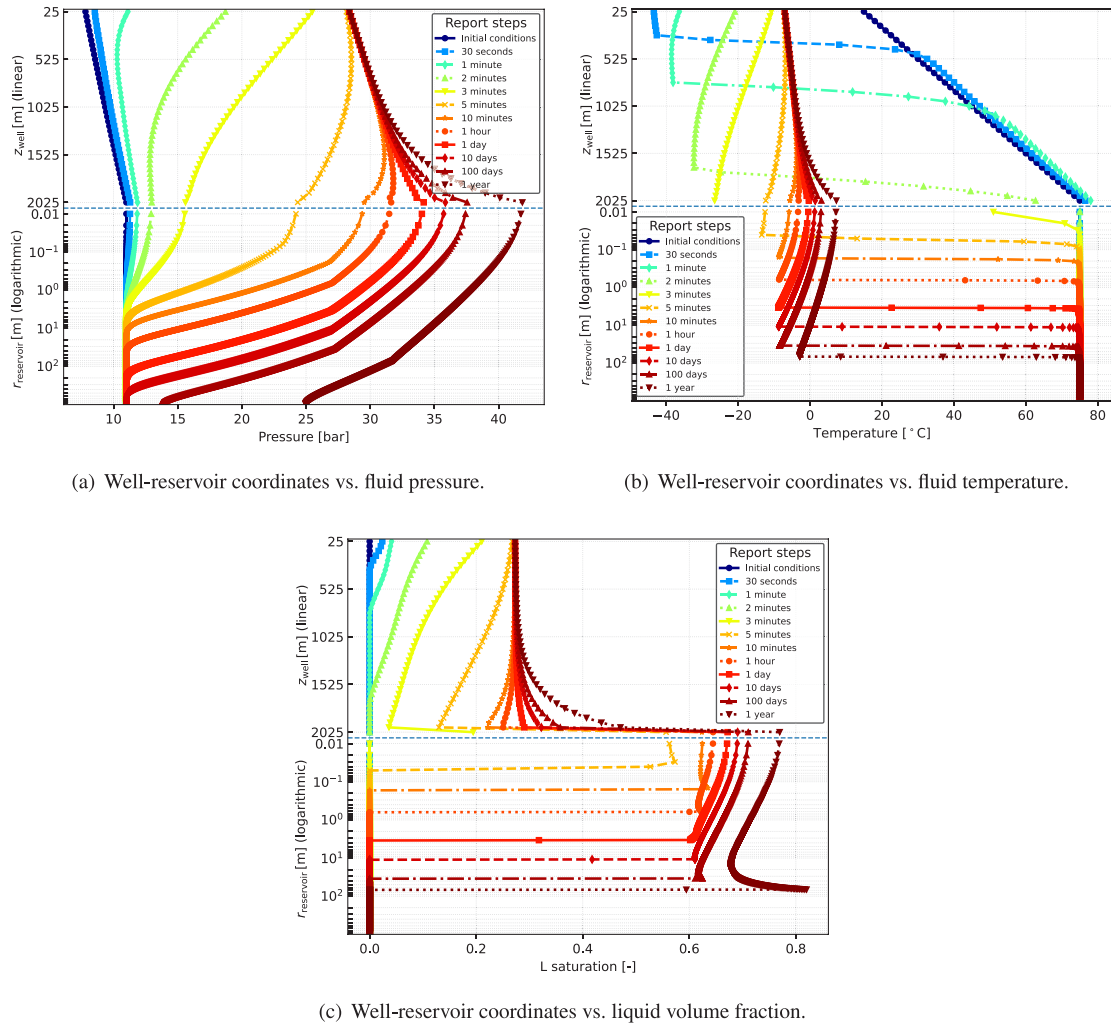
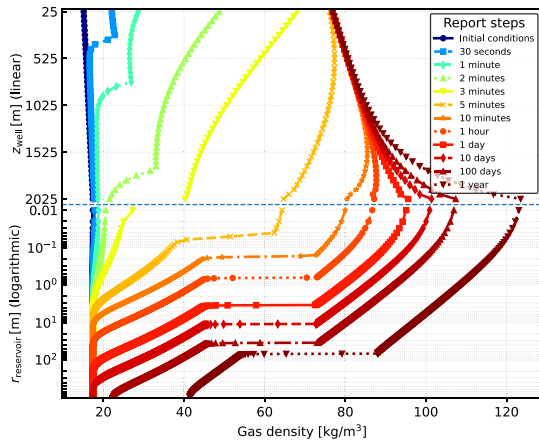


Fig. 10. Evolution of pressure, temperature, and liquid volume fraction along the vertical wellbore and 1D horizontal reservoir for the demonstrative example.

