Petroleum generation modeling

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Week 1

According to organic theory of petroleum genesis, oil and gas are the products of living organisms decomposition. Kerogen is a solid insoluble organic matter formed as a result of degradation of living matter biopolymers (diagenesis). Further high pressure and high temperature compaction of sediments (catagenesis) leads to bitumen, oil, and gas generation. Thus, let us consider the following system of chemical equations, which describes the evolution of various organic matter types:

$$\begin{cases} Kerogen \rightarrow a_1 Bitumen + a_2 Oil + a_3 Gas + a_4 Coke \\ Bitumen \rightarrow b_1 Oil + b_2 Gas + b_3 Coke \\ Oil \rightarrow c_1 Gas + c_2 Coke \\ Gas \rightarrow d_1 Coke \end{cases}$$

ere ai, bi, ci, and di – stoichiometric coefficients.

Task for Week 1

1. Using the law of mass action write down the system of kinetic differential equations.
2. Rewrite the system of differential equations in the form $\dot{x} = Ax$, where $\dot{x}$ denotes the derivative in time.
3. How can you describe the matrix A? How can you solve such matrix equation?
4. Find eigenvalues of matrix A. Describe in details the procedure how to find the analytical solution.

Solution

Subtask 1

According to law of mass action, velocity of decomposition reaction equal

$\omega = k \cdot C_{ker}^{n}$, when ω - velocity of the reaction, k - constant of velocity reaction, n - reaction order

It is a decomposition equation, that means the order of the reaction will be equal to 1.

Therefore, velocity of decomposition reaction for every component equal

$$\begin{cases} \omega_1 = -\frac{\partial C_{ker}}{\partial t} = k_{ker} \cdot C_{ker} \\ \omega_2 = -\frac{\partial C_{bit}}{\partial t} = k_{bit} \cdot C_{bit} \\ \omega_3 = -\frac{\partial C_{oil}}{\partial t} = k_{oil} \cdot C_{oil} \\ \omega_4 = -\frac{\partial C_{gas}}{\partial t} = k_{gas} \cdot C_{gas} \\ \omega_5 = -\frac{\partial C_{coke}}{\partial t} = 0 \end{cases}$$

In the next step, we need to find velocity of formation reaction every component

$$\begin{cases} \dot{C}_{ker} = -\omega_1 = -C_{ker} \\ \dot{C}_{bit} = a_1\omega_1 - \omega_2 \\ \dot{C}_{oil} = a_2\omega_1 + b_1\omega_2 - \omega_3 \\ \dot{C}_{gas} = a_3\omega_1 + b_2\omega_2 + c_1\omega_3 - \omega_4 \\ \dot{C}_{coke} = a_4\omega_1 + b_3\omega_2 + c_2\omega_3 + d_1\omega_4 \end{cases}$$

Subtask 2

$$A = \begin{pmatrix} -k_{ker} & 0 & 0 & 0 \\ k_{ker} \cdot a_1 & -k_{bit} & 0 & 0 \\ k_{ker} \cdot a_2 & k_{bit} \cdot b_1 & -k_{oil} & 0 \\ k_{ker} \cdot a_3 & k_{bit} \cdot b_2 & k_{oil} \cdot c_1 & -k_{gas} \\ k_{ker} \cdot a_4 & k_{bit} \cdot b_3 & k_{oil} \cdot c_2 & k_{gas} \cdot d_1 \end{pmatrix}.$$

$$A = \begin{pmatrix} -k_{ker} & 0 & 0 & 0 & 0 \\ k_{ker} \cdot a_1 & -k_{bit} & 0 & 0 & 0 \\ k_{ker} \cdot a_2 & k_{bit} \cdot b_1 & -k_{oil} & 0 & 0 \\ k_{ker} \cdot a_3 & k_{bit} \cdot b_2 & k_{oil} \cdot c_1 & -k_{gas} & 0 \\ k_{ker} \cdot a_4 & k_{bit} \cdot b_3 & k_{oil} \cdot c_2 & k_{gas} \cdot d_1 & 0 \end{pmatrix}.$$

$$\dot{C} = \begin{pmatrix} \dot{C}_{ker} \\ \dot{C}_{bit} \\ \dot{C}_{oil} \\ \dot{C}_{gas} \\ \dot{C}_{cok} \end{pmatrix}.$$

$$C = \begin{pmatrix} C_{ker} \\ C_{bit} \\ C_{oil} \\ C_{gas} \\ C_{cok} \end{pmatrix}.$$

$$\dot{C} = AC$$

Subtask 3

Matrix A is a square matrix of size 5x5. The type of the matrix - triangular. The matrix equation can be solved with the following methods:

- Kramer's method:
- Reverse matrix method:
- Gausse's method.

$$C = A^{-1}\dot{C}$$

Subtask 4

$$det(A - \lambda E) = 0$$

$$\begin{vmatrix} -k_{ker} - \lambda & 0 & 0 & 0 & 0 \\ k_{ker} \cdot a_1 & -k_{bit} - \lambda & 0 & 0 & 0 \\ k_{ker} \cdot a_2 & k_{bit} \cdot b_1 & -k_{oil} - \lambda & 0 & 0 \\ k_{ker} \cdot a_3 & k_{bit} \cdot b_2 & k_{oil} \cdot c_1 & -k_{gas} - \lambda & 0 \\ k_{ker} \cdot a_4 & k_{bit} \cdot b_3 & k_{oil} \cdot c_2 & k_{gas} \cdot d_1 & -\lambda \end{vmatrix} = 0$$

$$(-k_{ker} - \lambda)\begin{vmatrix} -k_{bit} - \lambda & 0 & 0 & 0 \\ k_{bit} \cdot b_1 & -k_{oil} - \lambda & 0 & 0 \\ k_{bit} \cdot b_2 & k_{oil} \cdot c_1 & -k_{gas} - \lambda & 0 \\ k_{bit} \cdot b_3 & k_{oil} \cdot c_2 & k_{gas} \cdot d_1 & -\lambda \end{vmatrix} = 0$$

$$(-k_{ker} - \lambda)(-k_{bit} - \lambda)\begin{vmatrix} -k_{oil} - \lambda & 0 & 0 \\ k_{oil} \cdot c_1 & -k_{gas} - \lambda & 0 \\ k_{oil} \cdot c_2 & k_{gas} \cdot d_1 & -\lambda \end{vmatrix} = 0$$

$$(-k_{ker} - \lambda)(-k_{bit} - \lambda)(-k_{oil} - \lambda)(-k_{gas} - \lambda)(-\lambda) = 0$$

$$\lambda = \begin{pmatrix} -k_{ker} \\ -k_{bit} \\ -k_{oil} \\ -k_{gas} \\ 0 \end{pmatrix}.$$