Optimization Strategies of CO$_2$ Injection for Sequestration and EOR

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Optimization Strategies of CO\textsubscript{2} Injection for Sequestration and EOR

by

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TU Delft
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Yuan Chen
Delft, August 2018
Abstract

The current situation with green gas emission requires the development of low carbon energy solutions. However, a significant part of the modern energy industry still relies on fossil fuels. To combine these two contradictory targets, we investigate a strategy based on a combination of CO$_2$ sequestration with Enhanced Oil Recovery (EOR) in the hydrocarbon reservoirs. In such technology, the development of miscibility is the most attractive strategy from both technological and economic aspects.

Modeling of this process involves solving complex nonlinear problem describing compositional flow and transport in highly heterogeneous porous media. An accurate capture of the miscibility development usually requires an extensive number of components to be present in the compositional problem which makes simulation run-time prohibitive for optimization. Here, we apply a multi-scale reconstructing of compositional transport to the optimization of CO$_2$ injection. In this approach, a restriction operator, based on the parametrization of injection and production tie-lines, is constructed following the fractional flow theory. This operator is tabulated as a function of pressure and pseudo-composition which then is used in the Operator-Based Linearization (OBL) framework for simulation. As a result, a pseudo two-component solution of the multidimensional problem will match the position of trailing and leading shocks of the original problem which helps to accurately predict phase distribution. Applying a simple prolongation operator, based on interpolation between injection and production compositions, a compositional solution with the correct reconstruction of two-phase region can be obtained.

The reconstructed multicomponent solution can be used then as an effective proxy-model mimicking the behavior of the original multicomponent system. In this study, we use this proxy-model in the optimization procedure which helps to improve the performance of the simulation with the increasing intricacy of the reservoir model. In this work, the nonlinear constrained optimization function is applied to find optimal pressure values for CO$_2$ injection process to acquire a highest Net Present Values (NPV). Starting with the limited number of the controls, the global extrema of the objective function can be determined from both full physics model and proxy model. The result shows that both models can converge to the similar extrema given various initial guesses. It is noting that for multicomponent system, the proxy model can also have salient accuracy to predict the NPV extrema compared with the original full model.

As a result, the reconstructed proxy model can be significantly cheaper than a full conventional compositional model. An additional benefit of the proposed methodology is based on the fact that important technological features of CO$_2$ injection process can be captured with lower degrees of freedom which accelerates the optimization process.
## Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acknowledgements</td>
<td>iii</td>
</tr>
<tr>
<td>Abstract</td>
<td>v</td>
</tr>
<tr>
<td>List of Figures</td>
<td>ix</td>
</tr>
<tr>
<td>List of Tables</td>
<td>xi</td>
</tr>
<tr>
<td>1 Introduction</td>
<td>1</td>
</tr>
<tr>
<td>2 Methodology</td>
<td>3</td>
</tr>
<tr>
<td>2.1 Compositional framework</td>
<td>3</td>
</tr>
<tr>
<td>2.2 Operator-Based Linearization</td>
<td>4</td>
</tr>
<tr>
<td>2.3 Multi-Scale Compositional Transport</td>
<td>5</td>
</tr>
<tr>
<td>3 Economic Model</td>
<td>9</td>
</tr>
<tr>
<td>4 Numerical Results</td>
<td>11</td>
</tr>
<tr>
<td>4.1 Restricted solution</td>
<td>11</td>
</tr>
<tr>
<td>4.1.1 Binary system</td>
<td>11</td>
</tr>
<tr>
<td>4.1.2 Four-component system</td>
<td>12</td>
</tr>
<tr>
<td>4.1.3 Eight-component system</td>
<td>13</td>
</tr>
<tr>
<td>4.2 Prolongation of proxy model</td>
<td>13</td>
</tr>
<tr>
<td>4.2.1 Four-component system</td>
<td>13</td>
</tr>
<tr>
<td>4.2.2 Eight-component system</td>
<td>14</td>
</tr>
<tr>
<td>5 Optimization Results</td>
<td>17</td>
</tr>
<tr>
<td>5.1 NPV with a limited number of control parameters</td>
<td>17</td>
</tr>
<tr>
<td>5.1.1 One control four-component system</td>
<td>17</td>
</tr>
<tr>
<td>5.1.2 Two controls four-component system</td>
<td>17</td>
</tr>
<tr>
<td>5.1.3 Two controls eight-component system</td>
<td>19</td>
</tr>
<tr>
<td>5.2 Optimization with multiple controls</td>
<td>20</td>
</tr>
<tr>
<td>6 Conclusions</td>
<td>23</td>
</tr>
<tr>
<td>7 Future Work</td>
<td>25</td>
</tr>
<tr>
<td>Bibliography</td>
<td>27</td>
</tr>
<tr>
<td>A Appendix</td>
<td>31</td>
</tr>
<tr>
<td>A.1 Fluid and rock interactions</td>
<td>31</td>
</tr>
<tr>
<td>A.2 The other operators for a proxy model</td>
<td>32</td>
</tr>
<tr>
<td>A.3 Optimization parameters and results</td>
<td>33</td>
</tr>
<tr>
<td>A.3.1 One-control optimization four-Component system</td>
<td>33</td>
</tr>
<tr>
<td>A.3.2 Two-control optimization four-Component system</td>
<td>33</td>
</tr>
<tr>
<td>A.3.3 Muti-control optimization four-Component system</td>
<td>34</td>
</tr>
</tbody>
</table>
List of Figures

2.1 Gas-injection solution in ternary system: (a) ternary diagram with displacement path and two key tie-lines and (b) fractional-flow curves for component CO₂ with solution path. ................................................................. 5
2.2 Analytical fractional flow for CO₂ ........................................... 6
2.3 Operators for a restricted compositional system parameterized at N=64 .... 6

3.1 General economic parameters for CO₂ injection project ...................... 9
3.2 General sensitivity study for Net Present Value (NPV) .......................... 10

4.1 First stage reconstruction of binary system: (a) fractional flow curve for CO₂ (b) full and reconstructed solution for CO₂ .............................................. 11
4.2 Shock reconstruction of the four-component system for two different BHP controls at production well (K-values) ......................................................... 12
4.3 Shock reconstruction of the four-component system for two different BHP controls at production well (EoS model) ......................................................... 13
4.4 Shock reconstruction of the eight-component system for two different BHP controls at production well (K-values) ......................................................... 13
4.5 Proxy model for a four-component system (K-value based) .................... 14
4.6 Proxy model for a four-component system (EoS based) ............................ 14
4.7 Proxy model for an eight-component system (K-value based) ................. 15