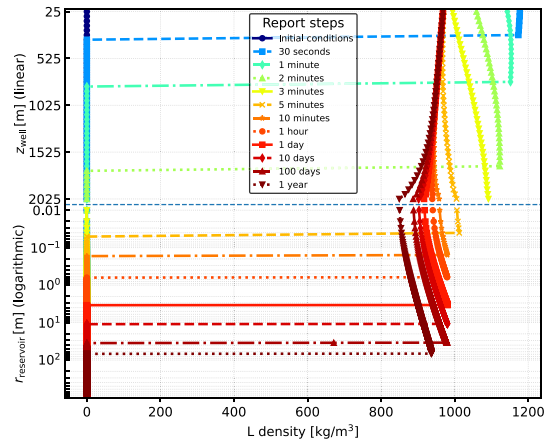
the temperature behavior: under gravity-dominated conditions, the fluid undergoes Joule–Thomson heating, whereas under friction-dominated conditions, the fluid undergoes Joule–Thomson cooling, leading to a temperature drop from the top to the bottom of the wellbore, shown in Fig. 10b.

During the first few minutes of injection, however, the temperature profile is governed primarily by a different mechanism than the along-wellbore pressure gradient: strong cooling near the wellhead at the choke, caused by the rapid pressure drop and liquid vaporization as injected liquid CO₂ expands into the low-pressure wellbore. At the same time, in intervals of the wellbore that have not yet been reached by the injected cold CO₂, temperature of gaseous CO₂ slightly increases. This heating results from initial pressure propagation along the wellbore induced by injection, and its magnitude also depends on the composition of the fluid in place. Fig. 10b also indicates that as the injected CO₂ moves through the reservoir, it experiences further cooling, reaching a local minimum in temperature at each reported time as a result of a further pressure drop and liquid evaporation in the reservoir. After a sufficient injection time, the high pressure and low temperature of the near-wellbore region provides formation of liquid CO₂ at the cold front, as depicted in Fig. 10c. Fig. 10c shows that once injection starts, injected liquid CO₂ flashes (i.e., vaporizes) at the wellhead. As the pressure of the wellhead increases over time (and so the rest of the wellbore), the liquid hold-up increases as well. There is also some accumulation of liquid CO₂ observed at the bottom of the well, which occurs due to the lower mobility of liquid CO₂ compared to gaseous CO₂.

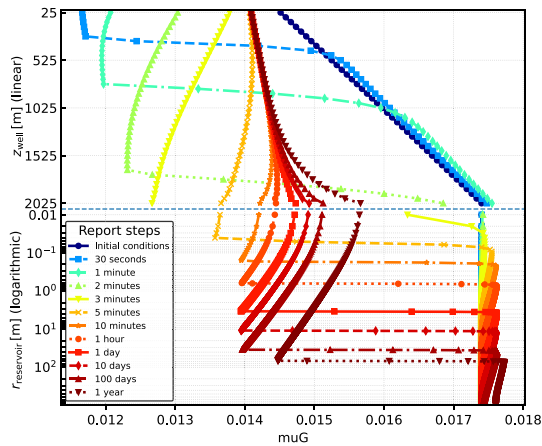
The evolution of the gas and liquid density and viscosity is shown in Figs. 11 and 12, respectively (zero liquid density and viscosity due to the zero liquid volume fraction). Fig. 11-a shows that gas density increases with time, driven by the combined effects of pressure buildup and cooling in the wellbore and reservoir. However, ahead of the cold front, the increase in gas density is solely induced by pressurization. As shown in Fig. 11-b, the liquid phase has the highest density once injection starts because



