The forward and inverse problems in oil shale modeling

Ne-Zheng Sun (email: nezheng@ucla.edu)
Civil & Environmental Engineering Department, UCLA, USA

Alexander Y. Sun (email: alexsunda@gmail.com)
Sunda Environmental Technology, LLC, USA

Brian Gallagher (email: bjgla@sbcglobal.net)
Ecotonics Environmental Scientists, USA

Abstract

This paper presents a preliminary outline for modeling the in-situ oil shale heating process in the field scale. The proposed model consists of a number of coupled and highly nonlinear partial differential equations. Numerical methods for solving these equations are described shortly. Some parameters in the model must be identified by solving the inverse problem with lab and field data. The paper gives an algorithm for identifying the process dependent parameters, such as the porosity and permeability. Finally, the model reduction and reliability problems are considered with a new concept of constructing objective-oriented models.

Introduction

Mathematical modeling is a very useful tool for oil shale development research. A reliable model can be used not only for feasibility and mechanism studies, but also for optimal engineering design and process management. In recent years, new in-situ retorting technologies have been reported (RAND, 2005). To model an in-situ oil shale development process we need three models: a dewatering model, a retorting model, and an environmental recovering model. The ending condition of the first model provides the initial condition for the second model, and then the ending condition of the second model provides the initial condition for the third model. The dewatering model and the environmental recovering model are relatively simple and have been considered in groundwater hydrology and environmental engineering. Developing a retorting model, however, is a very challenging topic because of its high complexity. This kind of model has not been studied very well in petroleum engineering.

A model that can simulate an in-situ retorting process may consist of:

- A set of multiphase flow equations for the oil, water and gas phases;
- A heat transport equation in porous media;
- A deformation equation for oil shale;
- A set of convection-dispersion-reaction equations when solvents are added.

There are difficulties in constructing such a model. First, the governing equations of the model are coupled and highly non-linear partial differential equations. Effective methods for solving such a complex system are needed. Second, most parameters in the model are unknown. They may vary not only with location but also with time and state variables, such as temperature and saturation. Third, the solutions and parameters are scale dependent. Their values obtained in the lab scale cannot be transferred directly in the field scale.

To overcome these difficulties, we must develop effective numerical methods for solving both the forward and inverse problems. The former gives the results of model prediction, while the latter gives the results of model calibration. Without the data collected from field experiments for model calibration, it is impossible to construct a useful oil shale model. Before a model is used for design and management purposes of oil shale development, its reliability must be studied.

This paper is a preliminary guideline to the oil shale modeling. A distributed parameter model is presented based on the physical process of in-situ heating technologies. Numerical methods for solving the forward problem are described shortly. A coupled inverse problem is formulated for parameter identification and model calibration. Our discussion is concentrated on the identification of the intrinsic permeability. During the heating process, permeability is a variable even for a homogeneous shale formation and is dependent on the temperature distribution. Based on the recent study of the first author on constructing objective oriented models, the paper also discusses how to reduce the complexity of an oil shale model while the accuracy requirement of model application can still be guaranteed.

A Proposed In-situ Oil Shale Heating Model

After the dewatering process is completed and the heating process is started, fluid oil and gas will be generated from the shale gradually. Multiphase flow is governed by a set of partial differential equations, one for each phase:

$$\frac{\partial}{\partial t}(\theta\rho_\alpha S_\alpha) = \nabla\cdot\left[\rho_\alpha k\frac{k_{r\alpha}}{\mu_\alpha}(\nabla P_\alpha + \rho_\alpha g\nabla z)\right] + \rho_\alpha q_\alpha \tag{1}$$

where the subscript α denotes a phase. Several different immiscible fluid and gas phases may exist during the retorting process, such as water, vapor, retorted oil, gas and other compounds with different densities and viscosities. Let the total number of phases be *n*. Solid can also be considered as a phase but it does not flow. The variables and parameters in equation (1) are defined as follows: *S* is the saturation, *P* the pressure, θ the porosity, ρ the density, μ the viscosity, *k* the intrinsic permeability, k_r the relative permeability, *g* the acceleration of gravity, and *q* the source term. For example, for the oil phase, q_o is the volume of oil generated from a unit volume of shale during unit time. All 2*n* state variables S_α and P_α can be solved from the *n* equations (1) with combining the following *n* constraints:

$$\sum_{\alpha=1}^{n} S_\alpha = 1 \tag{2}$$

$$P_\alpha - P_\beta = P_{\alpha\beta} \tag{3}$$

where α and β are two phases, and $P_{\alpha\beta}$ is the capillary pressure between the two phases. Note that Equation (3) contains only *n*-1 independent equations because the summation of all these equations is equal to zero.

