Modeling and Analysis

GREENHOUSE GASES SCIENCE AND TECHNOLOGY

An explicit finite difference model for prediction of wellbore pressure and temperature distribution in CO_2 geological sequestration

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Abstract: To conveniently realize the coupling calculation between wellbore pressure and temperature and consider the friction loss in the process of wellbore flow and heat transfer, this work takes the one-dimensional steady flow with homogeneous fluid in wellbores as the analysis object and divides the wellbore into finite micro-segments. Then we derive the explicit finite difference model (EFDM) about pressure in a certain micro-segment of wellbore, based on the mass and momentum equations. Next we deduce the EFDM about temperature reflecting the wellbore heat transfer in the same micro-segment according to the energy balance equation. After that, a coupling calculation method for the EFDM about pressure and temperature is presented. Finally, a comparison of the simulation results of the EFDM, other models, and the log data from engineering is implemented, which demonstrates that the prediction results of the EFDM are more consistent with the log data than the results of other models. Therefore, the reliability of the EFDM about pressure and temperature and their coupling calculation method is verified. Discussion of the friction loss in the energy balance equation and the isobaric specific heat capacity showed that both have a great impact on wellbore temperature distribution, which means the friction loss should not be ignored and the isobaric specific heat capacity should not be assumed as a constant in applications. Generally, the prediction of wellbore pressure and temperature distribution and the comprehension of the internal essence of wellbore flow and heat transfer will be effectively promoted by this work.

Keywords: explicit finite difference model (EFDM); wellbore pressure; wellbore heat transfer; steady flow; CO_2 geological sequestration

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Introduction

Carbon capture and storage (CCS) is an effective way of easing the global warming that has become a global consensus.[1–3] To implement the technology of carbon sequestration efficiently, a wellbore with large burial depth is generally selected as the channel of CO_2 injection into the appropriate reservoirs after the storage site has been determined, because the appropriate target reservoirs are normally buried at a depth of more than 800 meters.[1,4] Therefore, as the only access connecting the source (captured CO_2) and the sink (reservoirs) of CO_2, the wellbore is very significant in the carbon sequestration technology chain. Generally, pressure and temperature in wellbore are regarded as the most important dynamic quantities of fluid in wellbore,[5–7] which determine the safety and effectiveness of projects.[8,9] Hence, a clear knowledge of the wellbore flow and thermal behavior is needed.

As to the prediction of pressure and temperature of fluid in wellbore, various investigations have been done in the oil and gas industry and scholars have proposed a series of analytical solutions[10–23] and numerical models.[24–28] This literature has been reviewed in detail by Hasan and Kabir[16,21] and Livescu *et al.*;[28] thus, just a brief introduction is included in this work. Ramey's solution,[10] the first analytical model for wellbore heat transmission, has been widely used in the oil and gas industry. It assumes a steady single-phase flow with constant pressure in one dimension and neglects friction loss. Subsequently, Willhite[11], and Shiu and Beggs[12] improved some parameters of Ramey's solution. Hasan and Kabir,[14–16] Sagar *et al.*,[13] and Hasan *et al.*[19] further developed this model by considering two-phase flow, kinetic energy, and Joule-Thompson effects. However, some key parameters are regarded as constant and only consider the partial coupling between pressure (flow) and temperature (thermal) in the above analytical models. Stone *et al.*[24,25] presented a full coupling numerical model for thermal wellbore flow when they developed the reservoir simulator, which is called the black-oil model. Later, to grasp the slip between phases and to better handle unsteady flow, Shi *et al.*[29] introduced the drift-flux model (DFM) to describe the wellbore flow. Then, Livescu *et al.*[27,28] proposed a new full coupling numerical model by using the DFM, which has a higher computational accuracy.

As the main fluid media are CO_2 and CO_2-brine mixtures for CCS projects and CO_2 has significantly different fluid properties than water and oil, whether the above models can be applied depends on if CO_2 and its mixtures can satisfy the specific assumptions of those models. As we know, analytical solutions in the oil and gas industry concentrate on the steady flow, so CO_2 and its mixtures will satisfy the conditions when the flow gradually transforms into steady state. While the physical properties (e.g. density, specific heat capacity) of CO_2 strongly rely on its pressure and temperature,[5,30,31] a phase change will occur when the pressure and temperature approach a specific value. Therefore, when these analytical models are applied to predict the wellbore pressure and temperature distribution, the physical properties of CO_2 should be a function of pressure and temperature instead of constant. As a mesh generation about the wellbore is indispensable in the application, the solving process becomes a numerical method instead of a pure analytical method. Thus, Lu and Connell[5] developed a numerical procedure to study the flow behavior of CO_2 and its mixtures by solving the coupled mass, momentum, and energy equations combined with equation of state and thermodynamic relations for fluid properties.

As for the numerical models in consideration of transient flow in the oil and gas industry, apparently, they are not applicable because the behavior of CO_2 is more complicated than the fluid (oil, water, nitrogen) in the oil and gas industry under an unsteady flow state. Therefore, we must explore a new method for the transient flow of CO_2 in wellbore. Pan *et al.*[6] noted that the DFM can perfectly describe the complicated physical phenomenon based on the conclusion of Shi *et al.*[29] Consequently, they developed a numerical wellbore flow model to describe the transient flow of CO_2-brine mixtures by adopting the DFM to simulate the actual flow in the wellbore while the wellbore heat transfer is handled semi-analytically. Later, they applied this model to a steady two-phase flow and obtained an analytical solution under isothermal conditions.[32] They also presented a coupled wellbore-reservoir simulator by coupling this wellbore flow model with a standard reservoir simulator, TOUGH2/ECO2N, which is called T2Well/ECO2N.[33,34] Whereas the DFM involves a series of empirical parameters, which was determined by many experiments when Shi *et al.*[29] introduced it into the wellbore of the oil and gas industry, only the oil, water, and nitrogen were used as the fluid media in those experiments.[35] There is a significant difference between CO_2 and oil or nitrogen,

hence, whether the values of empirical parameters are appropriate for CO_2 and its mixtures is undetermined. The necessary discussion and experimental verification is barely found in Pan *et al.*,[6,32–34] thus, the above work still need to be further improved. Recently, Ruan *et al.*[36] proposed a two-dimensional wellbore flow and thermal model with consideration of the natural convection of fluid in the annulus and surrounding rock formation. Jiang *et al.*[37] generalized this model by including the reservoir. Unfortunately, the friction term is absent in the momentum equation. The conclusion of Bai *et al.*[7] showed that the friction term can be omitted only when the injection rate is low. In addition, other models can be found in Mireault *et al.*,[38,39] Lindeberg,[40] Sasaki and Sugai,[41] and Singhe *et al.*;[42] they also contribute to the development of wellbore flow and thermal model.

