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Numerical study of physico-chemical interactions for CO₂ sequestration and geothermal energy utilization in the Ordos Basin, China

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Promotion an der Technischen Universität Clausthal
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Abstract

The injection of CO₂ in geological formations for storage, especially in the widespread deep saline formations, is considered an optimal option to reduce CO₂ emissions in the atmosphere. However, geological sequestration of CO₂ in porous media must confront with comprehensive problems, for example, pollution of the shallow ground water, the damage of the caprock caused by overpressured effect, the corrosion of downhole equipments, which can only be addressed by synthetic solutions from studies of hydrology, geotechnology, geochemistry, rock mechanics, mathematics, computational technology and related sciences.

In order to understand the physical and chemical processes associated with CO₂ sequestration in the subsurface, numerical simulators, such as TOUGH2MP, TOUGHREACT, FLAC3D have been developed. These numerical investigations can provide important information on spatial and temporal evolution of CO₂ plume, pore pressure, effective stresses, formation uplifts, ion concentration, mineral volume fraction etc., under the consideration of reservoir heterogeneities at different scales, thus can provide an invaluable reference for a specific CCS project to ensure its safety and efficiency.

In this thesis, a pilot-scale (0.1 Mt/year) CO₂ sequestration site in the Ordos Basin of China has been selected to provide a case study of CO₂ storage in deep saline formations, by addressing a variety of aspects including two phase (CO₂ & water) flow, rock deformation, heat transport and CO₂-water-rock interactions. Besides, a simple case study for geothermal production associated with CO₂ sequestration in porous media has been carried out. In general, the basic research carried out in this thesis will be useful in assessing and evaluating the capacity, efficiency, safety, economics and feasibility of CO₂ sequestration in deep saline formations. To achieve these objectives, the study has further developed suitable criteria of site selection both for CO₂ sequestration and geothermal production utilizing CO₂ to enhance heat extraction.

In the course of this study, some general results have been obtained for the problems of coupled geo-processes that arise from CO₂ sequestration. The upward and lateral migration process of CO₂ is triggered off as soon as the injection starts, until it is restricted or stopped by some impermeable layers (caprocks) and structures for its storage, in the short-term. This is then, followed by its long-term trapping mechanisms, including solubility and mineralization, which may impart significant changes on the reservoir properties, especially in the vicinity of the injection well. If the multilayered injection strategy was used in a multilayered reservoir-caprock system, strong perturbation between aquifer layers may occur, especially if they are located close to each other. Sensitivity analysis shows that CO₂ plume migration can be affected by factors in the following sequence: injection rate, reservoir permeability and multi-layered injection strategy, while the impact of other parameters is not obvious. Under consideration of the coupled hydro-mechanical effect, the lateral movement of the CO₂ plume can be enlarged to some extent as a result of volumetric expansion of the reservoir. Among those factors that affect the uplift movement of formations, injection rate has the largest impact, followed by reservoir permeability. Furthermore, the risk of tensile or shear failure of rocks surrounding the injection wellbore can be induced due to use of a poorly designed injection scheme. With respect to the geological conditions at the pilot site in the Ordos Basin, simulation results suggest that the pressure buildup should be controlled not to exceed 13.7, 14.8, 17.0 and 17.5 MPa in the four injection layers from top to bottom, respectively, to achieve a safe long-term storage of CO₂. Geochemical interactions caused by CO₂ injection are complex and highly specific case-dependent (e.g. initial mineralogy and formation water chemistry, salinity, pH, temperature). In view of a short time (several tens of years), the impact of geochemical interactions on fluid flow can be negligible. Using the reservoir properties representative for the injected aquifers of the Ordos Basin, simulation results show that after 1000 years of chemical reactions, the maximum reduction of the reservoir porosity and permeability is about 3% and 8%, respectively.