The multiphase flow equations are similar to those used in the petroleum engineering, but the values of some parameters, such as the porosity and permeability, will change with the progress of the heating process as more oil and gas are produced from the shale. Even for a homogeneous shale structure, the porosity will depend on time and temperature of heating. Therefore, the following heat transport equations for all phases, including the solid phase, are needed:

$$\frac{\partial}{\partial t}(\rho_\alpha\theta S_\alpha c_\alpha T_\alpha) = \nabla\cdot(\rho_\alpha\theta S_\alpha \mathbf{D}_\alpha^h\nabla T_\alpha) - \nabla\cdot(\rho_\alpha\theta S_\alpha c_\alpha T_\alpha \mathbf{V}_\alpha) + I_\alpha + Q_\alpha \tag{4}$$

$$\frac{\partial}{\partial t}[\rho_s(1-\theta)c_s T_s] = \nabla\cdot[\rho_s(1-\theta)\mathbf{D}_s^h\nabla T_s] + I_s + Q_s \tag{5}$$

where the subscript α in Equation (4) denotes a fluid or a gas phase, $\mathbf{D}_\alpha^h$ is the heat dispersion coefficient, $\mathbf{V}_\alpha$ is the velocity, I_α is the heat exchange between phase α and other phases, and Q_α is the heat source term. The subscript s in Equation (5) denotes the solid phase. These heat transport equations are also highly nonlinear. For example, the porosity θ is a coefficient in these equations but is dependent on the heating process. The solutions of the flow equations depend on the temperature distribution, and in turn, the flow velocities in the heat transport equations are dependent on the solutions of the flow equations through Darcy's law:

$$\mathbf{V}_\alpha = -\frac{kk_{r\alpha}}{\theta\mu_\alpha}\left(\nabla P_\alpha + \nabla z\right) \quad (6)$$

For a chemical compound β, such as a solvent added to a phase α or generated from the oil shale, we also need the following reactive mass transport equation:

$$\frac{\partial}{\partial t}\left(\theta S_\alpha C_\alpha^\beta\right) = \nabla\cdot\left(\theta S_\alpha \mathbf{D}_\alpha \nabla C_\alpha^\beta\right) - \nabla\cdot\left(\theta S_\alpha C_\alpha^\beta \mathbf{V}_\alpha\right) + I_\alpha^\beta + R_\alpha^\beta + Q_\alpha^\beta \quad (7)$$

where C_α^β is the concentration of the compound β in phase α; $\mathbf{D}_\alpha$ is the hydrodynamic dispersion coefficient; I_α^β and R_α^β are the mass increments of compound β in phase α caused by mass exchanges and reactions, respectively, between phase α and other phases, and Q_α^β is the term of mass source. This equation is coupled with flow and heat transport equations through the state equations for each phase:

$$\rho_\alpha = \rho_\alpha(P_\alpha, T_\alpha, C_\alpha) \quad (8)$$

and

$$\mu_\alpha = \mu_\alpha(P_\alpha, T_\alpha, C_\alpha) \quad (9)$$

The deformation equation is not explicitly involved in the model. Instead, its effect is represented by the variable porosity, permeability, and density. The density ρ_s is determined by the following equation:

$$\frac{\partial}{\partial t}[\rho_s(1-\theta)] = -\rho_o q_0 - \rho_g q_g \quad (10)$$

Summarily, *n* multiphase flow equations with *n* constraints, *n* Darcy's law equations (in vector form), (*n*+1) heat transport equations, *m* mass transport equations for *m* chemical compounds, 2*n* state equations, and one solid density equation, with appropriate subsidiary conditions together form a complete in-situ oil shale retorting model.

This model can be significantly simplified by assuming that the heat transport process is much faster then the oil share retorting. In other words, the temperature distribution becomes steady state before the oil and gas start to generate from the shale. In this case, the model reduces to a model of multi-component transport in multiphase flow, except that the porosity, intrinsic permeability, and solid density are time dependent.