In conclusion, as the fluid properties of CO_2 and its mixtures are significantly different from those of water and oil, which strongly depend on its pressure and temperature, there is no appropriate and effective model that can be applied to predict the wellbore pressure and temperature distribution in CO_2 geological sequestration. Even for the simplest steady single-phase flow, these analytical or semi-analytical models are too simple to handle the coupling of pressure and temperature, while the coupled numerical models are complicated in form, inconvenient to understand and apply due to their heavy computational work, and still regard some key pressure and temperature dependent parameters as constants. As the models developed for transient flow or multi-phase flow lack the necessary experimental verification, they still need to be improved. Moreover, an interesting problem is that all these models ignore the friction loss work in their energy equation.

Therefore, this work will carry out an investigation on the basic steady single-phase flow and develop a new simple coupling numerical model including all terms both in the momentum and in the energy equation for wellbore flow and heat transfer. In addition, the more accurate specific calculation methods for some key parameters influenced by pressure and temperature are introduced in this paper, and will be updated in the full process of calculation. Finally, a comparison of this new model, other models, and the log data from engineering is implemented by simulating the practical project to verify the reliability of this new model.

Fundamental theory and mathematical model

Basic assumptions

The mathematical model of wellbore flow and heat transfer discussed in this work follows some basic assumptions:

1. One-dimensional steady single-phase flow in wellbores (pipes), homogeneous fluid, i.e., the density, velocity, pressure, temperature, and the other physical properties of different positions at the same cross section, are all uniform. Noting that, the homogeneous fluid of this work is not only the single-component flow but also refers to the homogeneous multi-component flow. Since this work aims to steady the flow, while the original fluid in the wellbore is displaced in the initial transient flow, the fluid in the wellbore is near to a single component when the flow approaches to steady state. Therefore, the assumption of homogeneous fluid for steady flow is relatively consistent with the actual case. To simplify the expression, this work only takes the single-component flow as an example to derive the coupled wellbore flow and thermal model. With regard to the multi- component flow, it will be okay if the basic physical properties (density, velocity, and isobaric specific heat capacity) are expressed in the form of mixture fluid.
2. It only considers the radial heat transmission between the fluid in the wellbore and its surrounding earth. The heat transfer from the surrounding earth to the second interface (cement/earth interface) is regarded as unsteady state, while it is assumed to be steady state between the second interface and the fluid in the wellbore.[10]
3. The impact of phase change induced by the transformation of pressure and temperature on the physical properties is neglected because the latent heat is difficult to calculate.
4. The integral wellbore is divided into finite micro-segments. All other physical properties except for the variable under study are supposed to be constant within a certain micro-segment, when establishing the wellbore flow and thermal model.

Wellbore Flow

Taking a micro-segment whose length is dx as the object of this study, a coordinate system is set as in

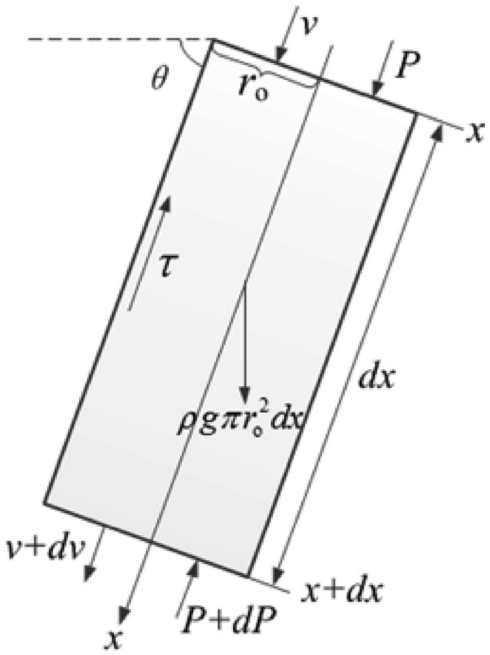

Figure 1. The micro-segment model of wellbore flow.

Fig. 1, whose positive direction is parallel to the center axis of wellbore downward. Supposing a homogeneous injection with the injection rate C [kg/s], the flow direction is consistent with the positive direction of the coordinate system. Based on the basic principle of flow dynamics, the mass (continuity) equation for one-dimensional steady flow is

$$\frac{d(\rho v)}{dx} = 0 \tag{1}$$

where ρ is the density of fluid, in kg/m^3;v is the velocity of fluid, in m/s; x is the wellbore coordinate, in m.

The momentum equation of fluid in wellbore can be described by

$$\rho g \pi r_o^2 dx \sin\theta - \pi r_o^2 dP - 2\tau\pi r_o dx = \rho\pi r_o^2 dx \frac{dv}{dt} \tag{2}$$

where,

$$\tau = \frac{\lambda}{8}\rho v^2 \tag{3}$$

Bringing Eqn (3) into Eqn (2), a formula of pressure gradient can be obtained:

$$\frac{dP}{dx} = \rho g \sin\theta - \lambda\frac{\rho v^2}{4r_o} - \rho v\frac{dv}{dx} \tag{4}$$

where P is the pressure of fluid in wellbore, in Pa; g donates the acceleration of gravity, in m/s^2; λ donates the friction coefficient; r_o is the inner radius of tubing, in m;θ donates the incline angle of wellbore; τ is the shear stress of fluid and well-face, in Pa; t is the injection time, in s.

On the right side of Eqn (4), the first term describes the effect of gravity on the pressure gradient, which is called gravity term; similarly, the second term and the third term reflect the effect of friction and acceleration on the pressure gradient, respectively, so-called acceleration term and friction term.[7]

The equation of state of fluid is

$$\rho = \frac{PM}{ZRT} \tag{5}$$

where Z is the compression factor; R is universal gas constant, in J/mol/K; T is the thermodynamic temperature of fluid in wellbore, in K; M is the gas molar mass, in kg/mol.

According to Bai *et al.*,[7] Eqn (1) indicates that

$$\rho v = \overline{C} \tag{6}$$

where $\overline{C}$ denotes the mass flow rate in unit cross section of wellbore, in kg/m^2/s, or,

$$\overline{C}\pi r_o^2 = C \tag{7}$$

Bringing Eqn (5) into Eqn (6), we have,

$$v = \frac{\overline{C}ZRT}{PM} \tag{8}$$

Substituting Eqn (5) and Eqn (8) into Eqn (4) yields,

$$\frac{dP}{dx} = \frac{PM}{ZRT}g\sin\theta - \frac{\lambda\overline{C}^2 R}{4r_o M}\frac{ZT}{P} - \frac{\overline{C}^2 R}{M}\frac{d}{dx}\left(\frac{ZT}{P}\right) \tag{9}$$

Though the pressure and temperature affect each other, and they will impact the compression factor and the friction coefficient, the temperature and the other physical properties of fluid are constants in a micro-segment, when deriving the wellbore flow model. Thus, Eqn (9) can be expressed by

$$\frac{dP}{dx} = \frac{PM}{ZRT}g\sin\theta - \frac{\lambda\overline{C}^2 R}{4r_o M}\frac{ZT}{P} + \frac{\overline{C}^2 R}{M}\frac{ZT}{P^2}\frac{dP}{dx} \tag{10}$$

or,

$$\frac{dP}{dx} = \left(\frac{PM}{ZRT}g\sin\theta - \frac{\lambda\overline{C}^2 R}{4r_o M}\frac{ZT}{P}\right)\Bigg/\left(1 - \frac{\overline{C}^2 R}{M}\frac{ZT}{P^2}\right) \tag{11}$$