In the case of CO₂-sequestration associated with geothermal production, some advantages can be achieved, i.e. an increased amount of heat extraction and additional CO₂-sequestration capacity of underground. After CO₂ breakthrough, the flowing enthalpy increases greatly, showing the great advantage of CO₂ as a heat extraction fluid. A favorable well configuration is achieved if geothermal production wells are perforated at the same depth of CO₂ injection wells or even deeper, because it can greatly delay the CO₂ breakthrough time if CO₂ is used as a pressure-driven fluid. Economical configuration of geothermal systems can also depend on other factors, including well spacing, completion depth, injection/production rate, reservoir temperature and pressure, etc. Therefore, further studies are still required before commercial applications.

Many uncertainties mar the evaluation of a suitable site for CO₂ sequestration and CO₂-associated geothermal production. These are, for instance, uncertainties in geological characteristics at the injection site and the simulation methods used. The site selection criteria further developed in this thesis, were based on different scales of the investigated site (e.g. basin scale, field scale, target formation scale, engineering operation scale). However, more studies in the future are still required to optimize the screening and ranking system. Under the guidance of the screening and ranking system, the optimization sequence of several sedimentary basins of China suitable for CO₂ sequestration and CO₂-associated geothermal production are studied. Bohaiwan, Songliao and Qiangtang Basins present the greatest potential for a geothermal production, while for only CO₂ sequestration purpose, top three sequences are the Ordos, Tarim and Bohaiwan Basins.

Keywords: CO₂ sequestration; numerical simulations; two phase flow; CO₂-water-rock interactions; geothermal production



Zusammenfassung

Die CO₂-Injektion zu Speicherungszecken in geologische Formationen, vor allem in weit verbreitete tiefe saline Formationen, kann als eine optimale Option für die Reduzierung des CO₂-Ausstoßes betrachtet werden. Jedoch muss die geologische CO₂-Sequestrierung in porösen Medien mit umfassenden Problemen konfrontiert werden, z. B. mit der Verschmutzung des flachen Grundwassers, dem Integritätsverlust des Deckgebirges, verursacht durch einen zu hohen Speicherdruck, der Korrosion einiger Bohrlochausrüstungen, die nur durch die kombinierte Anwendung von Hydrologie, Geotechnik, Geochemie, Felsmechanik, Mathematik, Computertechnologie und verwandten Fachdisziplinen gelöst werden können.

Um die physikalischen und chemischen Geo-Prozesse im Zusammenhang mit einer CO₂-Sequestrierung im Untergrund zu verstehen und zu quantifizieren, wurden die numerischen Simulatoren TOUGH2MP, TOUGHREACT und FLAC3D entwickelt. Diese numerischen Untersuchungen können wichtige Information über die räumliche und zeitliche Entwicklung von CO₂-Verteilung, Porendruck, effektiven Spannungen, Formationshebungen, Ionenkonzentration, Volumenanteil von Mineralien usw., unter Berücksichtigung von Reservoirheterogenitäten im unterschiedlichen Maßstab liefern und somit eine unschätzbare Referenz für ein bestimmtes CCS-Projekt zur Verfügung stellen, um seine Sicherheit und Effizienz zu gewährleisten.

In dieser Doktorarbeit wurde ein CO₂-Speicher-Pilotprojekt (CO₂-Injektionsrate: 0.1 Mt/Jahr) im Ordos-Becken (China) als Fallstudie für die CO₂-Speicherung in tiefen salinen Formationen ausgewählt, in dem eine Reihe von damit verbundenen Aspekten einschließlich des Zweiphasenflussprozesses von CO₂ und Wasser, der Gesteinsdeformation, des Wärmetransports sowie der Wechselwirkungen von CO₂, Wasser und Gestein behandelt werden. Darüber hinaus wurde eine vereinfachte Fallstudie für die geothermische Produktion in Verbindung mit der CO₂-Sequestrierung in porösen Medien betrachtet. Im Allgemeinen wird die im Rahmen dieser Arbeit durchgeführte Grundlagenforschung für die Beuteilung und Auswertung der Kapazität, Effizienz, Sicherheit, Wirtschaftlichkeit und Machbarkeit der CO₂-Sequestrierung in tiefen salinen Formationen von Nutzen sein. Um diese Ziele zu erreichen, wurden im Rahmen dieser Arbeit geeignete Kriterien zur Standortauswahl sowohl für die CO₂-Sequestrierung als auch für eine geothermische Produktion unter Anwendung von CO₂ zur Steigerung der Wärmegewinnung weiterentwickelt.