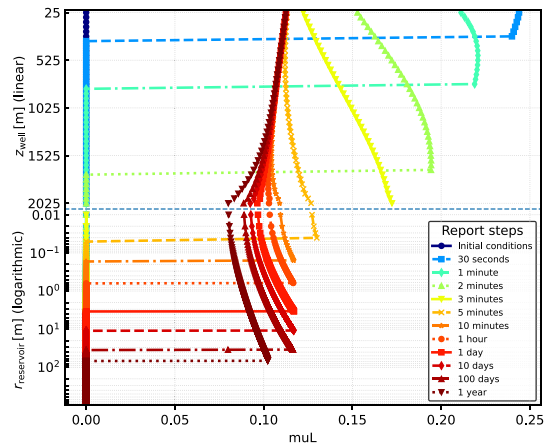
(a) Well-reservoir coordinates vs. gas density.



(b) Well-reservoir coordinates vs. liquid density.

Fig. 11. Evolution of gas and liquid density along the vertical wellbore and 1D horizontal reservoir for the demonstrative example.

(a) Well-reservoir coordinates vs. gas viscosity.



(b) Well-reservoir coordinates vs. liquid viscosity.

Fig. 12. Evolution of gas and liquid viscosity along the vertical wellbore and 1D horizontal reservoir for the demonstrative example.

the liquid phase entering the wellbore experiences the minimum temperature during the well start-up. While the gas density increases throughout the system over time, the liquid density decreases, depicted in Fig. 11b, since based on Fig. 10b, temperature increases throughout the system during the injection period. The evolution of phase viscosity in Fig. 12 indicates that viscosity is primarily controlled by temperature, but with opposite trends for the two phases: decreasing temperature reduces gas viscosity at low pressures, whereas it increases liquid viscosity. However, ahead of the cold front, the gas viscosity profile is controlled solely by pressure and increases with the induced pressure buildup in the reservoir.

The present simulation focuses on the coupled fluid and energy flow in a coupled well–reservoir system without lateral heat exchange or water-related effects. Future extensions can build on this formulation by incorporating lateral heat exchange with the surrounding formations and water-related processes, including near-wellbore dry-out, salt precipitation, and potential hydrate/ice formation/dissociation.

3.3.5. Computational and numerical performance

As shown in Table 9, replacing perturbation-based numerical differentiation with the OBL approach for Jacobian evaluation substantially reduces the simulation runtime. Moreover, the relative advantage of OBL becomes more pronounced as the number of well segments is larger. Since OBL produces simulation results that are nearly identical to those obtained with perturbation-based Jacobians while requiring substantially less simulation time, it provides a compelling and efficient choice for the coupled well–reservoir model. This conclusion follows up on similar results obtained in García-Navarrete et al. [50], where authors compared the performance of open-DARTS with the TOUGH2 simulator which uses perturbation-based numerical derivatives.

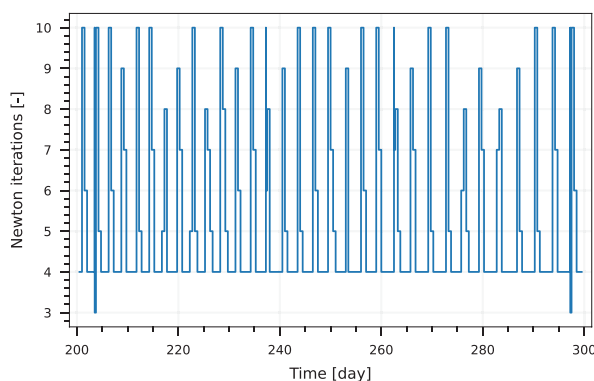


Fig. 13. Fluctuations of the number of Newton–Raphson iterations of the representative case study.

Table 9

Runtime comparison between OBL-based and perturbation-based numerical differentiation (OBND and PBND, respectively) for different numbers of well segments for one-hour simulated time.

No. of segments	OBND runtime (s)	PBND runtime (s)	Speedup (×)
9	85.9	11.8	7.3
11	89.1	9.3	9.6
21	441.8	14.9	29.7
41	1613.2	30.2	53.4
201	34 399.0	121.3	281.3

From a numerical standpoint, the solver faces oscillations in the number of Newton–Raphson iterations, shown in Fig. 13 (the maximum number of Newton–Raphson iterations is set to 10). While low-temperature CO₂ flows into the reservoir, when liquid CO₂ first appears in a previously gaseous-phase reservoir block, the nonlinear solver temporarily drives the liquid saturation to unity within a Newton–Raphson iteration. This behavior is non-physical, as liquid CO₂ should emerge gradually as the fluid enthalpy decreases. When such overshoots occur, additional Newton–Raphson iterations are required to recover the expected small liquid saturation, leading to oscillations in the iteration count over time. To mitigate such sharp state changes within a single Newton iteration, a trust-region Newton strategy could be considered.