Equation (11) is a first-order, non-linear, non-homogeneous, ordinary, differential equation about pressure in any micro-segment of the wellbore. Since the analytical solution cannot be obtained by an analytical integral method, numerical methods are the only way to solve Eqn (11). One of these is the classic numerical method, such as the fourth order Runge-Kutta method; another is the finite difference method. Here, the latter will be used for its simplicity in form and convenience in application. The ideal accuracy will be realized only if the step size of the iteration is better controled.[7] Hence, the explicit difference scheme of Eqn (11) under a known wellhead injection pressure is

$$\frac{P_{i+1} - P_i}{\Delta x} = \left(\frac{P_i M}{ZRT}g\sin\theta - \frac{\lambda\overline{C}^2 R}{4r_o M}\frac{ZT}{P_i}\right)\Bigg/\left(1 - \frac{\overline{C}^2 R}{M}\frac{ZT}{P_i^2}\right) \tag{12}$$

where the subscript i denotes the number of micro-segment of wellbore.

Or the explicit finite difference model (EFDM) about pressure is

$$P_{i+1} = P_i + \Delta x \cdot \left(\frac{Mg\sin\theta}{R}\frac{P_i}{ZT} - \frac{\lambda\overline{C}^2 R}{4r_o M}\frac{ZT}{P_i}\right)\Bigg/\left(1 - \frac{\overline{C}^2 R}{M}\frac{ZT}{P_i^2}\right) \tag{13}$$

Similarly, when knowing the bottom pressure, it is

$$P_{i-1} = P_i - \Delta x \cdot \left(\frac{Mg\sin\theta}{R}\frac{P_i}{ZT} - \frac{\lambda\overline{C}^2 R}{4r_o M}\frac{ZT}{P_i}\right)\Bigg/\left(1 - \frac{\overline{C}^2 R}{M}\frac{ZT}{P_i^2}\right) \tag{14}$$

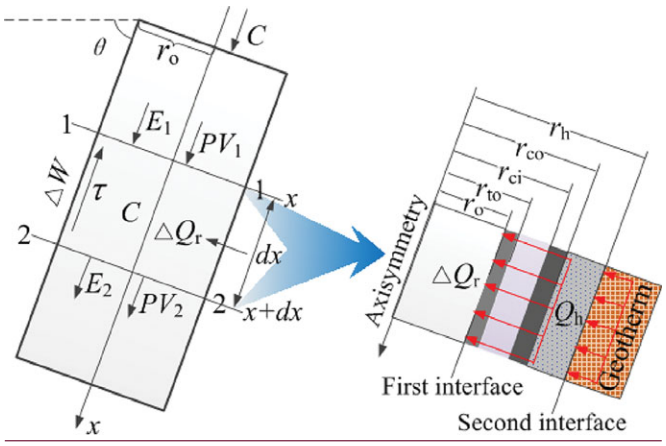

Figure 2. The micro-segment structure of wellbore and thermal model.

Wellbore heat transfer

As we know, the existence and movement form of mass in the flow field can be perfectly described by the mass and momentum equations for isothermal flow. And all physical parameters can be solved by combining the constitutive equation (equation of state) of fluid. However, the necessary constraint based on energy balance is needed for non-isothermal flow, so the energy equation should be added to describe the flow field.[43]

The heat transmission between the fluid in an injection well and its surrounding earth will occur because of their difference in temperature, inducing the change of fluid temperature. The change rate relies on the velocity of fluid and the heat transfer efficiency of its surrounding media. As Fig. 2 shows is the micro-segment structure of wellbore and thermal model, still taking the same micro-segment of wellbore as the study object. Thus, the mass of fluid through the micro-segment are m [kg] $= C^*dt$ for steady flow in time of dt, so the flux inflowing the cross section of 1-1, outflowing the cross section of 2-2, and remaining in the micro-segment are all equal to C^*dt at the same time. While their volumes are different in consideration of the compression property of fluid, V_1 [m^3] and V_2 [m^3] donate the volume of fluid inflowing the cross section of 1-1 and outflowing the cross section of 2-2, respectively, supposing that the total energy and the flow work of fluid inflowing the cross section of 1-1 are E_1 [J] and PV_1 [J] in the process, respectively. Similarly, these are E_2 [J] and PV_2 [J] for the cross section of 2-2. The radial heat transfer from the surrounding earth to the fluid in the micro-segment is ΔQ_r [J]; the friction

loss of this process is ΔW[J]. Since it is steady flow, the mass increment and the total energy increment of fluid in the micro-segment are both equal to zero after finishing this process. Therefore, according to the first law of thermodynamics, the energy balance equation with all terms of the process can be expressed by

$$E_1 + PV_1 + \Delta Q_r - (E_2 + PV_2 + \Delta W) = 0 \quad (15)$$

where

$$E = U + E_k + E_P \quad (16)$$

$$\begin{cases} U = H - PV \\ E_k = \frac{1}{2}mv^2 \\ E_P = mgx\sin\theta \end{cases} \quad (17)$$

where U is internal energy, in J; H is enthalpy, in J; E_k is kinetic energy, in J; E_p is potential energy, in J.

A further expression can be obtained from Eqn (15) to Eqn (17),

$$\begin{aligned} \Delta Q_r - \Delta W &= E_2 - E_1 + PV_2 - PV_1 \\ &= (U + dU - U) + \tfrac{1}{2}m[(v + dv)^2 - v^2] \\ &\quad + mg(x + dx - x)\sin\theta + P(V_2 - V_1) \\ &= dU + m(vdv + \tfrac{1}{2}dvdv) + mgdx\sin\theta + PdV \\ &= dH + m(vdv + \tfrac{1}{2}dvdv) + mgdx\sin\theta \end{aligned} \quad (18)$$

As for the calculation of enthalpy, the universal formula of actual gas is adopted here:

$$dH = c_P m dT + \left[\frac{1}{\rho} - T\left(\frac{\partial \frac{1}{\rho}}{\partial T}\right)_P\right] dP \quad (19)$$

where c_p denotes the isobaric specific heat capacity, in J/kg/K.