Im Rahmen dieser Doktorarbeit wurden einige allgemeingültige Ergebnisse bezüglich der Fragestellungen im Zusammenhang mit den gekoppelten Geo-Prozessen in der geologischen CO₂-Sequestrierung erzielt. Für die CO₂-Speicherung gilt zuerst der kurzfristige Bindungsmechanismus, nämlich dass, die nach oben und seitlich gerichtete Migration unmittelbar nach dem Beginn der CO₂-Injektion ausgelöst wird und erst durch undurchlässige Schichten, die sogenannten Deckgebirges, oder Strukturen für die CO₂-Speicherung gestopt wird. Danach wirken dann die langfristigen Bindungsmechanismen, wie Löslichkeit und Mineralisierung, die, insbesondere in der Nähe der CO₂-Injektionsbohrung, positive oder negative Auswirkungen auf die Reservoireigenschaften haben können. Im Fall der Anwendung der Mehrschichtinjektionsstrategie in ein mehrschichtiges Reservoir-Caprock-System, können starke Störungen zwischen Aquiferschichten auftreten, insbesondere wenn sie nahe beieinander liegen. Die Sensitivitätsanalyse zeigt, dass die CO₂-Migration durch folgende Faktoren in folgender Reihenfolge beeinflusst werden kann: Injektionsrate, Reservoirpermeabilität und Mehrschichtinjektionsstrategie, während die Auswirkungen anderer Parametern nicht offensichtlich sind. Unter Berücksichtigung des gekoppelten hydromechanischen Effekts, kann die seitliche Bewegung der CO₂-Verteilung wegen der Volumenausdehnung des Reservoirs zu einem gewissen Grad vergrößert werden. Unter den Faktoren, die sich auf die Hebung von Formationen auswirken, hat die Injektionsrate den größten Einfluss, gefolgt von der Reservoirpermeabilität. Weiterhin kann sich das

Risiko eines Zug- oder Scherversagens der Gesteine im Nahbereich der Injektionsbohrung aufgrund eines schlecht ausgelegten Injektionsschemas erhöhen. Gemäß den geologischen Bedingungen am Pilotstandort in dem Ordos Becken zeigen die Simulationsergebnisse, dass die Druckerhöhung in den vier Injektionsformationen von oben bis unten so kontrolliert werden soll, jeweils 13.7, 14.8, 17.0 und 17.5 MPa nicht zu überschreiten, für eine sichere langfristige Speicherung von CO₂. Die durch CO₂-Injektion verursachten geochemischen Wechselwirkungen sind komplex und hochspezifisch fallabhängig (z. B. initiale Mineralogie und Formationenwasserchemie, Salzgehalt, pH, Temperatur). In Anbetracht eines kurzen Zeitraums (mehrere Jahrzehnte) ist der Einfluss der geochemischen Wechselwirkungen auf den geohydraulischen Prozess vernachlässigbar. Mit repräsentativen Reservoireigenschaften für die Injektionsaquiferen im Ordos Becken zeigen die Simulationsergebnisse, dass die maximale Reduzierung der Porosität und Permeabilität nach 1000 Jahren jeweils ca. 3% und 8% beträgt.