4. Conclusions

In this work, we have developed a computationally-efficient, fully coupled well–reservoir model within the open-DARTS simulation framework to capture thermal, multiphase flow dynamics during subsurface energy-transition operations, particularly injection of high-pressure CO₂ into depleted hydrocarbon reservoirs. To this end, first, a multi-segment multiphase wellbore model is developed using the Drift-Flux Model, and then, the wellbore model is incorporated into and fully coupled with the open-DARTS reservoir simulator using the Operator-Based Linearization (OBL) approach. The fully coupled scheme and OBL approach are applied here to reduce the computational time and increase the solver stability for modeling the highly nonlinear physics of high-pressure CO₂ injection into depleted hydrocarbon reservoirs. The developed wellbore simulator and the well–reservoir coupling approach are verified and benchmarked against an analytical solution and commercial simulators, respectively. To demonstrate the applicability of the coupled well–reservoir model, liquid CO₂ injection into a depleted gas reservoir is simulated with properties representative of a North Sea GCS candidate reservoir, using optimal OBL, wellbore, and reservoir grid resolutions identified by convergence analyses. Ultimately, a comparison between the OBL approach and perturbation-based numerical differentiation is made, showing that the OBL approach significantly reduces computational time while maintaining identical simulation outcomes compared to perturbation-based numerical differentiation.

CRedit authorship contribution statement

Sajjad Moslehi: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis. **Siavash Kahrobaei:** Writing – review & editing, Validation. **Rouhi Farajzadeh:** Writing – review & editing, Validation, Supervision, Project administration, Funding acquisition, Conceptualization. **Denis Voskov:** Writing – review & editing, Validation, Supervision, Project administration, Methodology.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

The authors would like to acknowledge Shell Global Solutions International for financial support.

Appendix A. Drift-flux closure relations

This appendix summarizes the closure relations used with the DFM phase-velocity expressions in Eqs. (1) and (2). The average density and profile-adjusted average density are given by

$$\rho_m = s_g \rho_g + (1 - s_g) \rho_l, \quad (\text{A.1})$$

$$\rho_m^* = C_0 s_g \rho_g + (1 - C_0 s_g) \rho_l. \quad (\text{A.2})$$

The profile parameter, C_0 , is calculated using

$$C_0 = \frac{C_{\max}}{1 + (C_{\max} - 1)\eta^2}, \quad (\text{A.3})$$

where $C_{\max}$ is a maximum profile parameter that can be tuned to match observations and can vary between 1.0 and 1.5. It represents the value of the profile parameter in the bubble and slug flow patterns and was originally set to 1.2 in ECLIPSE [23]. In the denominator of Eq. (A.3), η is a parameter that reflects the effects of the flow status on the profile parameter and reduces C_0 to 1 at high gas saturations and mixture velocities:

$$\eta = \frac{\beta - B}{1 - B} \quad \text{subject to the limits} \quad 0 \leq \eta \leq 1. \quad (\text{A.4})$$

Here, β approaches 1.0 as gas saturation approaches 1.0 and also as mixture velocity approaches a high value. In these conditions, $\eta = 1$ and so $C_0 = 1$. The velocity for the onset of annular flow is chosen as the velocity at which the profile slip vanishes. The transition to annular flow occurs when the gas superficial velocity, v_{sg} , reaches the flooding value, v_{sgf} . Gas flooding superficial velocity is defined as the gas superficial velocity sufficient to support a thin annular film of liquid and prevent it from falling back against the gas flow:

$$v_{sgf} = K_u \sqrt{\frac{\rho_l}{\rho_g}} v_c. \quad (\text{A.5})$$

Accordingly, β is calculated as

$$\beta = \max \left(s_g, F_v \frac{s_g |v_m|}{v_{sgf}} \right) \quad \text{subject to the limits} \quad 0 \leq \beta \leq 1, \quad (\text{A.6})$$