Since the pressure in any micro-segment of wellbore is regarded as constant, the second term of the right side of Eqn (19) is zero. Therefore, substituting it into Eqn (18), we have

$$\Delta Q_r - \Delta W = m(c_P dT + vdv + \frac{1}{2}dvdv + gdx\sin\theta) \quad (20)$$

The calculation of radial heat transmission of the fluid in the wellbore and the surrounding earth can be divided into two parts in this process: the first one is the heat from surrounding earth that transmits into the second interface, i.e., the cement/earth interface, by heat conduction. As already mentioned, it is unsteady but satisfies the dimensionless time function of Ramey.[10] So the radial heat transfer from the surrounding earth to the second interface is

$$\Delta Q_h = \frac{2\pi k_e(T_e - T_h)}{f(t)}dxdt \quad (21)$$

where ΔQ_h denotes the radial heat transfer from the surrounding earth to the second interface, in J; k_e denotes the thermal conductivity of typical rock, in W/m/K; T_e denotes the initial temperature of earth, in K; T_h is the temperature of the second interface, in K; $f(t)$ is the dimensionless time function.

The second one is the heat transfer from the second interface to the fluid in the form of heat convection, radiation, and conduction, which is a steady process,[10] as Eqn (22) shows:

$$\Delta Q_r = 2\pi r_o dx U_t(T_h - T)dt \quad (22)$$

where U_t is the overall heat transfer coefficient, in W/m^2/K.

The value of heat transmission of the first part is equal to that of the second part in the same time for steady flow,[10] hence the temperature of the second interface is, according to Eqn (21) and Eqn (22) is

$$T_h = \frac{T_e k_e + f(t) r_o U_t T}{f(t) r_o U_t + k_e} \quad (23)$$

Bringing Eqn (23) back into Eqn (22) obtains

$$\Delta Q_r = \frac{2\pi r_o U_t k_e}{f(t) r_o U_t + k_e}(T_e - T)dxdt \quad (24)$$

The friction loss is calculated directly by the definition of work:

$$\Delta W = 2\pi r_o \tau dxdx = \frac{\lambda}{4}\rho v^2 \pi r_o dxdx \quad (25)$$

Substituting Eqn (6) and Eqn (7) into Eqn (25) yields

$$\Delta W = \frac{\lambda C v}{4 r_o}dxdx \quad (26)$$

Noting that although the friction loss turns the mechanical energy to heat, and the heat in turn leads to the increase of wellbore temperature. However, there is no doubt that the conversion ratio cannot approach 100%. Therefore, it is inappropriate to completely neglect the friction loss in the energy balance equation. As to the additional heat received from friction, it is implicitly included in the radial heat transmission in this work.

Bringing Eqn (24) and Eqn (26) into Eqn (20) produces

$$\frac{2\pi r_o U_t k_e}{f(t) r_o U_t + k_e}(T_e - T)dxdt - \frac{\lambda C v}{4r_o}dxdx = m(c_P dT + vdv + \frac{1}{2}dvdv + gdx\sin\theta) \quad (27)$$

Letting Eqn (27) be divided by dt, obtains

$$\frac{2\pi r_o U_t k_e}{f(t) r_o U_t + k_e}(T_e - T)dx - \frac{\lambda C v^2}{4r_o}dx = C(c_P dT + vdv + \frac{1}{2}dvdv + gdx\sin\theta) \quad (28)$$

A part of the kinetic energy term is second order infinite, while the other terms are all first order infinite in Eqn (28). Therefore, the second order infinite can be ignored from the perspective of mathematics:

$$\frac{2\pi r_o U_t k_e}{C[f(t) r_o U_t + k_e]}(T_e - T)dx = c_P dT + vdv + gdx\sin\theta + \frac{\lambda v^2}{4r_o}dx \quad (29)$$

Similarly, the left side is a heat transmission term; the four terms on the right side are enthalpy, kinetic energy, potential energy, and friction term, in that order.

Letting $A = \frac{2\pi r_o U_t k_e}{C[f(t) r_o U_t + k_e]}$, Eqn (29) can be expressed by

$$c_P \frac{dT}{dx} + AT = AT_e - g\sin\theta - \frac{vdv}{dx} - \frac{\lambda v^2}{4r_o} \quad (30)$$

For Eqn (30), one study[13] assumed the last three terms on the right side to be constants, so the analytical solution of temperature could be obtained by an analytical integral method. The problem there is that the gradient of v is unknown, and it is unreasonable to regard the gradient of v as a constant. Thus, the analytical solution produced by this method is not rigorous. in contrast, Ramey's solution with more constraint conditions is more meaningful and widely used in the oil and gas industry. The reason why Ramey's solution is not adopted in this work is that its assumptions are too ideal to apply in CCS projects because of their higher safety requirements, the process of solving temperature is not linked with pressure, and the coupling effect of pressure field and temperature field is neglected. Therefore, this work aims to realize the coupling of pressure field and temperature field by as few assumptions as possible, and to develop the thermal model. Thus, a further derivation for Eqn (30) is obtained by taking Eqn (5) and Eqn (8) into Eqn (30):

$$c_P \frac{dT}{dx} + AT = AT_e - \left[g\sin\theta + \left(\frac{\overline{C}ZR}{PM}\right)^2 T\frac{dT}{dx} + \frac{\lambda}{4r_o}\left(\frac{\overline{C}ZR}{PM}\right)^2 T^2 \right] \quad (31)$$

The initial temperature of earth is a function of depth (coordinate), or

$$T_e = ax + b \quad (32)$$

where a is the gradient of initial temperature, in K/m; b is the temperature of earth surface, in K.

According to Eqn (31) and Eqn (32), a formula about the temperature gradient can be expressed by

$$\frac{dT}{dx} = \left[A(ax + b - T) - g\sin\theta - \frac{\lambda}{4r_o}\left(\frac{\overline{C}ZR}{PM}\right)^2 T^2 \right] \Big/ \left[c_P + \left(\frac{\overline{C}ZR}{PM}\right)^2 T \right] \quad (33)$$

Equation (33) is also a first-order, non-linear, non-homogeneous, ordinary differential equation about temperature in a micro-segment of the wellbore. Apparently, the analytical integration is impractical, so this work still chooses the finite difference method to solve it. When the wellhead injection temperature of fluid is known, we have

$$\frac{T_{i+1} - T_i}{\Delta x} = \left[A(ax + b - T_i) - g\sin\theta - \frac{\lambda}{4r_o}\left(\frac{\overline{C}ZR}{PM}\right)^2 T_i^2 \right] \Big/ \left[c_P + \left(\frac{\overline{C}ZR}{PM}\right)^2 T_i \right] \quad (34)$$

So, the explicit finite difference model (EFDM) about temperature is:

$$T_{i+1} = T_i + \Delta x \left[A(ax + b - T_i) - g\sin\theta - \frac{\lambda}{4r_o} \left(\frac{\overline{C}ZR}{PM}\right)^2 T_i^2 \right] \Big/ \left[c_P + \left(\frac{\overline{C}ZR}{PM}\right)^2 T_i \right] \quad (35)$$

Similarly, when knowing the bottom temperature, it is:

$$T_{i-1} = T_i - \Delta x \left[A(ax + b - T_i) - g\sin\theta - \frac{\lambda}{4r_o} \left(\frac{\overline{C}ZR}{PM}\right)^2 T_i^2 \right] \Big/ \left[c_P + \left(\frac{\overline{C}ZR}{PM}\right)^2 T_i \right] \quad (36)$$

Key parameters

The derivation of wellbore flow and heat transfer models involves some key P and T dependent parameters, and their calculation will influence the accuracy of the models. The specific calculation methods of those parameters are as follows.