Die CO₂-Sequestrierung in Verbindung mit geothermischer Produktion bringt einige wesentliche Vorteile mit sich, wie z. B. ein erhöhtes Potential zur Wärmegewinnung und eine zusätzliche CO₂-Aufnahmekapazität des Untergrundes. Nach dem CO₂-Durchbruch, steigt die Fließenthalpie stark an, was den großen Vorteil von CO₂ als Wärmeextraktionsflüssigkeit zeigt. Eine günstige Bohrlochkonfiguration wird erreicht, wenn die geothermische Produktionsbohrung in der gleichen Teufe der Injektionsbohrung oder noch tiefer perforiert wird, weil sich der Durchbruch von CO₂ verlangsamt, falls CO₂ als ein druckgetriebenes Fluid benutzt wird. Die Wirtschaftlichkeit geothermischer Systeme hängt darüber hinaus von weiteren Faktoren ab wie z. B. Bohrungsdurchmesser, Komplettierungstiefe, Injektions-/Produktionsrate, Reservoirtemperatur und Reservoirdruck usw. Aus diesem Grund sind vor einer kommerziellen Anwendung weitere Untersuchungen erforderlich.

Viele Unsicherheiten beeinträchtigen die Bewertung einer für die CO₂-Sequestrierung und CO₂-assoziierte geothermische Produktion geeigneten Lokalität, da sie beispielsweise hinsichtlich der Unwägbarkeit bezüglich der geologischen Gegebenheiten am Standort und damit der anzuwendenden Simulationsmethoden aufweisen. Die in dieser Arbeit weiterentwickelten und angewendeten Standortauswahlkriterien basieren auf verschiedenen Bewertungsmaßstäben für das Untersuchungsgebiet, wie z. B. auf den Maßstäben des Beckensystems, des Felds, der Zielformation sowie des ingenieurtechnischen Betriebes. Es werden jedoch auch zukünftig weitere Studien erforderlich sein, um das Screening- und Ranking-System zu optimieren. Nach diesem Screening- und Ranking-System, wurde mehrere Hauptsedimentbecken in China auf Eignung für die CO₂-Speicherung und CO₂-assoziierte geothermische Produktion untersucht. Das Bohaiwan, das Songliao und das Qiangtang Becken stellen das größte Potenzial für eine geothermische Produktion, während das Ordos-, Tarim- und Bohaiwan- Becken am besten für den Zweck der CO₂-Sequestrierung geeignet sind.

Keywords: CO₂-Sequestrierung; numerische Simulationen; Zweiphasenströmung; CO₂-Wasser-Gesteins-Wechselwirkungen; geothermische Produktion



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**Nomenclature**

A	Cross sectional area, m^2
A_m	Specified surface area of mineral m , m^2
B	Biot's modulus, MPa
B_f	Fluid formation volume factor, bbl/STB for oil, bbl/scf for gas
B_g	Gas formation volume factor, bbl/scf
B_o	Oil formation volume factor, bbl/STB
B_s	Skempton coefficient (compressibility coefficient), -
C	Chemical component concentration, mol/L
C'	Internal cohesion of the rock, N
C_s	Mass of CO_2 dissolved per unit volume of water
c	Compressibility, $1/\text{Pa}$
c_b	Compressibility of bulk rock, $1/\text{Pa}$
c_{eff}	Effective compressibility, $1/\text{Pa}$
c_f	Fluid compressibility, $1/\text{Pa}$
c_o	Isothermal oil compressibility, $1/\text{Pa}$
c_p	Pore compressibility, $1/\text{Pa}$
c_s	Compressibility of solid skeleton material, $1/\text{Pa}$
c_w	Water compressibility, $1/\text{Pa}$
D	Diffusion coefficient, m^2/s
D_e	Effective molecular diffusion coefficient, m^2/s
E_a	Activation energy, J
E_b	Elastic modulus of bulk rock, Pa
E_s	Elastic modulus of solid skeleton, Pa
F	Mass flux term, $\text{kg}/(\text{m}^2 \cdot \text{s})$
fr_m	Volume fraction of the reactive mineral m in the rock, -
fr_u	Volume fraction of the nonreactive minerals, -
G	Shear modulus, N/m^2
g	Gravitational acceleration, m/s^2
$\Delta H^\ominus$	Standard enthalpy change, J/mol
h	Specific heat, $\text{J}/(\text{kg} \cdot ^\circ\text{C})$
$\hat{h}$	Formation thickness, m
I	Ion strength = $0.5 \sum_j c_j \bar{z}_j^2$, mol/L
IAP/Q	Ion activity product, -
J	Hydraulic gradient, -
J_d	Diffusion flux per unit area per unit time, $\text{mol}/\text{m}^2\text{s}$
J_{inj}	Injectivity index, $\text{kg}/(\text{Pa} \cdot \text{s})$
K	Drained bulk modulus, N/m^2
$\hat{K}$	Equilibrium constant in chemical reactions, -
K_c	Permeability coefficient/hydraulic conductivity, m/s
$K_{c\alpha}$	Permeability coefficient of phase α , m/s
K_f	Fluid bulk modulus, N/m^2
K_s	Solid bulk modulus, N/m^2
K_{sp}	Solubility product constant under a certain temperature, -
K_u	Bulk modulus under undrained state, N/m^2
k	Intrinsic permeability/absolute permeability, m^2



