AN OPTIMAL MODEL AND ITS IDENTIFICATION FOR THE THERMODYNAMICS OF KEROGEN EVOLUTION*

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Abstract In this paper, a mathematical model with respect to the optimal identification of the thermodynamic parameters is established. The identifiability of the dynamics problem is proved and necessary conditions of the optimality are given.

1. Introduction

There are parameters in many evolution equations, such as $a_{10}$, $a_{11}$, $a_{12}$, $a_{20}$, $a_{21}$, $a_{22}$ in the 2-dimensional Volterra model [5], or the birthrate, the natural death rate, the fatality rate, and the lifelong immunity rate in the dynamics of an infectious disease [3,4]. Obviously, these parameters are related to the actual states, e.g., time and space, of the models used. Mathematical models for describing dynamical developing process will not have much practical value or theoretical significance unless these parameters can be determined from the concrete situations. Consequently, identifying these parameters is very important. But not enough work is done in connection with their identification [1]. Using the dynamics equation of the generation of oil and gas, we first establish in this paper a mathematical model for the optimal identification parameters, such as the activated energy and the frequency factor parameters. Then, using the continuity of functionals, we prove the identifiability of this problem. Finally, we prove that the solution of this dynamics equation is weak Gâteaux differentiable and give necessary conditions of the optimality of this optimal identification problem.

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2. Optimal Identification Problem

In the early 1970's, B. P. Tissot gave a mathematical model for the generating process of oil and gas as follows:

\[
\begin{align*}
\text{DES: } & \quad \dot{x}_i(t) = -k_i(t)x_i(t), \quad i = 1, \cdots, 6, \quad t \in I = [0, T_0], \\
& \quad \dot{x}_s(t) = k_\gamma(t)x_\gamma(t), \\
& \quad \dot{x}_g(t) = k_\delta(t) \sum_{i=1}^{6} x_i(t), \\
& \quad \sum_{i=1}^{9} x_i(t) = \sum_{i=1}^{9} x_{0i} = g_0, \\
& \quad x_i(0) = x_{0i}, \quad i = 1, \cdots, 9,
\end{align*}
\]

where \(x_i(t), \ i = 1, \cdots, 6,\) are the contents of the \(i\)-th bonding kerogen at time \(t \in I,\)
\(x_\gamma(t)\) is the content of fluid hydrocarbon (i.e., petroleum) generated by kerogen thermal degradation, and \(x_\delta(t)\) is the natural gas generated by fluid hydrocarbon and \(x_\delta(t)\) is the natural gas generated directly at time \(t.\) So, \(x_\delta(t) + x_\delta(t)\) is the content of the natural gas. Therefore these variables satisfy

\[
0 \leq x_i(t) < 1, \quad i = 1, \cdots, 9, \quad 0 \leq x_\delta(t) + x_\delta(t) < 1, \quad t \in I.
\]

The initial values of these variables satisfy

\[
0 < x_{0i} < 1, \quad i = 1, \cdots, 6, \quad x_{07} = x_{08} = x_{09} = 0, \quad 0 < g_0 < 1.
\]

\(T_0 > 0\) is the finish time of kerogen thermal degradation. Then we have

\[
0 \leq x_i(T_0) < 1, \quad i = 1, \cdots, 6.
\]

\(k_i(t)\) is the degradation rates of the \(i\)-th bonding kerogen and it satisfies

\[
k_i(t) = A_i \exp\left(-E_i/(R \times T(t))\right), \quad i = 1, \cdots, 8,
\]

where the frequency factor \(A_i \in L_a = [10^5, 10^{35}]\) and the activated energy \(E_i \in L_e = [35, 350]\) are undetermined constants, \(R\) is a positive constant and \(T(t)\) is the stratigraphic temperature at time \(t.\) From geology, we know that \(T(t)\) has

**Property 1.** The stratigraphic temperature \(T(t)\) at time \(t\) is a monotone increasing linear function of \(t \in I,\) and \(T(t) > 0, \ t \in I.\)

According to (9), Property 1 and the existence and uniqueness of solution for initial values problem of ordinary differential equations, we know that the solution for \(DES(1) - (5)\) exists and is unique. See [2].