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Short Communication

Characterization of wax using potential energy and nanocalculation

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ABSTRACT

Most reservoir fluids contain heavy paraffinic compounds that may precipitate as a solid or solid like material called wax if the fluid is cooled down. Wax precipitation is a phenomenon of considerable importance in oil industry. An increase in aggregation results in enhanced oil viscosity. This however causes significant negative effects on production, transportation and processing of crude oil. So, structural characterization of wax is considered to be important topic. In this work, normal paraffin molecules C_{20}, C_{21}, C_{23}, C_{24}, C_{25}, C_{27}, and C_{29} have been considered as representatives of wax molecule. Intermolecular forces have been calculated using quantum mechanics and statistical analysis. Second virial coefficients have been obtained for these molecules by applying intermolecular potential energy. Finally SRK and PR equation of states parameters have been achieved to have molecular consideration of wax structure.

Keywords: *Wax; Intermolecular force; Second virial coefficient; SRK; PR.*

INTRODUCTION

Precipitation of the heavy deposit in the course of petroleum production is a costly process and hampers production activities in many part of the word. So it is vital to have deep understanding of these molecules [1-4]. The equation of state and the transport properties of matters are intimately related to the force between the molecules. The statistical mechanical theories which relate the bulk properties to the intermolecular forces are highly developed for dilute gases and developed to a lesser extent for dense gases and liquids. In this study it is attempted to consider intermolecular potential energy between wax molecules and finally relate it to SRK and PR equation of state parameters to have molecular understanding of wax structure for further studies [5].

One of the bio-sensing mechanisms is mechanical. Than measuring shift in resonance frequency, we adopt to measure the change in spring constant due to adsorption, as one of the fundamental sensing mechanism. This study entails determination of spring constant of a surface functionalized micro machined micro cantilever, which resonates in a trapezoidal cavity-on Silicon <100> wafer [4][5][6], with the resonating frequency of 7000 cycles per second. This thin-flimsy-oxide micro-cantilever has a typical shape, and the tip of the micro-cantilever is dip-coated with chemically and biologically active material.
The change in mass, due to adsorption, is detected by measuring the change in spring constant. The Force-Distance spectroscopy is used to detect the change in spring constant.

EXPERIMENTAL

In this study normal paraffin molecules C_{20}, C_{21}, C_{23}, C_{24}, C_{25}, C_{27} and C_{29} have been considered as wax molecule. Intermolecular potential energy has been calculated by using statistical thermodynamics and quantum mechanics as: E(C_{20}-C_{20})-EC_{20}-EC_{20}.

Intermolecular potential energies Versace distance has been drawn for these molecules. By assuming Lennard-Jonse as potential model its constants parameters (ε, σ) have been obtained [6].

$$u(r) = 4\varepsilon\left\{\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right\} \qquad (1)$$

At $r = \sigma$ the potential energy is zero, and therefore σ is the distance of closest approach of two molecules, which collide with zero relative kinetic energy. The parameter ε is the maximum energy of attraction of two molecules, which occurs at a separation of $r = 2^{\frac{1}{6}}\sigma$ [7].

By applying these parameters, second virial coefficients have been calculated by integrate mentioned bellow [8]:

$$B_2(T) = -2\pi\int_0^{\infty}\left[e^{-\frac{u(r)}{kT}} - 1\right]r^2 dr \qquad (2)$$

SRK and PR equation of states parameters have been calculated using mentioned relations [9].

$$\left(P + \frac{a}{v(v+b)}\right)(v-b) = RT \qquad (3)$$

$$\frac{Pv}{RT} = \frac{1}{1-\frac{b}{v}} - \frac{a}{RT(v+b)} \qquad (4)$$

$$\frac{Pv}{RT} = 1 + \frac{b}{v} + \frac{b}{v^2} + \ldots - \frac{a}{RT(v+b)} = 1 + \frac{b}{v} + \frac{b}{v^2} + \ldots - f(v) \qquad (5)$$

$$f(v) = f\left(\frac{1}{x}\right) = \frac{a}{RT\left(\frac{1}{x}+b\right)} \qquad (6)$$

$$f(x) = \left(\sum_{n=0}\frac{1}{n!}x^n\frac{\partial^n f}{\partial x^n}\right)_{x=0} \qquad (7)$$

$$\frac{Pv}{RT} = 1 + \frac{b}{v} + \frac{b}{v^2} - \frac{a}{RTv} + \ldots = 1 + \frac{1}{v}\left(b - \frac{a}{RT}\right) + \ldots = 1 + \frac{B_2}{v} + \ldots \qquad (8)$$

$$B_2 = b - \frac{a}{RT} \qquad (9)$$

$$b = \frac{16N}{3}\pi\sigma^3 \qquad (10)$$

$$\left(P + \frac{a}{v(v+b)+b^*(v-b)}\right)(v-b) = RT \qquad (11)$$

$$\frac{Pv}{RT} = \frac{1}{1-\frac{b}{v}} - \frac{a}{RT}\left(\frac{1}{(v+b)+b(1-\frac{b}{v})}\right) = 1 + \frac{b}{v} + \ldots - \frac{a}{RT}\left(\frac{1}{(v+b)+b\left(1-\frac{b}{v}\right)}\right) \qquad (12)$$