Compression factor Z

The compression factor (Z) is used to distinguish the actual fluid and the ideal gas, which is a function of pressure and temperature. Some widely used methods to obtain Z include a look-up table, empirical formulae, and the equation of state method. The Peng-Robinson's equation,[44] suited for both gas and fluid,[45] is used to calculate Z here, as Eqn (37) shows:

$$Z^3 - (1-Y)Z^2 + (X - 3Y^2 - 2Y)Z - (XY - Y^2 - Y^3) = 0 \quad (37)$$

where

$$X = 0.45724\xi \frac{P}{P_c}\left(\frac{T_c}{T}\right)^2 \quad (38)$$

$$Y = 0.0778 \frac{P}{P_c}\frac{T_c}{T} \quad (39)$$

where ξ is a proportional coefficient detailed in Peng and Robinson,[44] and P_c and T_c are the critical pressure [Pa] and temperature [K], respectively.

Friction coefficient λ

There is an accurate implicit method to solve λ, i.e., the Colebrook equation. However, the numeric iteration calculation is the only choice to solve it. Consequently, some appropriate explicit methods are developed from the Colebrook equation, such as the Wood equation, the Churchill equation, and the Chen(46)equation.[46] Compared with the other explicit equation, the Chen equation is simpler but still accurate, and suits all Reynolds numbers and roughness,[46] which means the effect of flow state need not to be considered. Hence, the Chen equation is applied to calculate λ,

$$\frac{1}{\sqrt{\lambda}} = -2.0\lg\left[\frac{1}{3.7065}\frac{\varepsilon}{2r_o} - \frac{5.0452}{Re}\lg\left(\frac{1}{2.8257}\left(\frac{\varepsilon}{2r_o}\right)^{1.1098} + \frac{5.8506}{Re^{0.8981}}\right)\right] \quad (40)$$

$$Re = 2r_o\rho v/\mu = 2r_o\overline{C}/\mu \quad (41)$$

where ε is the roughness of the well-face, in m; Re denotes the Reynolds number; μ means the viscosity of fluid, in Pa·s.

Note that the viscosity in Eqn (41) is also a function of pressure and temperature. The calculation method of Fenghour *et al.*[47] and Vesovic *et al.*[48] is used here. The applicable ranges of pressure and temperature are very wide, and the relative error is less than 0.3% under normal pressure and temperature; the relative error is below 5% even for high pressure and high temperature. Based on this method, the viscosity of CO_2 consists of three independent parts:

$$\mu = \mu_0(T) + \Delta\mu(\rho, T) + \Delta\mu_c(\rho, T) \quad (42)$$

The three terms on the right are the viscosity in the zero-density limit, the viscosity influenced by the increment of density, and the incremental viscosity in critical point. Their specific calculation is detailed in Fenghour *et al.*[47] and Vesovic *et al.*[48]

Dimensionless time function $f(t)$

Since the $f(t)$ of Ramey's solution only suits the case over a long time (more than 7 days), Hasan and Kabir[14] presented a new function that can work for both long-time and short-time scenarios,

$$f(t) = \begin{cases} 1.1281\sqrt{t_D}\left(1 - 0.3\sqrt{t_D}\right) & , t_D \le 1.5 \\ (0.5\ln t_D + 0.4063)\left(1 + \frac{0.6}{t_D}\right) & , t_D > 1.5 \end{cases} \quad (43)$$

where $t_D = \alpha t/r_h^2$, denotes the dimensionless time; α is the thermal diffusivity of earth, in m^2/h; r_h is the radius of injection well, in m.

Overall heat transfer coefficient U_t

The overall heat transfer coefficient reflects the summation of all thermal resistances in the process of heat transfer from the second interface to the fluid, including the cement, casing, annulus, and tubing. The conclusion of Willhite[11] demonstrated that: (i) the thermal resistance of tubing and casing can be neglected because the thermal conductivity of the tubing and casing made from steel is considerably higher than that of the other materials in the wellbore, which means $T_{ci} = T_{co}$, $T_{ti} = T_{to}$; (ii) the temperature at the inside tubing-face and the fluid in the tubing is the same because the film coefficient and condensation coefficient of the fluid are both large enough, i.e., $T_{ti} = T$. Thus, the overall heat transfer coefficient can be described by

$$U_t = \left[\frac{1}{h_c + h_r} + \frac{r_{to}\ln\frac{r_h}{r_{co}}}{k_{cem}}\right]^{-1} \tag{44}$$

where

$$h_c = \frac{k_{hc}}{r_{to}\ln\frac{r_{ci}}{r_{to}}} \tag{45}$$

$$h_r = \sigma F_{tci}\left(T_{to}^2 + T_{ci}^2\right)\left(T_{to} + T_{ci}\right) \tag{46}$$

where h_c is the heat transfer coefficient for natural convection of annulus, in $W/(m^2\cdot K)$; h_r is the heat transfer coefficient for radiation, in $W/(m^2\cdot K)$; r_{to} is the outside radius of tubing, in m; r_{co} and r_{ci} are the outside radius and inner radius of casing, in m, respectively; σ is the Stenfan-Boltzmann constant; k_{cem} is the thermal conductivity of the cement, in $W/(m\cdot K)$; k_{hc} is the thermal conductivity of fluid in annulus, in $W/(m\cdot K)$;F_{tci} is the effective factor of radiation between the outside tubing-face and inside casing-face; T_{to} is the temperature of outside tubing-face, in K; T_{ci} is the temperature of inside casing-face, in K.

The F_{tci} in Eqn (46) can be expressed by

$$F_{tci} = \left(\frac{1}{\varepsilon_{to}} + \frac{r_{to}}{r_{ci}}\left(\frac{1}{\varepsilon_{ci}} - 1\right)\right)^{-1} \tag{47}$$

$$T_{ci} = T_h + \frac{r_o U_t \ln\frac{r_h}{r_{co}}}{k_{cem}}(T - T_h) \tag{48}$$

where ε_{to} is the radiation coefficient of outside tubing-face; ε_{ci} is the radiation coefficient of inside casing-face.

The steps of iterative calculation for the overall heat transfer coefficient are as follows:

1. Estimate the initial value of U_t based on the characteristic of the wellbore structure.
2. Calculate $f(t)$ based on Eqn (43).
3. Determine T_h by using Eqn (23).
4. Determine T_{ci} by using Eqn (48).
5. Calculate h_c and h_r according to Eqn (45) and Eqn (46), respectively.
6. Obtain the new value of U_t from Eqn (44).
7. Compare the new value of U_t with the initial value. If the deviation is above the upper limit, update the initial value of U_t with the new value and repeat step (2) to step (6), then compare again until an agreement is reached. Take the last one as the value of U_t. Generally, three iterations are enough.

