Oil Shale, 2005, Vol. 22, No. 3
pp. 291-303
ISSN 0208-189X

ATOMISTIC MOLECULAR SIMULATION OF THERMAL VOLUME EXPANSION OF ESTONIAN KUKERSITE KEROGEN

T. KAEVAND[(a)], Ü. LILLE[* (b)]

[(a)] Chair of Information Technology, Estonian Business School
3 Lauteri Str., Tallinn,10114 Estonia

[(b)] Department of Chemistry, Tallinn University of Technology
15 Akadeemia Rd., Tallinn, 12618 Estonia

Thermal volume expansion of Estonian kukersite kerogen was simulated with the aim to predict the response of kerogen to thermal stress in laboratory and geological conditions. The simulation was performed using a general amber force field evaluated by the calculation of non-polar cohesive energy density based on atomic interactions and value of corresponding solubility parameter. At constant pressure in the range 1–1,000 bars the specific volume vs. temperature plots were registered, and two linear regions at 150–525 and 550–900 K (at the pressure one bar) were identified. In the gap between these regions a changeover point, termed as apparent second-order polymer-like phase transition from the glassy to the rubbery state, is located. At higher pressures the changeover shifts to higher temperatures. Its possible meaning in kerogen transformations at retorting and geological conditions is discussed. A further experimental study of the observed phenomenon is needed.

[*] Corresponding author: e-mail address *lille@chemnet.ee*