Numerical Solution

Before solving the forward problem for prediction, we have to determine the parameter values in all equations of the model. Due to the nonlinearity nature, most of them are functions of location, time and state variables (pressure, saturation, temperature, and concentration). We assume that the following functional relationships can be obtained based on the results of lab experiments:

- The volume of oil and gas produced per unit volume of oil shale as a function of time and temperature: $q_0(t,T)$ and $q_g(t,T)$. Figure 1 is a schematic figure of the function $q_o(t)$ for a given temperature *T*.
- The porosity of oil shale as a function of time and temperature: $\theta(t,T)$. Figure 2 is a schematic figure of the function $\theta(t)$ for a given temperature *T*.

The permeability depends on how the pores are connected. It is a macroscopic property of porous media and cannot be measured directly in the lab. During the retorting process, it tends to increase depending on the time period of heating and the heating temperature, i.e., $k = k(t,T)$. Figure 3 is a schematic figure of the function $k(t)$ for a given temperature *T*. In the next section, we will discuss how to identify such a function by solving the inverse problem with the field data.

Note that q, θ, k may also depend on location when (1) the oil shale structure is heterogeneous, or (2) the oil shale structure is homogeneous but the temperature distribution is inhomogeneous. These parameters may have different values at different locations because of the difference in the starting time of retorting.

After all parameters are determined, a finite difference or a finite element based numerical method (Sun, 1996; Helmig, 1997; Chen et al., 2006) can be used to solve the oil shale model. Due to the nonlinearity, the governing equations of the model must be solved iteratively and the values of parameters must be updated in each step of iteration until a convergent criterion is satisfied. The solution procedure for each time step consists of the following nine steps:

Step 1. Solve temperatures T_α and T_s from the heat transport equations (4) and (5) with given heat sources and initial parameter values.

Step 2. Update the values of production volume, porosity, intrinsic permeability and solid density when the retorting process starts.

Step 3. Solve pressure P_α and saturation S_α from the multiphase flow equations (1) and the constraints in equations (2) and (3) with the updated values of parameters.

Step 4. Use the P-S-k constitutive relations to update the values of relative permeability.

Step 5. Use Darcy's law to calculate the velocity $\mathbf{V}_\alpha$ distribution for each phase α.

Step 6. Use the state equations to update the density ρ_α and viscosity μ_α of each flow phase.

Step 7. Use the updated parameter values to solve the heat transport equations in (5) to obtain updated temperature distributions T_α.

Step 8. Check the convergence of the calculation by comparing the temperature distributions calculated in Step 1 and Step 7.

Step 9. Move to the next time step when a convergence criterion is satisfied. Otherwise, return to Step 1 for iteration.

Because of the high nonlinearity of the system, generally, the computational effort is huge and the convergence procedure is slow. The development of more effective numerical methods for oil shale modeling is an important research topic of interest.

Parameter Identification

We have mentioned in the last section that a number of parameters in the in-situ oil shale retorting model need to be determined before the forward problem is solved. Some of them can be measured in the lab, such as the parameters in the state equations, the heat capacities c_α, and the volumes $q_\alpha(t,T)$ of oil and gas generated from a unit of volume of oil shale (a function of time and temperature). The constitutive relationships can also be obtained in the lab but need to be calibrated with the field data.

This section concentrates on the identification of the intrinsic permeability *k* because it cannot be measured directly in the lab scale. It depends on the temperature and time of heating and varies with location even for homogeneous shale structures. In this paper, *k* is identified by solving a coupled inverse problem (Sun and Yeh, 1990) based on the values of state variables measured in the observation wells during the field scale in-situ retorting research.

The initial value of the intrinsic permeability, k_0, can be obtained by well testing and calibrated using the data of head values measured in the dewatering process. The inverse problem may be formulated as:

$$k_0^* = \arg \min_{k_0} \left\{ \left\| \mathbf{h}^{cal}(k_0) - \mathbf{h}^{obs}(k_0) \right\|^2 + \lambda \left\| k_0 - k_0^{pri} \right\|^2 \right\} \quad (11)$$

where k_0^* is the identified permeability, $\mathbf{h}^{cal}$ and $\mathbf{h}^{obs}$ are calculated and observed head values, respectively, λ is the regularization factor, and k_0^{pri} is the permeability estimated by prior information.