Isobaric specific heat capacity c_P

The isobaric specific heat capacity of ideal gas is only a function of temperature, while it is a function of both pressure and temperature for actual fluid. Therefore, the calculation model of Span-Wagner[31] based on the dimensionless Helmholtz energy is selected in this work. The equation of solving c_P is

$$\frac{c_P}{R} = -\chi^2\left(\frac{\partial^2\Phi^o}{\partial\chi^2} + \frac{\partial^2\Phi^r}{\partial\chi^2}\right) + \left(1 + \delta\frac{\partial\Phi^r}{\partial\delta} - \delta\chi\frac{\partial^2\Phi^r}{\partial\chi\,\partial\delta}\right)^2 \Bigg/ \left(1 + 2\delta\frac{\partial\Phi^r}{\partial\delta} + \delta^2\frac{\partial^2\Phi^r}{\partial\delta^2}\right) \tag{49}$$

$$\chi = T_c/T,\ \delta = \rho/\rho_c \tag{50}$$

where Φ^o and Φ^r denote the ideal part and the residual part of the dimensionless Helmholtz energy, respectively; ρ_c is the critical density, in kg/m^3; χ and δ denote the inverse reduced temperature and the reduced density, respectively.

Coupling calculation method

This work established an EFDM about pressure and temperature for the same micro-segment of the wellbore in the sections, Wellbore flow and Wellbore heat transfer, respectively. Then the specific calculation method of some key parameters was presented in the

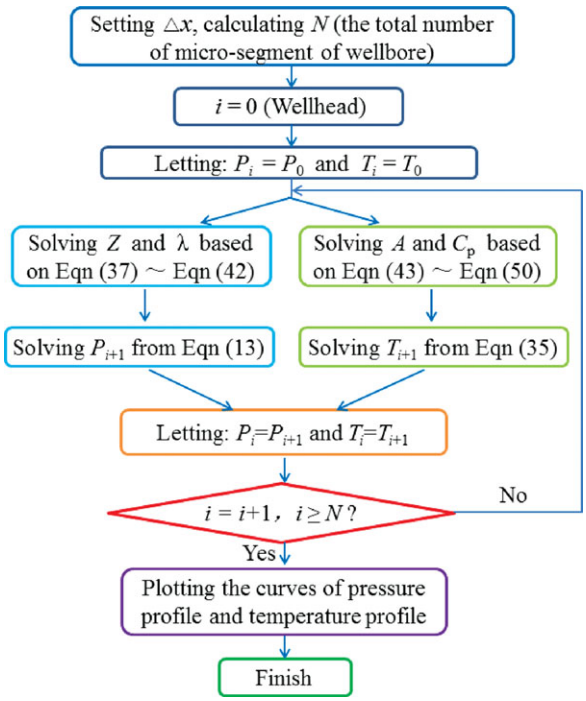

Figure 3. The specific coupling calculation method given the wellhead injection parameters.

section, Key parameters. To realize the decoupling of the pressure field and the temperature field, all the other physical parameters except for pressure are regarded as constants when deriving the model of pressure. Similarly, all the other physical parameters except for temperature are assumed as constants when deriving the model of temperature. However, this decoupled method is only valid in the micro-segment of the wellbore. To generalize the EFDM to the whole wellbore, the recoupling of pressure and temperature is needed. Hence, the specific coupling calculation method is presented here, taking the known wellhead injection parameters (injection rate, wellhead injection pressure (P_0) and temperature (T_0) of injected fluid) as an example, as shown in Fig. 3. It is similar if the bottom parameters are known. As to the determination of Δx in Fig. 3, the calculation results of Bai *et al.*[7] show that it will satisfy the requirement of accuracy and efficiency simultaneously, when Δx ranges from 0.1 to 1 m.

Verification

To verify the reliability of this work, two practical projects are taken as the analysis objects, and the results calculated by this work are compared with the log data from engineering and the simulation results of other models in this part.

Table 1. The main parameters of ZSZ1.[7,37]

Parameter	Value	Parameter	Value
Depth (m)	2500	k_{cem} (W/m/K)	0.35
r_o (mm)	31	k_{hc} (W/m/K)	0.6
r_{to} (mm)	36.5	k_e (W/m/K)	2.2
r_{ci} (mm)	62.13	α(m^2/h)	0.0037
r_{co} (mm)	68.95	ε(mm)	0.03
r_h (mm)	107.95	a (K/m)	0.026*
θ	$\pi/2$	b (K)	288.15

* : a = 0.016 at the depth of 1680 m to 2500 m.

Example 1

The Shenhua CCS demonstration project is the first large-scale CO_2 saline aquifer storage project with whole processes in China. Therefore, it was taken as the first example here. The main parameters of ZSZ1 (injection well in the Shenhua CCS project) are listed in Table 1, cited from Jiang *et al.*[37] The partial parameters (the parameters of the wellbore structure) are referred to in Bai *et al.*[7] Before doing the verification of comparing the simulated results with the log data from the project, a reliability verification of our algorithm was implemented. To verify the reliability of our algorithm, the classic fourth order Runge-Kutta method (FRKM) was applied as the comparison algorithm to solve the differential Eqns (11) and (33). The designed wellhead injection parameters are listed in Table 2. The other calculation parameters are consistent with Table 1. The calculation results of EFDM and FRKM are also shown in Table 2.

According to Table 2, the relative error of calculation results between EFDM and FRKM are all small under different wellhead injection parameters, which means the explicit finite difference method applied to solve Eqn (11) and Eqn (33) is reliable, and the EFDM about pressure and temperature in the wellbore expressed by Eqn (13) and Eqn (35) is no problem in the algorithm.

Later, a further verification of whether this work can predict the actual pressure and temperature in the application of practical projects was carried out. According to the data of Jiang *et al.*,[37] $P_o = 6$ MPa, $T_o = 0\ ^\circ$C, $C = 0.9$ kg/s. The curves of pressure and temperature in the wellbore calculated by this work

Table 2. Wellhead injection parameters and comparison of calculation results between EFDM and FRKM (Only verifying the reliability of algorithm here, so the injectivity is not considered).