5.1 Transport solution and pressure profile for five different BHP controls at the producer ........................................................................................................ 18
5.2 NPV with one control parameter ....................................................... 18
5.3 NPV with two controls: four-component system ..................................... 19
5.4 Optimization trajectory for quaternary system .................................... 19
5.5 NPV with two controls: eight-component system .................................. 20

A.1 Operators for a restricted compositional system parameterized at N=64 (second component) ............................................................... 33
A.2 Optimization results of an one-control system for full and proxy models ... 33
A.3 Optimization results with the same initial guess at BHP = 70 bars for full and proxy models ....................................................................................... 34
A.4 Optimization results with initial guess close to the optimal value for full and proxy models ................................................................. 34
A.5 Optimization results with initial guess starting at BHP = 70 bars for full and proxy models ................................................................. 35
A.6 Optimization results with initial guess starting at BHP = 100 bars for full and proxy models ................................................................. 35
List of Tables

3.1 The values for economic parameters .................................................. 10
5.1 Optimization results for two constant initial BHP ............................... 20
5.2 NPV result and optimal pressure sets for eight component system .......... 20
5.3 Optimization results for five controls starting from different initial guesses ... 21
A.1 Hydrodynamic parameters ............................................................... 31
A.2 Thermodynamic properties quaternary system ..................................... 31
A.3 Thermodynamic properties for eight-component system ......................... 32
A.4 Binary system .................................................................................... 32
A.5 Quaternary system .............................................................................. 32
A.6 Eight-component system .................................................................... 32
A.7 K-value table for quaternary system .................................................. 32
A.8 K-value table for eight-component system .......................................... 32
Greenhouse gas emission together with high demand of energy have long been concerned by contemporary society. Near-miscible CO\textsubscript{2} injection is among the most efficient strategies for a tertiary recovery of oil (Lake, 1989) which can also reduce the carbon emission. The produced hydrocarbons can already be seen as a low carbon fuel due to the significant amount of CO\textsubscript{2} left in subsurface as the results of Enhanced Oil Recovery (EOR) application. Nevertheless, the heterogeneity of subsurface with complex multi-scale characteristics requires a suitable and high resolved model to comprehend the details of flow and interactions of subsurface. Current economy situation, especially the modest oil price and formidable cost of CO\textsubscript{2}, introduces extra challenges on applying miscible regime of gas injection. However, in combined objective of enhanced oil recovery and CO\textsubscript{2} sequestration, the development of miscibility may become the most attractive strategy from both technological and economic sides. In addition, the effective miscible injection can increase a storage capacity of CO\textsubscript{2} sequestration in virgin or depleted hydrocarbon fields. It is strongly recommended to develop a plausible techno-economic model to meet both oil recovery and carbon dioxide sequestration goal. This serves as a primary motivation for our study.

To simulate the miscible gas injection process, compositional modeling is inevitably employed. Compositional models require numerical solution of nonlinear equations which involve mass conservation and thermodynamic equilibrium. The phase behavior of a multiphase multi-component mixtures is usually resolved by applying Equation-of-State (EoS) (Coats, 1980). In every time step, thermodynamic equilibrium is performed in every grid block to check phase behavior and compositions of the components (Watts, 1986), which is expensive in terms of total simulation time.

Thermodynamic equilibrium usually consists of two stages: phase stability test (Michelsen, 1982a) and flash calculation (Michelsen, 1982b). Various EoS were proposed to enunciate thermodynamic equilibrium process of a hydrocarbon mixture system starting with classic cubic EoS (Peng and Robinson, 1976; Soave, 1972). However, the growing accuracy of reservoir fluid characterization and better recognition of complex physical processes, imposed by components interactions, requires an application of more complicated EoS such as Statistical Association Fluid Theory (SAFT) (Chapman et al., 1989) or Cubic-Plus-Association (CPA) (Kontogeorgis et al., 1996). In addition, coupling with chemical reactions requires a combination of thermodynamic and chemical equilibrium (Lucia et al., 2015; Paterson et al., 2018). This can significantly increase the cost of phase behavior computations in compositional simulation (Voskov et al., 2017).

Conspicuous efforts are made to improve the performance of the compositional reservoir simulators by improving phase behavior computations (Voskov and Tchelepi, 2009a; Pan and Tchelepi, 2011; Iranshahr et al., 2010), spatial coarsening of compositional models (Iranshahr et al., 2014; Salehi, 2016) or reformulation of compositional nonlinear problem (Za-
In this work, a newly proposed Multi-Scale Compositional Transport (MSCT) approach by Ganapathy (2017) is utilized for production optimization. The Algebraic Multi-Scale (AMS) approach were initially proposed to solve an elliptic flow problem in Jenny et al. (2003). Several extensions of this method has been successfully developed. However, the most of the AMS methods were focused exclusively on flow solver and did not address transport problem except Zhou et al. (2012), where an adaptive Multiscale Finite Volume Method was proposed to accelerate transport solver. On the basis of these idea, an MSCT method for reconstruction of compositional transport problem with arbitrary number of components was developed in Ganapathy (2017).

This approach suggests two-stage reconstruction where in the first stage, the boundary of a two-phase region are recovered, and the detailed solution in two-phase region is reconstructed in the second stage. This approach utilized an Operator-Based Linearization (OBL) method proposed in Voskov (2017). In OBL method, terms of discretized governing equations are factorized into space and state depended operators. The state-dependent operators are adaptively discretized in parameter space of the problem and multi-linear interpolation is applied for continuous representation (Khait and Voskov, 2017). This formulation helps to avoid the performance issues associated with an accurate phase-split evaluation and reduce the nonlinearity of the problem. Recently, this approach was extended for adaptive parametrization of thermal-compositional problems with buoyancy Khait and Voskov (2018).

The original study on MSCT method has been limited by an isothermal two-phase flow conditions with fixed phase equilibrium ratios (K values) (Ganapathy, 2017). In this work, we introduce an application of MSCT using PR-EOS (Peng and Robinson, 1976). Due to the high nonlinearity of the CO₂ injection system, constrained nonlinear optimization strategy is utilized to determine the optimal production scenario. For production optimization, we used only the first-stage MSCT reconstruction as a physics-based proxy model and compare its result with optimization of full compositional solution. Both approaches were compared on an idealized conceptual model with growing optimization complexity.
Methodology

In this chapter, a concise simulation framework based on Voskov and Tchelepi (2012) is presented.