During the heating process, the oil and gas start to generate from a time t_0, depending on the heating temperature. After time t_0, the porosity of oil shale increases and that causes the increase of pore connection and the increase of permeability. For a fixed temperature *T*, the permeability can be regarded as a function of time, i.e., $k(t)$. This function can be parameterized by a series of times $t_0 < t_1 < t_2 < \cdots < t_n < t_f$ called the basis points of parameterization (Figure 4). The unknown vector

$$\mathbf{k} = \left[k(t_1), k(t_2), \cdots, k(t_n) \right] \quad (12)$$

then can be identified by solving a coupled inverse problem (Sun and Yeh, 1990). Assume the observed values of pressure, saturation, and temperature of each phase are $\mathbf{P}_\alpha^{obs}$, $\mathbf{S}_\alpha^{obs}$ and $\mathbf{T}_\alpha^{obs}$, respectively. The coupled inverse problem can be formulated as follows:

$$\mathbf{k}^* = \arg \min_{\mathbf{k}} \{ \sum_\alpha [w_{P,\alpha} \left\| \mathbf{P}_\alpha^{cal}(\mathbf{k}) - \mathbf{P}_\alpha^{obs} \right\|^2 + w_{S,\alpha} \left\| \mathbf{S}_\alpha^{cal}(\mathbf{k}) - \mathbf{S}_\alpha^{obs} \right\|^2 + w_{T,\alpha} \left\| \mathbf{T}_\alpha^{cal}(\mathbf{k}) - \mathbf{T}_\alpha^{obs} \right\|^2] \} \quad (13)$$

where the summation is for all phases, and $w_{p,\alpha}, w_{S,\alpha}, w_{T,\alpha}$ are weighting coefficients. This problem can be solved by a numerical optimization algorithm with appropriate constraints (Sun, 1994). The number *n* and locations $\mathbf{v}_n$ of the basis points of parameterization can also be optimized by solving the following extended inverse problem (Sun and Sun, 2002):

$$(\mathbf{k}^*, \mathbf{v}_n^*) = \arg \min_{\mathbf{k}} \min_{\mathbf{v}_n} \{ \sum_\alpha [w_{P,\alpha} \left\| \mathbf{P}_\alpha^{cal}(\mathbf{k}, \mathbf{v}_n) - \mathbf{P}_\alpha^{obs} \right\|^2 + w_{S,\alpha} \left\| \mathbf{S}_\alpha^{cal}(\mathbf{k}, \mathbf{v}_n) - \mathbf{S}_\alpha^{obs} \right\|^2 + w_{T,\alpha} \left\| \mathbf{T}_\alpha^{cal}(\mathbf{k}, \mathbf{v}_n) - \mathbf{T}_\alpha^{obs} \right\|^2] \} \quad (14)$$

Algorithms for solving this kind of combinatorial optimization problem are considered by many researchers as reviewed in Sun (2005). Finding effective algorithms for identifying time dependent permeability is also a very important research topic of interest.

Model Reduction and Parameter Upscaling

Theoretically, an in-situ oil shale model should be a 3-D model involving multiphase flow, deformation, heat transport, and mass transport. To solve the forward and inverse problems for such a complex system is time consuming and the reliability of the model prediction is not guaranteed. Design of an effective observation system for model calibration is also a very challenging problem because the model complexity is difficult to determine. Constructing a more complex model requires more data.

How is a model's complexity determined? Can we find a simple model structure with representative parameters to replace the true system while keeping the model results reliable? Sun (2005) and Sun and Yeh (2006a,b) developed a new methodology for constructing so called objective-oriented models. This methodology could be applied to the oil shale model construction to find a reliable model with minimum cost. In this methodology, the model complexity is determined by the objectives of model application; the model reliability is guaranteed by the use of sufficient data; and the sufficient data are obtained from a robust experimental design.

There are different objectives that can be presented for constructing an oil shale model. The following is a possible statement:

To design a heating system S with minimum cost C=C(S) while the oil production P is maximized.