Nomenclature

k_0	Permeability under zero stress condition, m^2
k_i	Initial permeability, m^2
k_α	Permeability of phase α , m^2
k^m	Permeability coefficient (mobility coefficient), $k^m = \frac{K_c}{\rho_f g}$, $m^2/Pa/s$
$k_{r\alpha}$	Relative permeability of phase α , -
k_{rg}	Relative gas permeability ratio, -
k_{rw}	Relative water permeability ratio, -
k_{rl}	Liquid phase relative permeability ratio, -
$\bar{k}$	Reaction rate constant, -
L	The distance between the two cross sections perpendicular to the flow direction, m
M	Mass accumulation term, kg/m^3
$\bar{M}$	Fluid mobility, $kg/(m^3 \cdot cP)$
N	Number of chemical basic components, -
P_c	Capillary pressure, Pa
P_d	Air entry pressure, Pa
P_{fm}	Fracture margin pressure of rocks, Pa
P_g	Gas partial pressure, Pa
P_i	Initial reservoir pressure, Pa
P_l	Water partial pressure, Pa
P_{max}	Maximum capillary pressure, Pa
P_0	Strength coefficient, Pa
P_{sc}	Critical shear slip pore pressure, Pa
p	Pore pressure, Pa
Δp	Pressure difference, Pa
q	Source/sink term, $kg/(m^3 \cdot s)$
$\hat{q}$	Total filtration amount per unit time, kg/s
q_c	Injection rate of CO_2 , kg/s
R_e	Ion radius, m
R_s	Solution gas oil ratio, scf/stb
R_t	Formation electrical resistivity factor, -
R_w	Well radius, m
$\bar{R}_n$	Radius of capillary tubes of non-wetting phase, m
$\bar{R}_w$	Radius of capillary tubes of wetting phase, m
r_m	Dissolution/precipitation rate of mineral m
r_t	Throat radius, m
r_p	Pore radius, m
S	Saturation, -
S_{gr}	Residual gas saturation, -
S_l'	Critical liquid saturation for fluid flow, -
S_{lr}	Residual liquid saturation, -
$S_{r\alpha}$	Residual saturation of phase α , -
S_{wi}	Connate water saturation, -
S_{wr}	Residual water saturation, -
$\hat{S}$	Effective saturation, $\hat{S} = (S_w - S_{wr}) / (1 - S_{wr})$