2.1. Compositional framework

For simplicity, the thermal changes, capillarity, gravity, and diffusion are neglected in the following description. The general mass-conservation equation for component $i$ in the two-phase compositional problem is defined as follows:

$$\frac{\partial}{\partial t} \left( \phi \sum_{j=1}^{2} x_{i,j} \rho_j S_j \right) + \nabla \cdot \left( \sum_{j=1}^{2} x_{i,j} \rho_j u_j \right) + \sum_{j=1}^{2} x_{i,j} \rho_j q_j = 0, \quad i = 1, \ldots, N_c$$

(2.1)

In eq. (2.1), $t$ is time, $\phi$ is the porosity of the reservoir, $\rho_j$ is molar phase density, $S_j$ is phase saturation, $x_{i,j}$ is the mole fraction of component $i$ in phase $j$, $q_j$ is the source or sink term of phase $j$, and $N_c$ is number of the components. The Darcy velocity $u_j$ is defined as

$$u_j = -K \frac{k_{rj}}{\mu_j} \cdot \nabla p, \quad j = 1, 2,$$

(2.2)

where $K$ is absolute permeability, $k_{rj}$ is the relative permeability of phase $j$, $\mu_j$ is viscosity of phase $j$ and $p$ is pressure. The equilibrium relations between oil and gas phase are required to close the system

$$\hat{f}_{i,o} (p, T, x_o) = \hat{f}_{i,g} (p, T, x_g), \quad i = 1, \ldots, N_c,$$

(2.3)

where $\hat{f}_{i,o}$ and $\hat{f}_{i,g}$ are the fugacities for the component $i$ in oil phase and gas phase, respectively. Fugacity is a function of pressure ($p$), temperature ($T$) and phase compositions ($x_{i,j}$), which are determined by EoS-based flash computations. Additional equations are given as follows to close the system of governing equations:

$$\sum_{i=1}^{N_c} \left( x_{i,1} - x_{i,2} \right) = 0, \quad i = 1, \ldots, N_c,$$

(2.4)

$$s_o + s_g = 1.$$

(2.5)

The overall composition of $i$ component can be expressed as:

$$z_i = \sum_{j=1}^{2} v_j x_{i,j}, \quad i = 1, \ldots, N_c,$$

(2.6)
where, \( v_j \) is the molar fraction of the phase \( j(o,g) \). Solving the eqs. (2.3) to (2.6) is a procedure called multiphase flash (Michelsen, 1982b), which will provides phase composition \( x_{ij} \) and phase fraction \( v_j \).

Finally, the phase saturation \( s_j \) can be found from

\[
s_j = \frac{v_g}{\rho_g} \frac{v_g}{\rho_g + v_o}
\]

(2.7)

Applying two-point finite-volume in space and backward Euler in time discretizations, the general mass-conservation equation is written as:

\[
V \left( \phi \sum_{j=1}^{2} x_{ij} \rho_j S_j \right)^{n+1} - \left( \phi \sum_{j=1}^{2} x_{ij} \rho_j S_j \right)^{n} - \Delta t \sum_{j=1}^{L} \left( \sum_{j=1}^{2} x_{ij} \rho_j T_j \Delta \Psi \right) + V \Delta t \sum_{j=1}^{2} x_{ij} \rho_j q_j = 0,
\]

(2.8)

where \( V \) is total control volume and \( L \) represents the interface which connects the control volume with another grid blocks. In the simplified assumptions, mentioned above, \( \Delta \Psi \) becomes a pressure difference between two connected grid blocks. Finally, \( T_j \) is the transmissibility of phase \( j \).

### 2.2. Operator-Based Linearization

The multi-scale technique is implemented on the basis of an Operator-based Linearization (OBL) approach proposed by Voskov (2017). To apply OBL, the discretized mass conservation equation (eq. (2.8)) is written in the following residual form:

\[
R_l(\xi, \omega, u) = a(\omega) (a_l(\omega) - a_l(\omega_0)) - \sum_{\nu} \beta_l^\nu(\omega) b^\nu(\xi, \omega) + \theta_l(\xi, \omega, u) = 0.
\]

(2.9)

The operators in eq. (2.9) are defined as follows:

\[
a_l(\omega) = \left( 1 + c_r (p - p_{ref}) \right) \sum_{j=1}^{2} x_{ij} \rho_j S_j,
\]

(2.10)

\[
a(\xi) = V(\xi) \phi_0(\xi),
\]

(2.11)

\[
\beta_l(\omega) = \sum_{j} x_{ij} \frac{k_{ij}}{\mu_j} \rho_j,
\]

(2.12)

\[
b(\xi, \omega) = \Delta t \tau_{ab}(\xi)(p^b - p^a),
\]

(2.13)

\[
\theta_l(\xi, \omega, u) = \Delta t \sum_{j=1}^{2} x_{ij} \rho_j q_j(\xi, \omega, u).
\]

(2.14)

In eq.(2.10) to eq.(2.14), \( c_r \) is rock compressibility and \( \tau_{ab} \) is the transmissibility between grid-blocks. The vector \( u \) contains well-control variables, \( \omega \) is the set of state variables and \( \xi \) are the set of spatial coordinates. In addition, \( a_i \) is the accumulation operator, \( \beta_l \) is the flux operator and \( \theta_i \) is the source/sink operator. The OBL approach is based on a simplified representation of the nonlinear operators in the parameter space of the simulation problem. For an isothermal reservoir simulation, the parameter space is defined by the range of pressure \( p \) between injection and production conditions and overall compositional \( z_l \) range from 0 to 1.

The fully implicit method (FIM) is utilized to resolve the given governing equation eq. (2.9) based on the unknowns set. The eq. (2.9) to eq.(2.14) represent a full conventional compositional model.
2.3. Multi-Scale Compositional Transport

A solution of a compositional transport problem can be shown in a phase diagram by the solution path in compositional space, which defines the compositional changes between the initial and injection mixtures. Conservation principles and fractional-flow theory form the foundation for the general solution method (Orr, 2007). Taking the ternary system as an example, the compositional path of the conventional compositional problem for gas injection process always results in two shocks (leading and trailing shocks) between single- and two-phase regions. In a ternary diagram (Fig. 2.1a), it is presented as yellow lines connecting the initial oil and injected gas composition.

Figure 2.1: Gas-injection solution in ternary system: (a) ternary diagram with displacement path and two key tie-lines and (b) fractional-flow curves for component CO\textsubscript{2} with solution path.