where F_v is a multiplier on the flooding velocity fraction. It is set to 1 by default and can be tuned to fit observations; profile flattening can be made more or less sensitive to gas velocity by adjusting this value [51]. In Eq. (A.4), B is the threshold parameter above which C_0 starts to drop below $C_{\max}$. Based on the T2Well formulation, it is a function of $C_{\max}$:

$$B = \frac{2}{C_{\max}} - 1.0667. \quad (\text{A.7})$$

This equation gives $B = 0.6$ for $C_{\max} = 1.2$, which is used in this work. In Eq. (A.5), K_u is the Kutateladze number, which is a function of Bond number (N_B):

$$K_u = \sqrt{\frac{C_{ku}}{\sqrt{N_B}}} \left(\sqrt{1 + \frac{N_B}{C_{ku}^2 C_w}} - 1 \right). \quad (\text{A.8})$$

N_B is the square of dimensionless wellbore diameter and characterizes the ratio of gravitational forces to interfacial tension forces:

$$N_B = d^2 \left[\frac{g(\rho_l - \rho_g)}{\sigma_{gl}} \right], \quad (\text{A.9})$$

where d is the wellbore diameter, g is gravitational acceleration, and σ_{gl} is the surface tension (ST) or interfacial tension (IFT) between gas and liquid phases. A value of $N_B < 1$ implies that the flow is weakly dependent on gravitational forces, whereas $N_B > 1$ implies that gravitational forces dominate over interfacial tension forces. In Eq. (A.8), C_{ku} is a constant. It was 75 in Richter's original formula, but this value overestimated K_u for smaller dimensionless diameters ($= \sqrt{N_B}$). Pan et al. [51] found that 142 better fits the experimental data provided in the same paper. C_w is a wall friction factor and is assumed to be a constant of 0.008. In Eq. (A.5), v_c is the characteristic velocity, a measure of the velocity of bubble rise in a stagnant liquid column:

$$v_c = \left[\frac{g \sigma_{gl} (\rho_l - \rho_g)}{\rho_l^2} \right]^{1/4}. \quad (\text{A.10})$$

The drift velocity, v_d , is another important parameter in Eqs. (1) and (2). The original formula for drift velocity proposed by Shi et al. [23] is calculated as a function of gas saturation and fluid properties. It is applicable for bubble to film, or annular, flow patterns, but not mist flow [51]:

$$v_d = \frac{(1 - C_0 s_g) v_c K(s_g, K_u, C_0) m(\theta)}{C_0 s_g \sqrt{\rho_g / \rho_l + 1 - C_0 s_g}}. \quad (\text{A.11})$$

The correlation above gives the gas-rise drift-velocity magnitude. In the DARTS-well implementation, the well coordinate is positive from the wellhead to the bottomhole, so the signed drift velocity used in Eqs. (1) and (2) is assigned with the opposite sign for gas drift. In Eq. (A.11), $m(\theta)$ accounts for the effect of wellbore inclination on drift velocity for wells up to 88° from vertical [52], and is defined as [51]

$$m(\theta) = m_0 (\cos \theta)^{n_1} (1 + \sin \theta)^{n_2}, \quad (\text{A.12})$$

where m_0 , n_1 , and n_2 are fitted parameters equal to 1.27, 0.24, and 1.08, respectively, at $C_{\max} = 1.2$. The function $K(s_g, K_u, C_0)$ interpolates from 1.53 to $C_0 K_u$ and provides a smooth transition of drift velocity between the bubble-rise and film-flooding stages. Different from the linear interpolation suggested by Shi et al. [23], we use the following smooth and so differentiable function following [30]:

$$K = \begin{cases} 1.53 & s_g \leq a_1 \\ 1.53 + \frac{C_0 K_u - 1.53}{2} \left[1 - \cos \left(\pi \frac{s_g - a_1}{a_2 - a_1} \right) \right] & a_1 < s_g < a_2 \\ C_0 K_u & s_g \geq a_2. \end{cases} \quad (\text{A.13})$$

The transition gas saturations a_1 and a_2 are equal to 0.06 and 0.12 at $C_{\max} = 1.2$, where the flow-pattern transition starts and ends as suggested by Shi et al. [23]. Because K is independent of gas saturation for $s_g \leq a_1$ and $s_g \geq a_2$, the function K is constructed such that $dK/ds_g = 0$ in the neighborhoods of a_1 and a_2 , making this derivative continuous over the entire range of s_g .

