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Sea water-mineral substance-living matter system

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Abstract

Formation of hydrocarbons in the seawater - mineral substance - living matter system is modeled. Some systems of various living matter compositions and stoichiometry and also at several sets of T,P parameters are simulated. During diagenesis kerogens and hydrocarbons are formed. The equilibrium constant of the reaction between oily kerogen and oxidized one, methane and CO_2 is evaluated: $\Phi_1 C_{292}H_{288}O_{12}$(kerogen, H/C 0.99, O/C 0.041) → $\Phi_2 C_{128}H_{68}O_7$(kerogen, H/C 0.53, O/C 0.055)+xCH_4+yCO_2+zH_2O, where Φ_1 and Φ_2 moles of kerogens; x, y, z – stoichiometry coefficients. In thermodynamically closed system the aqueous natural hydrocarbons are stable up to 300°C (at pressure above water saturated vapor) due to reductive environment formation (lg f $H_2 \approx 10^{-4}$ бар). Equilibrium mineral assemblages of the system include quartz, kaolinite, muscovite, ankerite, siderite, pyrite, $(Ca,Mg)CO_3$, $(Ca,Sr)CO_3$ and paragonite. High salinity Cl-HCO_3-Na aqueous solution also contains CO_2 of tens g/l and ammonium nitrogen.

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Keywords: Simulation, Water-Rock System, Sea Water, Mineral Assemblage, Living Matter, .Hydrocarbons, Hydrogeochemistry

1. Introduction

Our previous results of thermodynamic modeling of hydrocarbons formation in the seawater - mineral substance - living matter system are published in[1,2]. We confirmed Helgeson's opinion[3] on natural hydrocarbons stability in aqueous solutions at least up to 300°C and pressure higher then saturated vapor pressure *but it occurs in reductive environment* (lgf$H_2 \approx 10^{-4}$bar) only. Thermodynamic properties of hydrocarbons and kerogens taken from publications[4-6] have been used. Our modeling system differed from Helgeson's in that it included carbonate and clay substances and standard sea water.

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2. The influence of initial living matter composition and the set of hydrocarbon species adopted for examining its influence on reaction products.

At the beginning three types of living matter composition (seagrass, bacteria and green plant), have been chosen for simulation. They are shown in Table 1. Each type of the living matter produces all groups of natural hydrocarbons but in various proportions. According to the results of our modeling *bacteria (bacterioplankton) produces the hydrocarbon mixture with highest alkane contents.*

Table 1. Chemical elemental composition of living matter[7]

Elements	Seagrass (phytoplankton)	Bacteria (bacterioplankton)	Green plant
C	34.5	54.0	45.4
H	4.1	7.4	5.5
O	47.0	23.0	41.0
N	1.5	9.6	3.0
S	1.2	0.53	0.34

Then the influence of hydrocarbon species set on the modeling results has been also studied. Three sets of hydrocarbons have been adopted and used in stoichiometry matrix: (a) methane, ethane, benzene, toluene; (b) methane, ethane, propane, benzene, toluene, methylbenzene, propylbenzene; (c) eighty hydrocarbons and their derivatives. Simulation of the seawater - mineral substance - living matter system with the adopted stoichiometry of the above sets of hydrocarbons shows weak dependence of the number of hydrocarbons in the set on hydrocarbon production but *insignificant increase of hydrocarbon mass produced but no influence on mineral assemblage and geochemical type of aqueous solution*.

Total hydrocarbon aqueous concentration (C atoms), other aqueous solution properties, amount of kerogens formed from 30 kg of living matter in the seawater - mineral substance - living matter system are shown in fig.1.

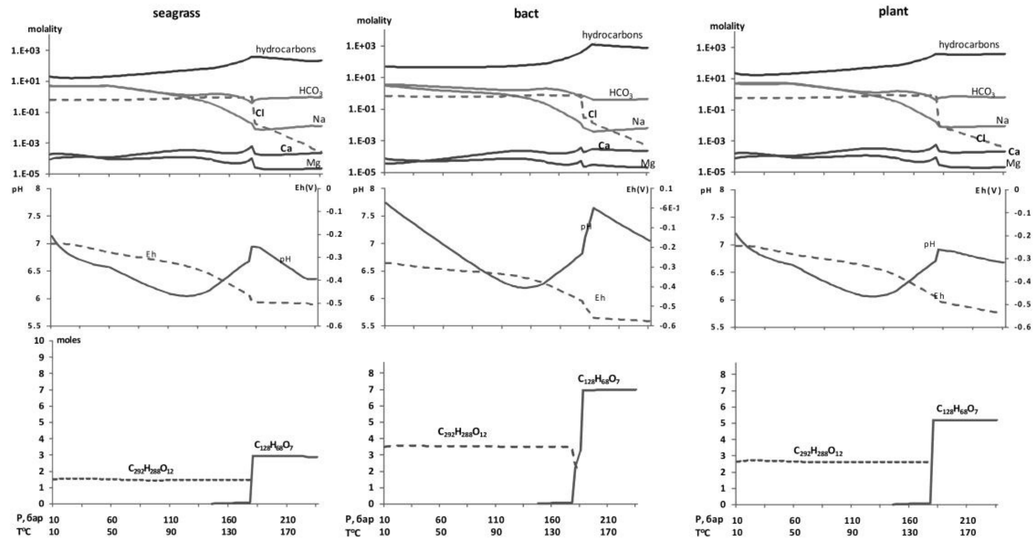

Fig.1. Aqueous hydrocarbon and inorganic species concentrations and amount of kerogens formed from 30 kg of living matter in the seawater - mineral substance - living matter systems

3. The influence of temperature and total pressure on living matter destruction and hydrocarbons formation

Thermodynamically closed seawater - mineral substance - living matter system has been studied at two linear