The shocks between single- and two-phase regions are always aligned along two key tie-lines (black dashed lines) defined by liquid $x_i$ and vapor $y_i$ fractions of each component. For a fixed pressure, $x_i$ and $y_i$ remain constant and it is possible to construct the fractional-flow curve corresponding with compositional transport, see eq. (2.15). Fig. 2.1b gives the injection and initial fractional-flow curves for CO\textsubscript{2} in a ternary system corresponding to the injection and initial tie lines in Fig. 2.1a.

\[ F_i = x_i (1 - f_g) + y_i f_g, \quad i = 1, \ldots, n_c - 1 \]  \hspace{1cm} (2.15)

The proposed Multi-Scale Compositional Transport (MSCT) approach consists of two stages (Ganapathy et al., 2018). The first stage utilizes the set of restriction-prolongation operators for reconstructing two-phase boundaries (the trailing and leading shocks). The restriction here reduces the $n_c - 1$ transport equations to a single equation with a special flux operator based on the pseudo-fractional-flow curve. In the second stage, the set of restriction-prolongation operators is applied in the two-phase region to reconstruct the solution structure of the two-phase displacement. This stage is based on the invariance of two-phase solutions in tie-line space reported in Voskov and Entov (2001) and adapted for practice in Voskov and Tchelepi (2009b).

The proxy model for compositional simulation, utilized in this work, uses the first-stage multi-scale reconstruction from Ganapathy et al. (2018). A restriction operator combines two fractional-flow curves for injection and production tie-lines, defined as:

\[ F_i^{\text{ini}} = x_i^{\text{ini}} (1 - f_g) + y_i^{\text{ini}} f_g, \quad F_i^{\text{ini}} = x_i^{\text{ini}} (1 - f_g) + y_i^{\text{ini}} f_g. \]  \hspace{1cm} (2.16)

The equivalent fractional-flow curve, serving as the restriction operator, is constructed by taking a convex hull on the union of both curves:
In Fig. 2.2, this curve is shown in green. Next, the equivalent values of \( F_i \) and \( z_i \) from the green curve are tabulated into the restriction operator and the reduced system is solved. The reduced system of equations includes the convenient pressure equation and the restricted transport equation based on the constructed pseudo-fractional-flow curve. In structure, this system is very close to the conventional binary compositional problem. Fig. 2.3 gives an example of the operators which are tabulated from the analytical fractional flow curve. Fig 2.3a and Fig 2.3b are accumulation and flux operators corresponding to the first component in binary system. In order to construct our proxy model, the operators for the second component are required, which shows in Appendix. Those operators are utilized in the OBL framework (Khait and Voskov, 2017) to solve the first-stage restricted system.

Once the solution of the restricted system is found, the full system is reconstructed based on
2.3. Multi-Scale Compositional Transport

the prolongation operator. This operator applies interpolation between initial and injection compositions using solution of the restricted system \( \kappa(z_R) \) as an indicator:

\[
\kappa(z_R) : \mathbb{R}^1 \rightarrow \mathbb{R}^{n_c-1} : z = I_{z_{ini},z_{ini}}(z_R).
\]

(2.18)

Here, \( \kappa \) is the interpolation-prolongation operator, \( z_R \) is the restricted solution and \( I \) is the piecewise linear interpolation function. Referring to this linear interpolation, the transport solution of other components in the multicomponent system is reconstructed and used as a proxy model in place of the full compositional model. Notice that this system can accurately predict only the boundaries of the two-phase region and their dynamic propagation in space; for a really accurate solution, the second-stage multi-scale reconstruction should be applied (Ganapathy et al., 2018).
Economic Model

The techno-economic model is applied to evaluate the economics of a combined CO₂ EOR and sequestration application. Several economic studies of CO₂ injection processes have been performed by Tayari et al. (2018); Kwak and Kim (2017); Ettehadtavakkol et al. (2014); Rubin et al. (2007). McCoy and Rubin (2009) proposed several regression equations for assessment of the capital cost of CO₂ injection projects, which are validated by Wei et al. (2015) and Ettehadtavakkol et al. (2014). Referring to Tayari et al. (2018), this techno-economic model uses simulation input data and oil production rate, gas injection rate and Bottom-Hole Pressure (BHP) to define different costs and revenues of the project.

On the basis of reservoir-simulation data, an economic model is developed to estimate the profitability of CO₂ injection for Enhanced Oil Recovery (EOR) and CO₂ sequestration, which will reflect on the Net Present Value (NPV). The general economic parameters of a CO₂ injection process are listed in Fig. 3.1. This figure shows that the cost of a CO₂ injection project can be divided into two parts, which are capital cost and operational cost. Dominant revenues from the gas-injection project mainly originate from oil sales and carbon sequestration incen-

![Diagram](image)

**Figure 3.1:** General economic parameters for CO₂ injection project
tives. A previous economic study of CO₂-injection projects (Kwak and Kim, 2017) indicates that CO₂ purchasing cost is one of the most sensitive parameters when NPV is evaluated. In this work, according to the general parameters and equations provided in Kwak and Kim (2017), a spider plot is constructed in Fig. 3.2, which shows that CO₂ processing cost has a similar impact on NPV as CO₂ purchasing cost. The CO₂ processing-cost model in this work is based on Tayari et al. (2018), and is expressed in terms of the pump capital cost as follows:

\[ C_{\text{pump}} = (1.35 \times 10^3 \times W_p) + 0.085 \times 10^6, \]

(3.1)

where \( W_p \) is pumping power requirement, which is expressed in kW, which in turn varies with CO₂ injection pressure. Other parameters in the economic model are listed in Table 3.1. Some of them are obtained by introducing the regression equations listed in McCoy and Rubin (2009), such as those for well engineering cost and CO₂ processing equipment cost.

**Table 3.1: The values for economic parameters**

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Units</th>
<th>Remarks</th>
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<tr>
<td>CO₂ storage incentives</td>
<td>12 $/t</td>
<td>Kwak and Kim (2017)</td>
</tr>
<tr>
<td>Well engineering cost</td>
<td>501644 $</td>
<td>McCoy and Rubin (2009)</td>
</tr>
<tr>
<td>CO₂ processing equipment</td>
<td>10637265 $</td>
<td>McCoy and Rubin (2009)</td>
</tr>
<tr>
<td>Wells work-over</td>
<td>241429 $</td>
<td>McCoy and Rubin (2009)</td>
</tr>
<tr>
<td>CO₂ purchase cost</td>
<td>24 $/t</td>
<td>Kwak and Kim (2017)</td>
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<tr>
<td>CO₂ transportation</td>
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<td>CO₂ source in-situ</td>
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<tr>
<td>CO₂ processing cost</td>
<td>10 $/t</td>
<td>Rubin et al. (2007)</td>
</tr>
<tr>
<td>Lift facility maintenance</td>
<td>0.6 $/t</td>
<td>Rubin et al. (2007)</td>
</tr>
<tr>
<td>CO₂ net cost</td>
<td>12 $/t</td>
<td>Purchasing cost-Incentives</td>
</tr>
<tr>
<td>Tax rate(royalty, severance tax)</td>
<td>0.4 [-]</td>
<td>McCoy and Rubin (2009)</td>
</tr>
<tr>
<td>Depreciation</td>
<td>Linear over ten years $</td>
<td>McCoy and Rubin (2009)</td>
</tr>
<tr>
<td>Discount rate</td>
<td>12 [-]</td>
<td>Wei et al. (2015)</td>
</tr>
</tbody>
</table>
In this chapter, we demonstrate the comparison between solutions of the proxy model and the full compositional model. Here, we limit our investigation to a conceptual 1D reservoir model for simplicity. In this model, the injection well on the left operates at a constant gas rate when the production well is controlled by Bottom-Hole Pressure (BHP) which serves as a control variable for optimization.