Wellhead injection parameters			Bottom pressure (MPa)		Relative error (%)	Bottom temperature (°C)		Relative error (%)
C (kg/s)	P_o (MPa)	T_o (°C)	EFDM	FRKM		EFDM	FRKM	
0.5	6	0	27.682	27.690	0.029	55.612	55.610	0.0036
1	6	0	29.193	29.201	0.027	41.150	41.151	0.0024
1	10	0	34.030	34.036	0.018	42.809	42.812	0.0071
1	6	10	28.317	28.324	0.025	42.559	42.561	0.0047
2	10	0	35.069	35.075	0.017	25.325	25.330	0.020
5	10	0	35.725	35.732	0.020	7.034	7.038	0.057
10	20	0	46.564	46.569	0.011	1.032	1.033	0.097

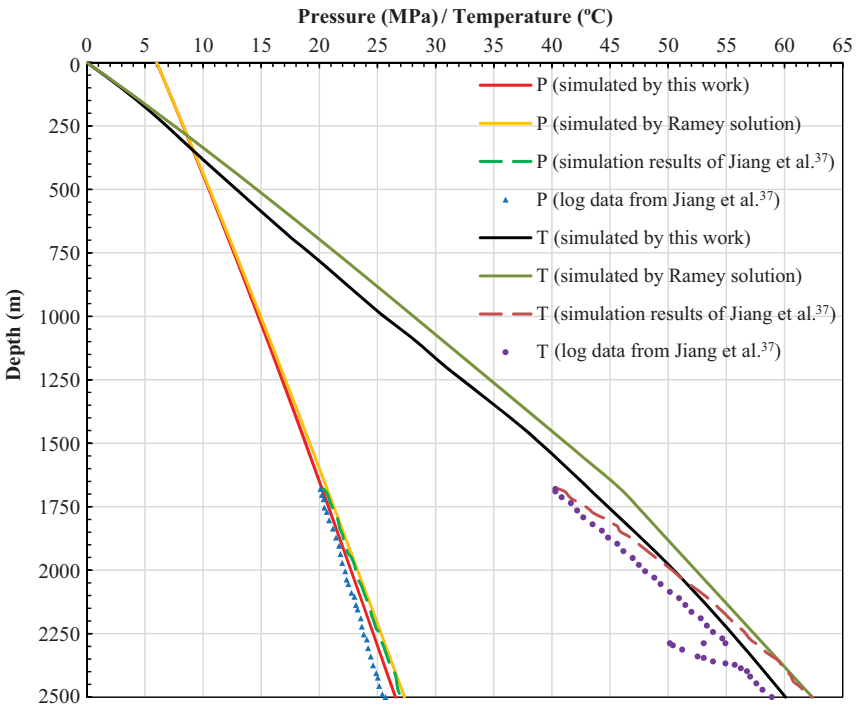

Figure 4. Comparison of pressure and temperature between simulation results and log data of ZSZ1.

and Ramey's solution are shown in Fig. 4, including the log data and the simulation results from Jiang *et al.*[37]

In Fig. 4, the EFDM in all ranges of pressure and temperature in the wellbore can better predict the actual pressure and temperature in the wellbore than the other models. Though the simulation results of Jiang *et al.*[37] are based on a two-dimensional numerical model, the result is not ideal because the friction loss is ignored in both momentum and energy equations. As to Ramey's solution, the results are higher not only than the log data but also than the results of this work, especially for temperature, because friction loss is not included in its wellbore heat transfer and the effect of pressure on temperature is not considered.

Example 2

The second analysis case is the pilot test project of CO_2-enhanced oil recovery managed by the Sinopec Group. The site is in the Caoshe oil field in China. The injection well is CS8, whose main parameters are listed

Table 3. The main parameters of CS8.[49]

Parameter	Value	Parameter	Value
Depth (m)	3100	α(m^2/h)	0.0037
r_o (mm)	31	ε(mm)	0.03
r_{to} (mm)	36.5	θ	$\pi/2$
r_{ci} (mm)	62.185	a (K/m)	0.03
r_{co} (mm)	68.5	b (K)	288.15
r_h (mm)	107.95	T_o (K)	293.15
k_{cem} (W/m/K)	0.52	P_o (MPa)	30
k_{hc} (W/m/K)	0.6	C (kg/s)	0.245
k_e (W/m/K)	2.09	—	—

in Table 3.[49] The calculation results based on the EFDM and the log data of CS8 are shown in Table 4. It is obvious that the model predictions of pressure and temperature in the wellbore are consistent with the log data based on Table 4. The maximum relative error is less than 2%, which satisfies the requirement of engineering in general.

Therefore, according to the verification results of Examples 1 and 2, it is convincing that the EFDM for pressure and temperature prediction and their coupling calculation method are reliable and applicable. The prediction of pressure and temperature in the wellbore and the understanding of the link between wellbore flow and heat transfer will be effectively promoted by this work for its reliability and simplicity.

Discussion

As described in the introduction, the friction loss of wellbore heat transfer is not considered in all the previously developed models, and is included in this work for the first time. Some scholars[27,41,50] assumed that the friction loss is small because of the small pipe friction factor and low fluid viscosity for CO_2 flow. However, the result of Example 1 in the verification demonstrated that there is a considerable deviation for the prediction of temperature between Ramey's solution (ignoring friction loss) and this work. Therefore, it is worth further discussing the effect of friction. Besides, based on Fig. 4, the maximum deviation of temperature between Ramey's solution and this work occurred at the bottom. Thus, the discussion about the friction loss will be carried out by comparing the prediction results of the bottom here.

If ignoring the friction term in Eqn (33), the explicit difference equation about temperature can be simplified to

$$T_{i+1} = T_i + \Delta x\left[A(ax+b-T_i) - g\sin\theta\right] \Big/ \left[c_P + \left(\frac{\overline{C}ZR}{PM}\right)^2 T_i\right] \tag{51}$$

The mass flow rate (also controlling velocity) is the main element impacting the quantity of friction loss based on Eqn (26), though the friction coefficient and velocity will change along with the variation of pressure and temperature. Therefore, it follows that the temperature at the bottom hole will be predicted by coupling Eqn (35) to include the friction loss and Eqn (51) to ignore the friction loss with Eqn (13) under a

Table 4. Comparison of pressure and temperature between the calculation results of EFDM and the log data of CS8.

	Pressure (MPa)			Temperature (°C)		
Depth (m)	Log data[49]	Calculated value	Relative Error (%)	Log data[49]	Calculated value	Relative Error (%)
0	30	30	0.00	20	20	0
100	30.89	30.98	0.29	18.22	18.56	1.87
650	35.8	36.19	1.09	30.84	29.77	3.47
700	36.24	36.64	1.10	32.34	31.24	3.40
1000	38.86	39.29	1.11	41.34	39.9	3.48
1950	46.93	47.63	1.49	69.87	67.82	2.93
2000	47.35	48.07	1.52	71.37	69.3	2.90
3000	55.54	56.57	1.85	100.14	97.65	2.49
3100	56.35	57.45	1.95	103.14	100.63	2.43

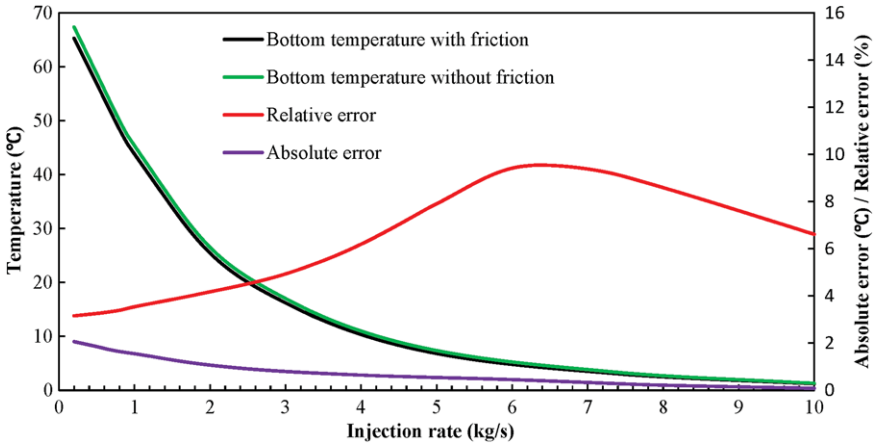

Figure 5. The temperature at bottom hole under different injection rate.

different injection rate to investigate the impact of the friction loss on temperature. As to the impact of the friction loss on pressure, this has been studied by Bai *et al.*[7] Thus, this part will not be repeated in this work. Still taking Example 1 as the analysis object, setting the wellhead injection pressure and temperature of injected fluid as 10 MPa and 0°C, respectively, the injection rate changes from 0 to 10 kg/s; the results are shown in Fig. 5.