As mentioned previously, the original drift-velocity formula was developed to cover two-phase flow patterns from bubble flow to film flow as controlled by gas saturation, but it cannot be applied to mist flow, which often occurs at high velocity and high gas fraction ($s_g \approx 1$). In the mist flow pattern, the gas velocity is so high that the small amount of liquid cannot form a film and instead forms tiny droplets that are uniformly distributed in the gas phase. As a result, slip between the two phases diminishes [30]. Cheng et al. [53] developed a flow-pattern map for CO_2 that suggests that mist flow occurs when mass flux, i.e., total mass flow rate per unit cross-sectional area ($G = \rho_m u_m$), exceeds 300 kg/m²/s at high gas mass fraction (X). To account for mist flow, Pan et al. [24] modified the original equation for drift velocity as

$$v_d = \frac{(1 - C_0 s_g) v_c K(s_g, K_u, C_0) m(\theta) f(G, X)}{C_0 s_g \sqrt{\rho_g / \rho_l + 1 - C_0 s_g}}, \quad (\text{A.14})$$

where $f(G, X)$ is an adjustment function that smoothly and quickly approaches zero as the state point in the $G - X$ plane enters the mist-flow pattern, while it equals one elsewhere. Pan et al. [24] simplified the mist-flow region boundary on the flow-pattern map as a straight line defined by its two end coordinates (X_{m1}, G_{m1}) , (X_{m2}, G_{m2}) . A given flow system with mass flow rate G and gas mass fraction X plots as a point on the flow-pattern map. Therefore, how far a system state (G, X) is away from the mist flow region can be measured by the distance from the state point (G, X) to the mist region boundary, $(X_{m1}, G_{m1}) - (X_{m2}, G_{m2})$. The distance D_m from this state point (G, X) to the mist-region boundary can be calculated as

$$D_m = \frac{\begin{vmatrix} X & \alpha G & 1 \\ X_{m1} & \alpha G_{m1} & 1 \\ X_{m2} & \alpha G_{m2} & 1 \end{vmatrix}}{[(X_{m2} - X_{m1})^2 + (\alpha G_{m2} - \alpha G_{m1})^2]^{1/2}}, \quad (\text{A.15})$$

where α is the scaling factor for mass flow rate and $|\cdot|$ is the determinant of the matrix. The value of D_m becomes negative when (G, X) is inside the mist-flow region and increases as the point moves away from the mist-flow region. Finally, the adjustment function is defined as

$$f(G, X) = \max \left[0.0, 1.0 - \min \left(1, \frac{G}{G_{m1}} \right) \exp(-\lambda D_m |D_m|) \right], \quad (\text{A.16})$$

where λ is a fitting parameter controlling the steepness of the function and the term G/G_{m1} accounts for the fact that the mist-flow region only occurs in the high-velocity region [53]. The parameter values are given in Table A.1 [24].

Appendix B. Relations for the fanning friction factor

The value of the Fanning friction factor is dependent on whether the flow regime in the pipe is laminar or turbulent, which is determined by the Reynolds number (ratio of inertial forces to viscous forces), expressed as

$$Re = \frac{\rho_m v_m d}{\mu_m}, \quad (\text{B.17})$$

Table A.1

Parameters used for the adjustment function.

Parameter	Value
X_{m1}	1.0
X_{m2}	0.94
G_{m1}	300.0 kg m ⁻² s ⁻¹
G_{m2}	700.0 kg m ⁻² s ⁻¹
α	0.001 m ² s kg ⁻¹
λ	199

where d is the pipe internal diameter and μ_m is the mixture viscosity. Saturation-weighted average is used to calculate the mixture viscosity of two phases [54]

$$\mu_m = S_g \mu_g + S_l \mu_l. \quad (\text{B.18})$$

In this study, if $Re < 2400$, the flow regime in the pipe is assumed to be laminar, and if $Re > 2400$, the flow regime in pipe is considered turbulent. If the flow regime is laminar, the Fanning friction factor is calculated using the following relation