4.1. Restricted solution
In this section, the multi-component system restricted solutions are demonstrating.

4.1.1. Binary system
In continuation to the previously described constant K-value implementation (Ganapathy, 2017), here we introduced the EoS-based methodology to determine the thermodynamic parameters. The validation of this reconstruction is carried out for a binary compositional system first and later for a quaternary system. In a binary system, the injection and initial tie-lines are equal for a fixed pressure due to the Gibbs phase rule. As a result, it implies that the first-stage reconstruction on a binary system yields the full solution of the problem. Initially, a single full scale fractional flow curve of CO$_2$ is determined. Taking the fractional flow dependency on CO$_2$ composition, a fine scale 1D two-component injection transport problem is solved. In this example, the temperature is 373K and the simulation time is defined as 1000 days. Fig 4.1a shows the fractional flow curve of CO$_2$ for a fixed pressure (100 bars).
based on the EoS computations, and Fig 4.1b gives the solution for the full system along with the reconstructed shock solution. According to the theory, the displacement path of the binary system is along a single tie-line, thereby resulting in a single fractional flow curve. As a result, only the shock solution reconstruction framework is plausible to construct the full transport solution of a binary system.

4.1.2. Four-component system

Fig. 4.2 shows the restricted solution $z_R$, which yields the shock reconstruction curves for simulation results for the growing BHP at the production well in a four-component system. All simulation results of this system are shown for the model with parameters specified in Appendix A after 1000 days of simulation. The K-value table in this work is obtained from the embedded Constant Composition Expansion (CCE) experiments in Geoquest (2008) based on the PR EoS, which is shown in Tab A.7. It is clear that the K-value system does not develop miscibility even when BHP provides the pressure at the displacement front close to the First-Contact Minimal Miscibility Pressure (FC MMP) for this system (around 126 bars at $T = 373K$). This happens due to the inability of the K-value model to predict miscibility accurately, since compositional dependency is not captured in this model. It can be overcome by either extension of the K-value parameterization with additional degrees of freedom (e.g. Rannou et al., 2013) or incorporation of EoS-based phase behavior (Voskov and Tchelepi, 2009b). However, it is clear that the two-phase boundaries can be accurately represented by the restricted model for K-value based physics. In addition, the complexity and structure of the restricted solution are invariant with respect to the number of components present and only depends on initial and injection tie-lines in the multi-component system (see Ganapathy et al., 2018, for details).

Next, the results of the restricted solution for the compositional problem based on the EoS is shown. The structure of the compositional transport solution depends on key tie-lines (Orr, 2007). For the restricted solution, we follow the same strategy as before and construct the restriction operator based on combined fractional flow (eq. (2.16)) according to the first stage of MSCT approach (Ganapathy et al., 2018). The solution of the restricted transport equation reconstructs the boundaries of the two-phase region using one transport equation instead of $n_c - 1$ equations in the conventional compositional model.

The results of quaternary system reconstruction are shown in Fig. 4.3. Here you can see that for a high BHP value, the structure of the solution is much closer to miscibility (leading and trailing shocks stays closer to each other) than in the K-value approximation. This
happens because the EoS-based phase behavior correctly represents the compositional dependency of the solution. Similar to the K-value model, the restriction stage requires the solution of only one equation instead of $n_c - 1$, where $n_c$ is the number of components.

### 4.1.3. Eight-component system

Next, we present the simulation results for more realistic multicomponent mixture. Here we used the eight-component system from Zaydullin et al. (2012) with compositional parameters shown in Tab. A.6 (see Appendix). In cooperating with the K-values table generating from Geoquest (2008), which shows in Tab. A.8, based on the first stage reconstruction of MSCT approach, the restricted solution is shown in Fig. 4.4.

![Figure 4.4: Shock reconstruction of the eight-component system for two different BHP controls at production well (K-values)](image)

**Figure 4.4:** Shock reconstruction of the eight-component system for two different BHP controls at production well (K-values)

### 4.2. Prolongation of proxy model

In this section, we show the solution of the first stage MSCT based on prolongation of the restricted solution for 4- and 8-components systems.

#### 4.2.1. Four-component system

We illustrate the construction of the proxy model using an interpolation-based prolongation operator (eq. (2.18)) for both cases. It can be seen in Fig. 4.5 and Fig. 4.6 that the prolongation operator does not reconstruct the full structure of the solution, but only one indicator

![Figure 4.3: Shock reconstruction of the four-component system for two different BHP controls at production well (EoS model)](image)

**Figure 4.3:** Shock reconstruction of the four-component system for two different BHP controls at production well (EoS model)
component. For the full solution, the second stage of the reconstruction should be applied; see Ganapathy et al. (2018) for details.

Figure 4.5: Proxy model for a four-component system (K-value based)

(a) Full solution for BHP = 85 bars  
(b) Full solution for BHP = 120 bars

4.2.2. Eight-component system

Here, we construct the proxy model for the eight-component. Similarly to the previous case, we apply an interpolation-based prolongation operator (eq. (2.18)) for K-values system which yields the first stage MSCT approach which shows in Fig. 4.7. The compositions of these components and K-values table show in the Appendix (Tab. A.6 and Tab. A.8). This proxy model still can’t fully represent the eight component model, the second-stage MSCT approach should be employed to reconstruct the two-phase region, the details show in Ganapathy et al. (2018).

The prolongation yields a full compositional solution at every gridblock, which then can be used in a multiphase flash procedure to predict phase behavior. This phase behavior provides the boundary of the two-phase region in space. In our proxy model, we are using this prediction to compute phase rates at wells. As a result, this proxy model will be applied to evaluate economic performance of the CO$_2$ injection project together with full eight-component model.
4.2. Prolongation of proxy model

This eight-component system is conducted under the K-values system, in order to precisely predict the development of the miscibility, the EoS based reservoir model should be introduced.