S_e	Normalized saturation, $S_e = \frac{(S_w - S_{wr})}{(S_w - S_{wr} - S_{gr})}$
$\bar{S}$	Brine salinity, -
SI	Mineral saturation index, -
T	Temperature, °C
T_c	Temperature at critical point, °C
t	Time, s
U	Internal energy, J/kg
u	Darcy velocity, m/s
$\hat{u}$	Solid grain displacement, m
$\hat{u}_i$	Solid grain displacement vector, m
V	Volume, m ³
V_b	Volume of bulk rock, m ³
V_m	Molar volume (V/n), L/mol
V_t	Total volume of porous media, m ³
V_p	Pore volume of porous media, m ³
V_{p1}	Pore volume of matrix medium, m ³
V_{p2}	Pore volume of the fracture, m ³
X	Mass fraction, -
x	Distance, m
Z_c	Compressibility factor at the critical point, -
$\tilde{z}_j$	Ion charge, -
z	Gas compressibility factor, -
α	Biot's coefficient, -
$\bar{\alpha}_j$	Activity of aqueous component j
β	Undrained thermal coefficient, 1/°C
Γ	Volumetric exchange rate (interporosity flow, transfer rate) between fractures and matrix blocks per unit bulk volume, m ³ /s
γ_j	Activity coefficient of aqueous component j , -
δ_{ij}	Kronecker delta ($i=j$, $\delta_{ij} = 1$)
ε_{ij}	Strain, $\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$
ε_v	Volumetric strain, -
θ	Contact angle between solid and fluid, -
λ	Heat conductivity, W/(m·°C)
μ	Fluid viscosity, cP or m.Pa/s
ν	Poisson's ratio, -
ν_u	Poisson's ratio of the undrained elastic rock skeleton, -
π	Variation of fluid content per unit volume of porous media, -
ρ	Density, kg/m ³
ρ_c	CO ₂ density, kg/m ³
ρ_f	Fluid density, kg/m ³
ρ_o	Oil density, kg/m ³
σ	Stress, Pa
σ'	Effective stress, Pa
σ_{ij}	Total stress, $\sigma_{ij} = \sigma'_{ij} + \alpha P$, Pa



σ'_{ij}	Effective stress, Pa
σ_h	Minimum horizontal stress, Pa
σ_m	Mean stress, Pa
σ_{s1}	Interfacial tension between solid and fluid 1, N
σ_{s2}	Interfacial tension between solid and fluid 2, N
σ_{wg}	Interfacial tension between water and gas, N
σ_v	Vertical stress, Pa
σ_1	Maximum principal stress, Pa
σ_3	Minimum principal stress, Pa
σ_{12}	Interfacial tension between fluid 1 and fluid 2, N
τ	Maximum shear stress, Pa
$\hat{\tau}$	Medium tortuosity, -
ϕ	Porosity, -
$\hat{\phi}$	Porosity at reference pore pressure p_0 , -
ϕ_e	Effective porosity, -
ϕ_r	Residual porosity under zero stress condition, -
ϕ_t	Total porosity, -
ϕ_0	Porosity under zero stress condition, -
ϕ_1	Porosity from matrix media, -
ϕ_2	Porosity from fracture part in the fractured media, -
φ'	Internal friction angle, °
Ω	Mineral saturation ratio, -
ω	Fugacity coefficient, -
$\tilde{\omega}$	Solubility, -
$\nabla \cdot$	Divergence, -
∇	Gradient, -

Superscripts

T	Under thermal mode condition
c	CO ₂ component
i	Chemical aqueous ions
m	Pore size distribution index, -
n	Power term
o	Initial state
w	H ₂ O component
λ	Pore size distribution index, -
κ	Mass component (water, CO ₂ , NaCl, heat etc.)
nu, H, OH	Reaction is under neutral, acid and base mechanism
θ	Parameter used in the calculation of reaction rate of mineral
η	Parameter used in the calculation of reaction rate of mineral

Subscripts

$g, l/w, s$	Gas phase, liquid phase and solid phase, respectively
$n = 1, 2$	Matrix and fracture media, respectively
α	Phase index