$$f_f = \frac{16}{Re}. \quad (\text{B.19})$$

If the flow regime is turbulent, different correlations are presented in the literature. First, we utilized the following correlation, which is used by Pan et al. [51]

$$\frac{1}{\sqrt{f_f}} = -4 \log \left[\frac{2\epsilon}{3.7d} - \frac{5.02}{Re} \log \left(\frac{2\epsilon}{3.7d} + \frac{13}{Re} \right) \right], \quad (\text{B.20})$$

where ϵ is the roughness or absolute roughness of the pipe. This correlation causes significant deviation of pressure profile and small deviation of temperature profile from those of OLGA. Instead, Colebrook's correlation (Eq. (B.21)) is used [55], and it significantly reduces the deviation of the results of the wellbore model from those of OLGA

$$\frac{1}{\sqrt{f_f}} = -4 \log \left(\frac{\epsilon}{3.7065d} + \frac{1.2613}{Re \sqrt{f_f}} \right). \quad (\text{B.21})$$

The Colebrook equation is implicit in friction factors. Hence, it has to be approximately solved using an iterative method (e.g., Newton–Raphson method) or using approximate explicit formulas which are already developed by many authors [55–57]. A famous example of these explicit formulas is the following equation developed by Chen [55]

$$\frac{1}{\sqrt{f_f}} = -4 \log \left\{ \frac{\epsilon}{3.7065d} - \frac{5.0452}{Re} \log \left[\frac{(\epsilon/d)^{1.1098}}{2.8257} + \left(\frac{7.149}{Re} \right)^{0.8981} \right] \right\}. \quad (\text{B.22})$$

Both the implicit Colebrook correlation and the explicit Chen correlation are evaluated for calculating the turbulent-flow friction factor. The two approaches produce nearly identical results, with comparable runtimes in the tested cases. While the implicit Colebrook formulation requires the solution of a nonlinear equation, its computational overhead is found to be negligible when solved with an efficient root-finding algorithm. In the present implementation, this nonlinear equation is solved using the fsolve routine available in the SciPy library. Therefore, the implicit Colebrook correlation is adopted in this study without imposing a significant computational burden.

Appendix C. Effect of uniform and phase-dependent injectivity indices on the results of the standalone wellbore model

In commercial well simulators, a uniform injectivity index can be used to calculate the rates of all phases at the perforated interval by

$$q_j = -J k_{rj} \Delta p, \quad j = 1, \dots, n_p. \quad (\text{C.23})$$

A uniform injectivity index, however, is not an accurate approach if two phases with different viscosity flow through perforations during the simulation time. Both uniform and phase-dependent injectivity indices are developed in the wellbore model in this study. The results of the two-phase benchmark scenario given in Section 3.1.3 are based on uniform injectivity indices used in both scenarios. If phase-dependent well injectivity indices are used in the developed well model, the wellbore results deviate from the solution of uniform injectivity once two-phase flow occurs at the perforation as shown in Fig. C.1.

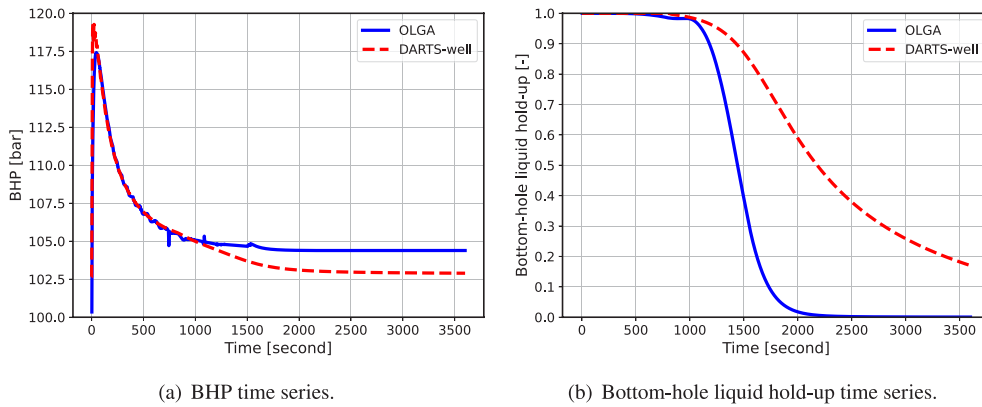


Fig. C.1. Comparison of the time series of bottom-hole pressure and liquid holdup in the standalone well model with phase-dependent injectivity indices and OLGA with a uniform injectivity index for the isothermal two-phase, two-component flow in a vertical wellbore.