(a) Full solution for BHP = 80 bars

(b) Full solution for BHP = 140 bars

Figure 4.7: Proxy model for an eight-component system (K-value based)
Optimization Results

Fig. 5.1 shows the transport solution for both fully compositional and proxy models for different BHP controls at the production well and a fixed rate at the gas-injection well. It is clear that with increasing pressure, both models capture the development of miscibility since the BHP control at production rate will apparently control the pressure at the displacement front. Due to the development of miscibility, the leading and trailing shocks getting closer to each other and the displacement efficiency growing. Next, we investigate optimal production strategies for this model.

In the optimization stage, the full four-component system together with the proxy two component system is used to determine oil production. Net Present Value (NPV) is used as an indicator to estimate the economic profitability of the project. The simulation time is divided into several periods where changes in BHP at production well are applied. Here we make sure that the time period for simulation covers the breakthrough of the trailing shock at the lower limit of pressure. Next, we estimate the optimal production strategy with a different numbers of control variables.

5.1. NPV with a limited number of control parameters
In this section, we will check the structure of objective function in optimization problems with a limited number of controls.

5.1.1. One control four-component system
The NPV distribution as a function of a single BHP control is evaluated here. We compare the NPV curve vs. BHP control for both the proxy and the full compositional model. The simulation time is defined to be long enough for the breakthrough of both leading and trailing shocks of the solution. NPV plot as a function of control BHP is shown in Fig. 5.2. Here, the green solid curve corresponds with NPV for the full four-component model, and red dashed curve is the NPV for the the proxy model. While there are some differences between the full physics solution and the proxy solution due to the limited application of the MSCT (only first stage of reconstruction), the model captures the correct boundaries of the two-phase region and yields the correct maximum of the NPV function. To improve the NPV evaluation, the second stage of the MSCT reconstruction can always be performed. For one-control optimization procedure, we use the ‘fminbnd’ function from the Matlab optimization toolbox (MathWorks, 2018) to find a local minimum value of the function in a given interval. The optimization result from the one-control system is conspicuous, which shows in Fig. A.2 that the optimal pressure solution for a four-component system is near the MMP value (118bars).

5.1.2. Two controls four-component system
Next, we introduce two simulation time periods and two control variables (BHP₁ and BHP₂) for NPV evaluation. Performing an exhaustive search in the space of control variables, we
5. Optimization Results

![Graphs showing transport solution and pressure profile for five different BHP controls at the producer](image1.png)

**Figure 5.1**: Transport solution and pressure profile for five different BHP controls at the producer.

![Graphs showing net present values](image2.png)

**Figure 5.2**: NPV with one control parameter.

evaluate the NPV function, shown in Fig. 5.3. While the NPV function is different for the proxy and the full model, the maximum NPV is reached at similar control values, i.e. around...
BHP₁ = 95 bars and BHP₂ = 118 bars. These values are conditioned by the obvious strategy for production controls when in the first time interval, the lower BHP at the production well provides the near-miscible pressure at the displacement front. In the second time interval, the pressure at the production well should be higher to provide near-miscible pressure at the displacement front until the gas breakthrough to the production well. The near-miscible strategy is optimal since it maximizes both the oil recovery and sequestration of CO₂.

In order to illustrate optimization procedure, the optimization trajectory is constructed. Fig. 5.4 gives the result of the optimization trajectory of the full physics model and proxy model respectively. For proxy model, the number of optimization steps is less than that of the full physics model. In addition, it is faster for proxy model to acquire near optimal NPV result within the same provided optimization strategy. The details of the optimization procedure is shown in Fig A.3 in Appendix. Tab. 5.1 presents results from constrained nonlinear optimization of the four-component model and the corresponding proxy model.

**5.1.3. Two controls eight-component system**

Finally, we look into optimization process for more realistic eight component system with compositions and corresponding thermodynamic characteristics show in the Appendix (Tab. A.3 and Tab. A.6). The objective function for two control variables is shown in Fig. 5.5. The pressure interval is corresponding to the lower and upper limit of the BHP values of the production
Table 5.1: Optimization results for two constant initial BHP

<table>
<thead>
<tr>
<th>Initial guess</th>
<th>Model</th>
<th># of iter.</th>
<th>NPV($)</th>
<th>Controls for time periods</th>
</tr>
</thead>
<tbody>
<tr>
<td>BHP = 70 bars</td>
<td>Full model</td>
<td>14</td>
<td>260,927</td>
<td>94.85 118.55</td>
</tr>
<tr>
<td></td>
<td>Proxy model</td>
<td>5</td>
<td>260,866</td>
<td>94.83 120.41</td>
</tr>
</tbody>
</table>

(a) Full model  
(b) Proxy model

Figure 5.5: NPV with two controls: eight-component system

wells, which ranges from 80 bars to 160 bars. In this eight-component system, the optimal pressure sets for the given reservoir and fluid properties show in the following table to capture the similar highest NPV value. The result shows in the Tab. 5.2.

Table 5.2: NPV result and optimal pressure sets for eight component system

<table>
<thead>
<tr>
<th>Model</th>
<th>NPV($)</th>
<th>Controls for time periods</th>
</tr>
</thead>
<tbody>
<tr>
<td>Full model</td>
<td>279,576</td>
<td>100 bars 138 bars</td>
</tr>
<tr>
<td>Proxy model</td>
<td>279,866</td>
<td>100 bars 137 bars</td>
</tr>
</tbody>
</table>

5.2. Optimization with multiple controls

Next, we apply production optimization based on five control variables (BHP’s) corresponding to five time periods in the simulation. In this study, we use the ’fmincon’ function from the Matlab optimization toolbox (MathWorks, 2018). In ’fmincon’, the ’sqp’ algorithm has been chosen. The optimizer is utilized to provide BHP controls at each time period and obtain an optimal NPV result during the CO$_2$-injection process. All BHP controls were bounded by BHP$_{min}$ = 60 bars and BHP$_{max}$ = 140 bars. Note, that the expected optimal strategy should include a gradual increase of BHP at each consecutive control interval to provide near-miscible conditions at the displacement front.

We test several initial guesses for the optimization with five control parameters. For this number of controls, several local minima can exist and the optimizer struggles with finding a single global extremum. However, based on the structure of solution in Fig. 5.1, we can predict a near-optimal BHP strategy where BHP should monotonically increase with time to provide the near-miscible pressure at the displacement front. Using this strategy with BHP =
[63; 77; 83; 102; 121] at five controls intervals as the initial guess, we perform the optimization. The results of optimization based on the full and proxy models are present in Table 5.3. You can see that the proxy model performed fewer iterations and obtained a similar NPV.