It is clear that the temperature of the fluid at the bottom hole decreased rapidly with the injection rate increasing, finally approaching the initial temperature of injected fluid gradually, according to Fig. 5. The effect of friction loss on temperature at the bottom hole, from the perspective of error analysis, is obvious. The relative error is below 5%, when the injection rate is small, while the absolute error is above 2°C. The absolute error decreased gradually and the relative error rose at first then reduced slowly with the increase of the injection rate. The maximum relative error is near 10%. Therefore, the previous assumption that the friction loss is small or not important is not appropriate. The friction loss cannot be neglected in the investigation of the thermal damage[51] induced by temperature difference.

Another problem that needs to be discussed is that the isobaric specific heat capacity is regarded as constant in the previous research, while it is strongly dependent on pressure and temperature. Thus, to improve the accuracy, the Span-Wagner model[31] is used in this work. However, how large the deviation of them is? To answer this question, this work still took Example 1 as the analysis case and applied the wellhead injection parameters of Table 2 directly to the analysis of the sensitivity of isobaric specific heat capacity for pressure and temperature in the wellbore. The calculation results demonstrated that the impact of isobaric specific heat capacity on pressure is small; however, it is large enough for temperature, as shown in Table 5. Therefore, the isobaric specific heat capacity should be treated as variable, as in this work, when having a high temperature requirement. Only when caring about the pressure distribution can it be regarded as constant.

There are two main points of significance for predicting the pressure and temperature distribution from the perspective of engineering. On the one hand, it is necessary to evaluate the safety of the wellbore. Whether the crack (an access of CO_2 leakage) induced by high pressure and high temperature will occur or not in the wellbore can be predicted and controlled when knowing the pressure and temperature distribution. It is useful to avoid the leakage of CO_2. On the other hand, it presents a fundamental basis for evaluating the injectivity and safety of reservoirs. Investigating only the wellbore is enough for the former, while the reservoir is also indispensable for the latter. This means the wellbore should be coupled with the reservoir. In a recent study, we proposed an explicit integral solution for pressure build-up in reservoirs under a steady flow,[52] which can be coupled with the simple numerical model developed in this paper for the wellbore. Then the simulation of full process that CO_2 through the injection well into reservoirs and diffuses here will be more actual and clearer. However, taking into consideration that Pan *et al.*[32,34] and Jiang *et al.*[37] have investigated this coupling problem of wellbore and reservoir based on the models developed by them,

Table 5. Wellhead injection parameters and the comparison of calculation results of EFDM with a variable c_P and with a constant c_P.

Wellhead injection parameters			Bottom pressure (MPa)			Bottom temperature (°C)		
C (kg/s)	P_o (MPa)	T_o (°C)	c_P = variable	c_P = 2040	Relative error (%)	c_P = variable	c_P = 2040	Relative error (%)
0.5	6	0	27.682	27.445	0.856	55.612	57.372	3.165
1	6	0	29.193	28.823	1.267	41.150	43.043	4.600
1	10	0	34.030	33.737	0.861	42.809	43.965	2.700
1	6	10	28.317	27.972	1.218	42.559	44.348	4.204
2	10	0	35.069	34.784	0.813	25.325	26.287	3.799
5	10	0	35.725	35.463	0.733	7.034	7.339	4.336
10	20	0	46.564	46.358	0.442	1.032	1.084	5.039

and only the steady flow is considered in this work. Therefore, this part of work will not be repeated here.

At last, it is worth noting the problem of CO_2 leakage through an abandoned well. It is a more complicated problem for CCS projects compared with the problem of injection, because the pressure becomes low toward the top of the leaky well and a phase change of CO_2 from supercritical phase to gas phase will occur. Therefore, it will become an inverse calculation process, if applying the EFDM to simulate the process of leakage. Theoretically speaking, it is feasible because the inverse calculation process can be realized on basis of the Eqn (14) and Eqn (36), if still ignoring the phase change. From the perspective of calculation, the problem is how to get the initial condition, because the pressure, temperature, and leakage rate at the bottom hole are all unknown and undetermined. Thus, for CO_2 leakage through an abandoned well, if the initial condition can be obtained by monitoring technology or other method, the EFDM is applicable to simulate the leakage situation of the wellhead. Of course, if considering phase change, a necessary modification to the EFDM for temperature is needed. It is a big challenge because the latent heat is difficult to calculate, so it will be investigated in the next work.

Conclusions

This paper took the one-dimensional steady flow as the analysis object, and developed the EFDM to predict pressure and temperature in the same micro-segment of the wellbore based on the mass, momentum and energy equations connected by the state equation of fluid. The specific coupling calculation method of pressure and temperature in the whole wellbore is presented. The more accurate calculation methods for some key parameters influenced by pressure and temperature are also introduced. Finally, the reliability of the EFDM is verified by two case studies using practical projects. The specific conclusions are as follows:

1. To solve the non-linear, non-homogeneous, ordinary, differential equation about pressure and temperature, the finite difference method was used to obtain the EFDM about pressure and temperature, which was compared with the classic fourth order Runge-Kutta method. The results show that the EFDM is scientific and reliable in algorithm. The EFDM is simple and convenient to use in form, similar to an analytical model. It is useful to understand the internal essence of wellbore flow and heat transfer.
2. The EFDM can predict pressure and temperature distribution better than the other models in the case studies using practical projects. Thus, it is applicable to the practical project.
3. The discussion on the friction loss in wellbore heat transfer showed that the impact of friction term on temperature rose first then reduced slowly along with increasing injection rate, the maximum relative error of which is near 10%. Therefore, friction loss cannot be neglected in the investigation of the thermal damage induced by temperature difference.
4. The sensitivity analysis of isobaric specific heat capacity suggested that its impact on pressure is small, while it is obvious for temperature. Therefore, the appropriate method to deal with isobaric specific heat capacity should be selected based on the practical requirement of projects in application.

5. Only the steady single phase flow is considered in this work. It is worth generalizing the EFDM to the transient flow and multi-phase flow with phase change in further work.

Acknowledgement

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