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Estimating the reaction parameters of oil shale pyrolysis and oil shale grade using temperature transient analysis and inverse modeling



Kyung Jae Lee^{a,*}, Stefan Finsterle^b, George J. Moridis^{a,c}

^a Energy Geosciences Division 74-316C, Lawrence Berkeley National Laboratory, Berkeley, 94720, CA, USA

^b Finsterle GeoConsulting, Kensington, CA, USA

^c Texas A&M University, College Station, TX, USA

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ABSTRACT

Grade of oil shale and reaction parameters of in-situ pyrolysis must be identified for the prediction of productivity before actual heating and production. Identification of oil shale grade and reaction parameters depends on laboratory experiments on core samples. However, laboratory-determined parameters can be different from those representing in-situ reservoir conditions. In this study, we use inverse modeling to determine oil shale grade and reaction parameters. The inversions are based on a forward model that simulates heat injection into a well. Temperature at the heating well is affected by a thermal skin effect as a result of a decrease of composite thermal conductivity around the heater due to the decomposition-induced porosity increase. Synthetic observations of heater temperature are generated from a forward simulation. Temperature difference and its derivative are used in synthetic inversions to estimate oil shale grade and parameters of active decomposition reactions with an error below 1%. The proposed methodology of inverse modeling is expected to successfully estimate the oil shale grade and reaction parameters without core sampling and subsequent surface experiments.

1. Introduction

Hydrocarbon production from oil shale significantly depends on the grade of oil shale and the parameters of decomposition reactions. Oil shale grade and reaction parameters are typically determined by laboratory experiments on core samples (Burnham and McConaghy, 2014; Campbell et al., 1978; Kar and Hascakir, 2017; Reynolds et al., 1991; Wen and Kobylinski, 1983). However, parameters estimated in the laboratory on the scale of a core sample tend to be conceptually and numerically different from those needed to represent the large-scale behavior under in-situ conditions. In this study, we develop an inversion methodology to estimate the oil shale grade and reaction parameters under in-situ reservoir conditions.

We propose an inverse modeling approach, which examines the use of temperature transient data and the concept of a thermal skin to estimate oil shale grade and decomposition parameters. Similar to pressure transient analyses, temperature transient analyses have been used in oil and gas reservoir engineering to determine productivity, transport properties, and the vertical formation structure (Bahrami and Siavoshi, 2007; Muradov and Davies, 2012; Onur and Cinar, 2017; Sui et al., 2012). In this study, we observe heater temperature as a system response during in-situ

pyrolysis of oil shale in a kerogen-bearing system. We analyze the temperature of an electrical heater operated at a constant heat output rate, while the previous studies analyzed the well temperature during injection or production of fluids.

In combination with the temperature transient analysis, we introduce the concept of a thermal skin effect. Positive hydraulic skin effects in a drawdown test lead to an additional pressure drop at the wellbore, which is induced by decreased permeability around the wellbore due to the mud filtration; and negative hydraulic skin effects lead to a reduced pressure drop at the wellbore, which is induced by increased permeability around the wellbore by stimulation (Lee, 1982). The proposed concept of a thermal skin implies an additional temperature increase at a heater, which is induced by the formation's decreased composite thermal conductivity due to the porosity increase following oil shale decomposition. The corresponding thermal skin factor thus contains information about decomposition reactivity, which is a function of oil shale grade and reaction parameters.

The objective of this study is to estimate oil shale grade and reaction parameters by inverting transient heater temperature data, as they are affected by the thermal skin. Temperature difference and its derivative are directly computed from the observed heater temperatures. Synthetic

* Corresponding author.

E-mail addresses: kjlee6@central.uh.edu (K.J. Lee), stefan@finsterle-geoconsulting.com (S. Finsterle), moridis@tamu.edu (G.J. Moridis).

Table 1

Most active decomposition reactions of oil shale pyrolysis (Braun and Burnham, 1992; Youtsos et al., 2013).

Reactions	Frequency factor [s ⁻¹]	Activation energy [kJ·mole ⁻¹]	Reaction enthalpy [kJ·mole ⁻¹]	Magnitude of reaction rate constant ^a [s ⁻¹]
Kerogen → 0.279 Heavy oil + 0.143 Light oil + 0.018 Hydrocarbon gas + 0.005 Methane + 0.555 Coke 1	3.0 × 10 ¹³	213.384	-335	10 ⁻⁸ ·10 ⁻⁵
Heavy oil → 0.373 Light oil + 0.156 Hydrocarbon gas + 0.03 Methane + 0.441 Coke 2	1.0 × 10 ¹³	225.936	-46.5	10 ⁻¹⁰ ·10 ⁻⁶
Coke 1 → 0.031 Hydrocarbon gas + 0.033 Methane + 0.936 Coke 2	1.0 × 10 ¹³	225.936	-46.5	10 ⁻¹⁰ ·10 ⁻⁶

^a Reaction rate constants were computed for temperatures between 250 and 350 °C, where the reactions were active.

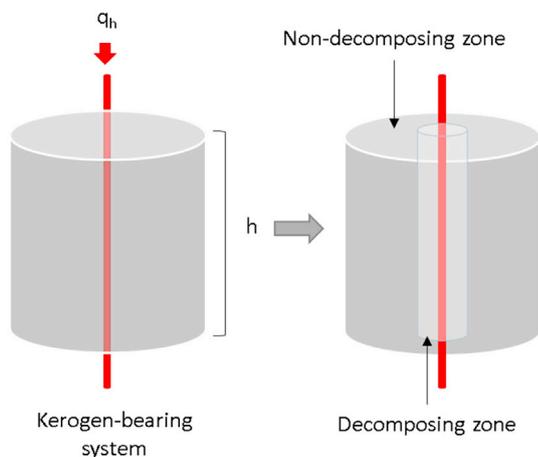


Fig. 1. Schematic concept of decomposing zone near the heater and non-decomposing zone, in the kerogen-bearing system.