In addition, we perform two more optimization runs with different initial guesses when all BHP controls have been set to 70 bars and 100 bars respectively. The results can also be seen in Table 5.3. In these optimization runs, both models cannot converge to the same optimal strategy, but getting close to it. The proxy model performs quite robustly and proves to be applicable for optimization of gas injection process in the idealistic reservoir.

### Table 5.3: Optimization results for five controls starting from different initial guesses

<table>
<thead>
<tr>
<th>Initial guess</th>
<th>Model</th>
<th># of iter.</th>
<th>NPV($)</th>
<th>Controls for time periods</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Near optimal</td>
<td>Full model</td>
<td>6</td>
<td>261,100</td>
<td>60.00</td>
</tr>
<tr>
<td></td>
<td>Proxy model</td>
<td>3</td>
<td>261,064</td>
<td>60.00</td>
</tr>
<tr>
<td>BHP = 70 bars</td>
<td>Full model</td>
<td>11</td>
<td>261,007</td>
<td>60.00</td>
</tr>
<tr>
<td></td>
<td>Proxy model</td>
<td>12</td>
<td>260,247</td>
<td>60.97</td>
</tr>
<tr>
<td>BHP = 100 bars</td>
<td>Full model</td>
<td>9</td>
<td>260,093</td>
<td>60.00</td>
</tr>
<tr>
<td></td>
<td>Proxy model</td>
<td>7</td>
<td>260,817</td>
<td>60.00</td>
</tr>
</tbody>
</table>
Conclusions

In this work, we extend the Multi-Scale Compositional Transport (MSCT) approach for the EoS-based gas-injection problems. In particular, we parametrize the restriction operator of the first stage MSCT reconstruction in the pressure interval and obtain the restricted solution using the Operator-Based Linearization framework. The restricted solution was prolonged to the full compositional solution using interpolation operator. The obtained proxy model can accurately predict the boundaries of the two-phase region and has been utilized in this work for production optimization.

Referring to previous economic assessments of CO₂-injection projects, a techno-economic model has been developed to analyze the revenues of CO₂ injection for the combined objective of EOR and sequestration. A general application of proposed proxy model for optimization of gas injection process is demonstrated in this study. Starting with a limited number of controls, we show that the objective function of full-physics compositional model and the proposed proxy model share similar extrema for a limited number of control parameters. To test the robustness of the proposed proxy model in a relatively complicated cases, the general form of the objective function was evaluated for a limited number of control parameters. Based on these comparisons, we demonstrate that both full-physics and proxy models share similar extrema.

In addition, a constrained nonlinear optimization is applied to determine an optimal production strategy for the gas injection operation. For optimization model with more control parameters, when the initial guess of controls is near the optimal solution, we show that both full-physics model and proxy model converge to similar optimal solution. For arbitrary initial guesses, the converged optimal strategy may differ for proxy and full compositional models due to a local extrema of both objective functions.

Through the optimization process in four-component system, we show that by providing optimizer with the same input parameters in both full-physics model and proxy model, the optimal solution with the proposed proxy model is usually more feasible (takes less iterations) than full-physics model. In addition, the forward simulation of the proposed proxy model is significantly cheaper (proportional to the reduction in the number of components) than full physics model and becomes comparable with the black oil model.
Future Work

In this work, we applied the first-stage of the MSCT approach to construct the proxy model which precisely capture the boundary of the two-phase region (leading and trailing shocks). The NPV result shows while there are some differences at the lower pressure region, they do not affect the position of extremum in the proposed proxy model compared with the full model. In order to fully capture the physics of the simulation, the second stage of the MSCT approach (e.g. Compositional Space Parameterization (CSP)) to reconstruct the two-phase region which can be applied to satisfy full complexity of near-miscible gas injection process.

In addition, we have implemented the first-stage MSCT approach in 1D reservoir models without capillarity and gravitational forces. Those unwieldy nonlinear physics should be included to develop a fully implicit model and accurately describe the the characteristics of the flow in porous media. In order to mimic the actual CO$_2$ injection procedure, more realistic models and scenarios should be employed which requires to extend the proposed methodology to 3D simulation problems.

As mentioned in the model description, this work is based on isothermal two-phase formulation. In the later work, we plan to extend this framework to the thermal-compositional problems with arbitrary number of phases.

In addition, the optimization approach in this work is the constrained gradient-free nonlinear optimization strategy, where we only provide the optimizer with upper and lower bounds of the system. To make the optimization more efficient, the adjoint gradients should be developed for the proxy model.
Bibliography


A.1. Fluid and rock interactions

The simulation model in this study is a 1D homogeneous model ($K = 20$ mD), 200 m long with one injection well on the left and one production well on the right boundaries. The finite volume discretization is applied based on the standard Cartesian grid with the block sizes: $\Delta x = 1$ m, $\Delta y = 10$ m, $\Delta z = 1$ m. For the well model, the Peaceman formula (Peaceman, 1978) is utilized with $r_w = 0.15$ m. The injection well is controlled by a constant gas rate $q_0 = 2m^3/day$. The rest of parameters are specified in tables below. For the K-value model, we perform the Constant Composition Expansion (CCE) using PVTi module (Geoquest, 2008) where we generate K-value table corresponding to given initial compositions in Tab. A.5. The K-value table is present as a function of pressure with three pressure values employed, see Tab. A.7 and Tab. A.8 for details.

<table>
<thead>
<tr>
<th>Table A.1: Hydrodynamic parameters</th>
<th>Oil</th>
<th>Gas</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rock compressibility, 1/bar</td>
<td>$10^{-5}$</td>
<td></td>
</tr>
<tr>
<td>Porosity</td>
<td>0.3</td>
<td></td>
</tr>
<tr>
<td>Residual saturation ($S_r$)</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>End point relative permeability ($K_{r,f}$)</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Saturation exponent ($n_f$)</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Viscosity, cP ($\mu_f$)</td>
<td>0.5</td>
<td>0.1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table A.2: Thermodynamic properties quaternary system</th>
</tr>
</thead>
<tbody>
<tr>
<td>Components</td>
</tr>
<tr>
<td>Critical pressure, bars</td>
</tr>
<tr>
<td>Critical temperature, K</td>
</tr>
<tr>
<td>Critical volume, m$^3$ / kg-mole</td>
</tr>
<tr>
<td>Acentric factor</td>
</tr>
<tr>
<td>Molar weight, g/mol</td>
</tr>
<tr>
<td>Binary interaction, CO$_2$</td>
</tr>
<tr>
<td>Binary interaction, C$_1$</td>
</tr>
</tbody>
</table>
### Table A.3: Thermodynamic properties for eight-component system