To solve this problem, a model *M* is used to predict the oil production *P* for a given design *S*, i.e., *P=M(S).* A representative model M^r that can be used to replace *M* should satisfy the following condition:

$$|P[M(S)]-P[M^r(S)]|<\varepsilon \qquad (15)$$

where ε is a given accuracy requirement. The problem of finding a representative model under this condition is called a generalized inverse problem (Sun and Sun, 2002). It can be solved by constructing a series of models, in which the complexity of model structure is increased gradually:

$$M_1^r, M_2^r, \cdots, M_m^r, M_{m+1}^r, \cdots \qquad (16)$$

Effective algorithm for constructing a non-nested model series is developed recently in Sun and Yeh (2006a,b) for groundwater modeling. A structure in (16) can be considered as a global upscaling of a distributed parameter system. We expect that the objective-oriented method can also be used for reducing the structure of an oil shale model under condition (15).

6. Conclusions

Mathematical models are important tools for optimally designing and operating complex systems. This paper presents a preliminary outline for in-situ oil shale retorting modeling. The proposed field scale model is based on the physical process of in-situ oil shale heating technologies reported recently. It consists of a number of coupled and highly nonlinear partial differential equations, including the multi-phase flow equations, movement equations, heat and mass transport equations, and state equations. This model is different from existing groundwater and petroleum models in such a way that the porosity and permeability become unknown functions even for homogeneous shale structure. As a result, solving the inverse problem for identifying these time and location dependent parameters in the field scale becomes the key of successful oil shale modeling.

Major steps of solving both the forward and inverse problems are preliminary described in the paper. Finally, the paper considers the possibility of using the objective-oriented method to find a simplified but reliable oil shale model. A more complicated model may not be more reliable. To develop a useful model for in-situ oil shale retorting, there are several important research topics of interest, including the inverse problem, scaling problem, reliability and model reduction problems introduced in this paper. These problems should be studied at the same time with the field experiments. A realistic oil shale model can be constructed only when sufficient field data become available.

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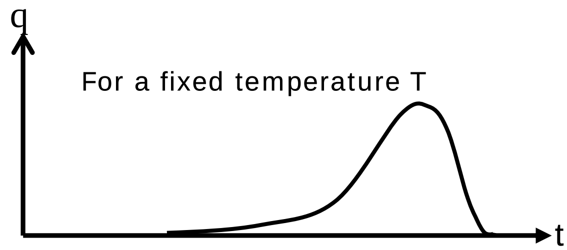

Figure 1. Volume rate of oil production as a function of time

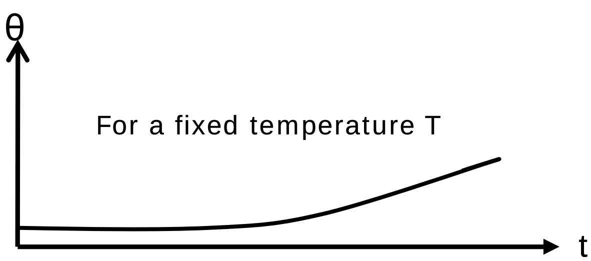

Figure 2. The porosity as a function of time

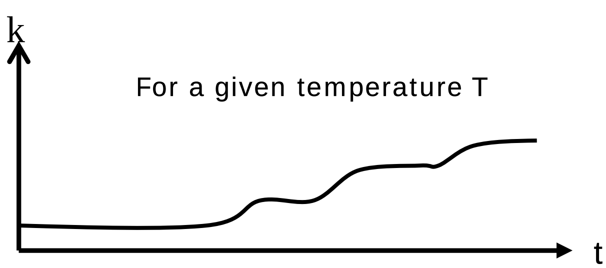

Figure 3. The permeability as a function of time

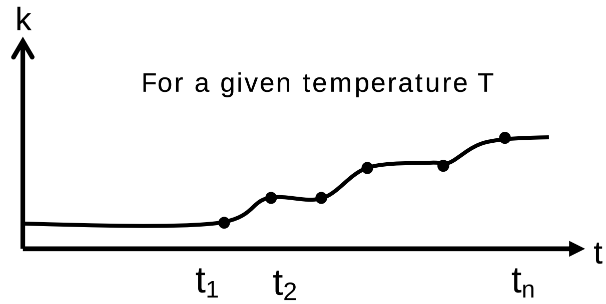

Figure 4. A parameterization method for identifying the permeability.