Table 2

Input parameters of the heating simulation.

Input parameters	Values	Input parameters	Values
ϕ_i [-] (Initial porosity)	0.015	P_i [MPa] (Initial system pressure)	20.7
$V_{\text{kerogen}, i}$ [-] (Initial kerogen volume fraction)	0.25	T_i [K] (Initial system temperature)	303.15
ρ_R [kg·m ⁻³] (Dry rock density)	2600	r_w [m] (Heating well radius)	0.1
$C_{p,R}$ [J·(kg·K) ⁻¹] (Dry rock specific heat capacity)	1500	h [m] (Thickness of heating interval)	10
K_R [W·(m·K) ⁻¹] (Dry rock thermal conductivity)	2.0	q_h [J·s ⁻¹] (Heat injection rate)	8500

data are generated by numerical simulations of heating and in-situ pyrolysis of oil shale, because of the absence of actual field or experimental data. These synthetic data are then used in notional inversions to examine efficacy and accuracy of the proposed method for different

thermal conductivities.

2. Mathematical and chemical models

The energy balance equation involving heat accumulation and heat transfer by conduction, convection, and reaction is described as follows (Maes et al., 2016):

$$\frac{\partial}{\partial t} \left[(1 - \phi) \rho_R C_{p,R} T + \phi \sum_{\beta} \rho_{\beta} S_{\beta} C_{p,\beta} T \right] = \nabla \cdot (K \nabla T) - \nabla \cdot (h_{\beta} \mathbf{F}_{\beta}) + \sum_j \Delta h_j r_j \quad (1)$$

In the heat accumulation terms on the left-hand side, ϕ is the medium porosity; T [K] is the system temperature; ρ_R [kg·m⁻³] is the rock grain density; and $C_{p,R}$ [J·(kg·K)⁻¹] is the rock grain specific heat capacity. S_{β} is the saturation; and $C_{p,\beta}$ [J·(kg·K)⁻¹] is the specific heat capacity of phase β . We consider the same temperature of fluid phases and a rock grain in each element, regarding that the time for a rock grain to absorb the heat of fluids is about 10⁻⁷ s, which means that all fluid phases are at same temperature as a rock grain in a same discrete element (Phillips, 1991; Woods, 1999; Youtsos et al., 2013). In the heat flux terms on the right-hand side, K [W·(m·K)⁻¹] is the composite thermal conductivity of the formation; h_{β} [J·kg⁻¹] is the specific enthalpy of phase β ; and \mathbf{F}_{β} [kg·m⁻²·s⁻¹] is the flow rate of phase β , which is described by Darcy equation. In the reactive heat term on the right-hand side, Δh_j [J·kg⁻¹] is the reaction enthalpy; and r_j [kg·m⁻³·s⁻¹] is the reaction rate of j -th reaction. The detailed equations for $C_{p,\beta}$, \mathbf{F}_{β} , and h_{β} can be found in Lee et al. (2016).

The most active decomposition reactions of oil shale pyrolysis are summarized in Table 1 (Braun and Burnham, 1992; Youtsos et al., 2013). When kerogen in a porous medium is heated to a high temperature, it decomposes into fluid and solid components. Heavy oil and coke 1, which are generated from the kerogen decomposition, also decompose into secondary products. The reaction rate of each reaction is determined by using the Arrhenius law of first order as follows:

$$r_j = A_j \exp\left(-\frac{E_j}{RT}\right) C_j = K_j C_j \quad (2)$$

where, C_j [kg·m⁻³] is the concentration of reactant j ; A_j [s⁻¹] is the frequency factor; E_j [kJ·mol⁻¹] is the activation energy; K_j [s⁻¹] is the reaction rate constant; and R ($= 8.314 \cdot 10^{-3}$) [kJ·mol⁻¹·K⁻¹] is the gas constant.

Dynamic change of the reservoir porosity, which is defined by the volumetric ratio of void space to the bulk formation, can be computed by accounting for the amount of individual solid components:

$$\phi = \phi_i + \frac{V_{\text{kerogen}, i}}{C_{\text{kerogen}, i}} (C_{\text{kerogen}, i} - C_{\text{kerogen}} - C_{\text{coke}}) \quad (3)$$

where, ϕ_i is the initial porosity; $V_{\text{kerogen}, i}$ is the initial volume fraction of kerogen in the porous media; $C_{\text{kerogen}, i}$ [kg·m⁻³] is the initial concentration of kerogen; and C_{kerogen} [kg·m⁻³] and C_{coke} [kg·m⁻³] are the concentrations of kerogen and cokes, respectively. In Eq. (3), the pore expansion by increasing temperature and the heating-induced pressurization is not included because of its insignificant magnitude. Assuming a pore compressibility of 4.35×10^{-10} Pa⁻¹ and a thermal expansivity of 10⁻⁵ K⁻¹, factors of the pore expansion by the pressurization and increasing temperature are on the order of 10⁻⁴ and 10⁻³, respectively. Changes in porosity due to changing temperature and pressure are fully accounted for in our numerical model. In addition to this, dynamically changing permeability, tortuosity, and composite thermal conductivity are accounted in the numerical model, so that we can accurately simulate the flow of heat and fluid with changing porosity. Kozeny-Carman equation and Millington-Quirk equation are used for porosity-

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