<table>
<thead>
<tr>
<th>Components</th>
<th>CO₂</th>
<th>C₁</th>
<th>C₂</th>
<th>C₃</th>
<th>NC₄</th>
<th>C₆</th>
<th>C₈</th>
<th>C₁₅</th>
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<tr>
<td>Critical pressure, bars</td>
<td>73.87</td>
<td>43.04</td>
<td>48.84</td>
<td>42.45</td>
<td>37.47</td>
<td>30.10</td>
<td>28.79</td>
<td>17.60</td>
</tr>
<tr>
<td>Critical temperature, K</td>
<td>304.7</td>
<td>190.60</td>
<td>305.43</td>
<td>369.80</td>
<td>419.5</td>
<td>507.5</td>
<td>575.00</td>
<td>724.00</td>
</tr>
<tr>
<td>Critical volume, m³ / kg-mole</td>
<td>0.094</td>
<td>0.098</td>
<td>0.148</td>
<td>0.200</td>
<td>0.200</td>
<td>0.289</td>
<td>0.433</td>
<td>0.779</td>
</tr>
<tr>
<td>Acentric factor</td>
<td>0.225</td>
<td>0.013</td>
<td>0.0986</td>
<td>0.1524</td>
<td>0.1966</td>
<td>0.299</td>
<td>0.312</td>
<td>0.55</td>
</tr>
<tr>
<td>Molar weight, g/mol</td>
<td>44.01</td>
<td>16.04</td>
<td>30.07</td>
<td>44.097</td>
<td>58.12</td>
<td>84.00</td>
<td>107.00</td>
<td>206.00</td>
</tr>
</tbody>
</table>

### Table A.4: Binary system

<table>
<thead>
<tr>
<th>Compositions</th>
<th>CO₂</th>
<th>C₁₀</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Oil Compositions</td>
<td>0.33</td>
<td>0.67</td>
</tr>
<tr>
<td>Injection gas Compositions</td>
<td>1.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

### Table A.5: Quaternary system

<table>
<thead>
<tr>
<th>Compositions</th>
<th>CO₂</th>
<th>C₁</th>
<th>NC₄</th>
<th>C₁₀</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Oil Compositions</td>
<td>0.33</td>
<td>0.03</td>
<td>0.24</td>
<td>0.40</td>
</tr>
<tr>
<td>Injection gas Compositions</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

### Table A.6: Eight-component system

<table>
<thead>
<tr>
<th>Compositions</th>
<th>CO₂</th>
<th>C₁</th>
<th>C₂</th>
<th>C₃</th>
<th>NC₄</th>
<th>C₆</th>
<th>C₈</th>
<th>C₁₅</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial Oil Compositions</td>
<td>0.01</td>
<td>0.10</td>
<td>0.01</td>
<td>0.01</td>
<td>0.10</td>
<td>0.10</td>
<td>0.20</td>
<td>0.47</td>
</tr>
<tr>
<td>Injection gas Compositions</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

### Table A.7: K-value table for quaternary system

<table>
<thead>
<tr>
<th>Pressure (bars)</th>
<th>CO₂</th>
<th>C₁</th>
<th>NC₄</th>
<th>C₁₀</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>6.70</td>
<td>8.60</td>
<td>1.20</td>
<td>0.00085</td>
</tr>
<tr>
<td>80</td>
<td>2.05</td>
<td>4.70</td>
<td>0.54</td>
<td>0.005</td>
</tr>
<tr>
<td>120</td>
<td>1.33</td>
<td>2.51</td>
<td>0.31</td>
<td>0.09</td>
</tr>
</tbody>
</table>

### Table A.8: K-value table for eight-component system

<table>
<thead>
<tr>
<th>Pressure (bars)</th>
<th>CO₂</th>
<th>C₁</th>
<th>C₂</th>
<th>C₃</th>
<th>NC₄</th>
<th>C₆</th>
<th>C₈</th>
<th>C₁₅</th>
</tr>
</thead>
<tbody>
<tr>
<td>65</td>
<td>4.31</td>
<td>6.73</td>
<td>4.33</td>
<td>3.05</td>
<td>1.22</td>
<td>0.50</td>
<td>0.23</td>
<td>0.0016</td>
</tr>
<tr>
<td>100</td>
<td>1.88</td>
<td>3.25</td>
<td>2.12</td>
<td>1.56</td>
<td>0.95</td>
<td>0.48</td>
<td>0.27</td>
<td>0.08</td>
</tr>
<tr>
<td>140</td>
<td>1.21</td>
<td>1.38</td>
<td>0.99</td>
<td>0.81</td>
<td>0.65</td>
<td>0.45</td>
<td>0.33</td>
<td>0.12</td>
</tr>
</tbody>
</table>

### A.2. The other operators for a proxy model

In order to fully reconstruct the proxy model, the operators for the second component is constructed, together with the operators in Fig. 2.3. The format of these operators show as follows,
A.3. Optimization parameters and results

Here we present the illustration for the convergence of optimization process.

A.3.1. One-control optimization four-Component system

In this section, we give the optimization result of single variable control for the a four-component system. In order to find one optimal pressure corresponding to optimal NPV value, by passing the pressure range limited by injection and production pressure which are implemented as lower bound and upper bound, the optimizer 'fminbnd' will automatically find the maximum NPV value for the function.

A.3.2. Two-control optimization four-Component system

In this section, following figures give the details of the whole optimization for both full physics model and proxy model in four-component system (Fig A.3). On the basis of the constrained nonlinear multi-variable function of of our objective function, 'fimincon' optimizer (MathWorks, 2018) is applied to find the optimal value. In this nonlinear programming optimizer, we are supposed to provide initial value ($x_0$ vector), linear inequality constraints ($A$ matrix and $b$ vector), linear equality constraints ($Aeq$ matrix and $beq$ vector), lower bounds ($lb$ vector), upper bounds ($ub$ vector) and so on. In this work, we provided the optimizer exclusively with initial values, lower bounds and upper bounds which are also defined by the injection
and production pressure to cover pressure values in entire system. 'fmincon' has five algorithm, which are interior-point, trustregion, sqp, sqp-legacy, active-set. In this work, sqp algorithm is employed.

A.3.3. Muti-control optimization four-Component system
The optimization runs are illustrated here with the graphs below which contained the optimal solution (five BHP controls), number of function evaluations and NPV dynamics. All results are shown for (a) full physics (four-component) compositional model and (b) proxy (two-components) model. The same tolerance, algorithm and etc. as we used in two-control optimization system are applied in this multi-control optimization system.
A.3. Optimization parameters and results

(a) Full physics model

(b) Proxy model

Figure A.5: Optimization results with initial guess starting at BHP = 70 bars for full and proxy models

Figure A.6: Optimization results with initial guess starting at BHP = 100 bars for full and proxy models