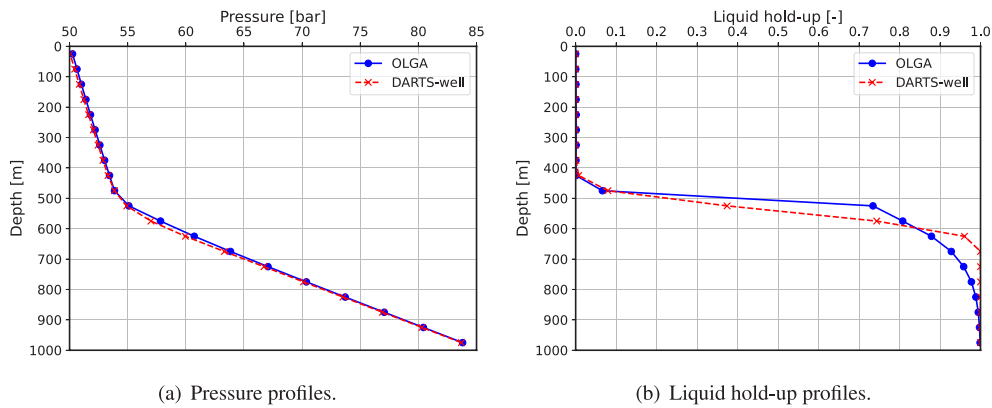


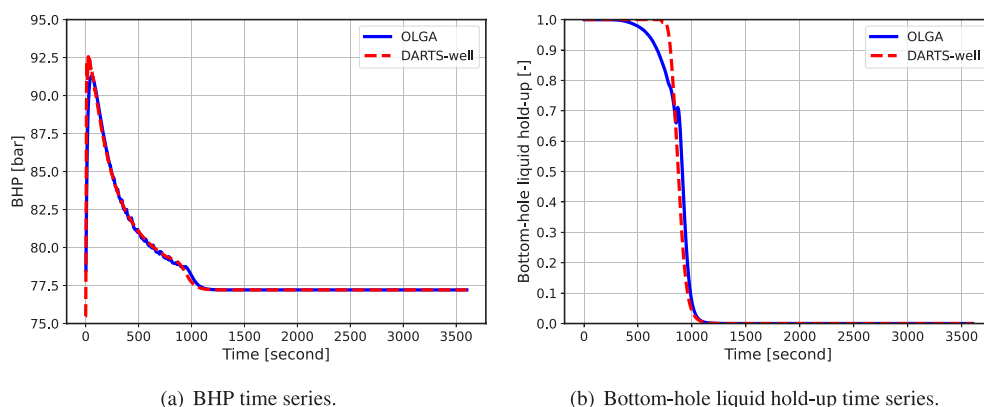
Fig. D.2. Comparison of pressure and liquid hold-up profiles in the standalone well model and OLGA for the isothermal two-phase two-component fluid flow in an inclined wellbore.

Appendix D. Benchmarking of the standalone wellbore model for an inclined wellbore

This scenario is the same as the benchmark scenario presented in Section 3.1.3 except that the wellbore is inclined at 45 degrees. The total length of the wellbore is still 1 km, which means that in this case, the true vertical depth of the wellbore is $1000 \times \cos 45^\circ$ (≈ 707.1 m). The final pressure and liquid hold-up profiles and BHP and bottom-hole liquid hold-up time series obtained from the developed well model are compared with those from OLGA, as shown in Figs. D.2 and D.3, respectively. Note that the vertical axis in Fig. D.2 is a measured depth. As in the case of Fig. 6-b, the difference in liquid hold-ups in Fig. D.2-b is also caused by the difference in mathematical formulations employed.

Data availability

Data will be made available on request.



(a) BHP time series.

(b) Bottom-hole liquid hold-up time series.

Fig. D.3. Comparison of the time series of bottom-hole pressure and liquid holdup in the standalone well model and OLGA for the isothermal two-phase, two-component flow in an inclined wellbore.

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