$$f(v) = f\left(\frac{1}{x}\right) = -\frac{a}{RT}\left(\frac{1}{\left(\frac{1}{x}+b\right)+b(1-bx)}\right) \qquad (13)$$

$$\frac{Pv}{RT} = 1 + \frac{b}{v} + \ldots - \frac{a}{RTv} = 1 + \frac{1}{v}\left(b - \frac{a}{RT}\right) + \ldots = 1 + \frac{B_2}{v} + \ldots \qquad (14)$$

$$B_2 = b - \frac{a}{RT} \qquad (15)$$

$$b = \frac{16N}{3}\pi\sigma^3 \qquad (16)$$

RESULTS AND DISCUSSION

ε parameter has been calculated for these molecules as shown in Table. 1. This parameter increases by increasing the chain length of hydrocarbon.

Table 1. ε parameter for C_{20}, C_{21}, C_{23}, C_{24}, C_{25}, C_{27}, C_{29}

ε (Hartree)* 10^4						
C_{20}	C_{21}	C_{23}	C_{24}	C_{25}	C_{27}	C_{29}
6.57	6.91	7.58	7.91	8.24	8.91	9.59

Intermolecular potential energy verses distance has been drawn for these molecules as shown in Figures (1-7). σ parameter has been obtained 5.18 ºA with a good approximation for all these molecules [10].

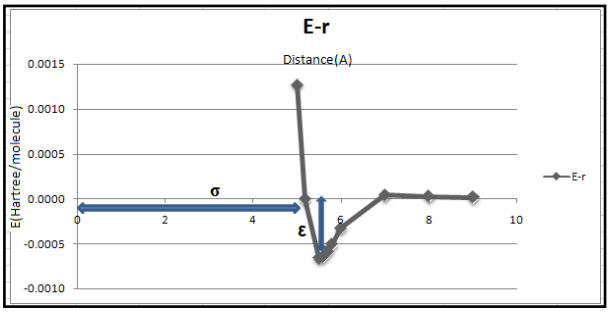

Fig. 1. Intermolecular potential energy Versace distance for normal paraffin c_{20}

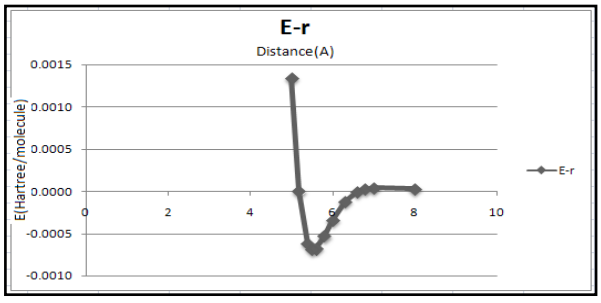

Fig. 2. Intermolecular potential energy Versace distance for normal paraffin c_{21}

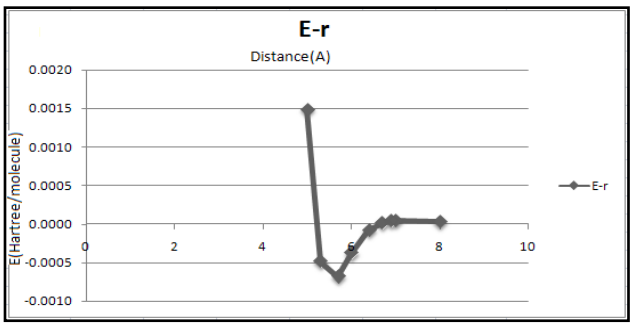

Fig. 3. Intermolecular potential energy Versace distance for normal paraffin c_{23}

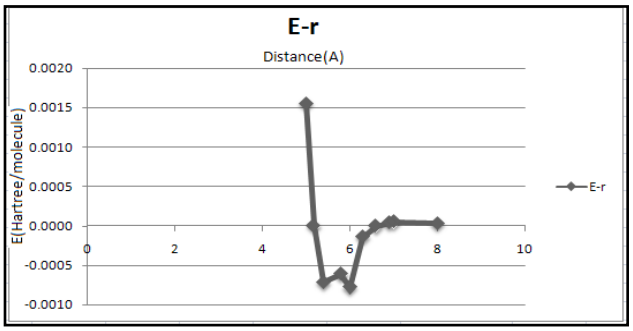

Fig. 4. Intermolecular potential energy Versace distance for normal paraffin c_{24}

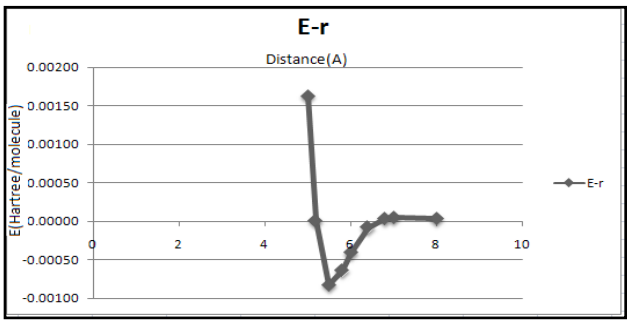

Fig. 5. Intermolecular potential energy Versace distance for normal paraffin c_{25}

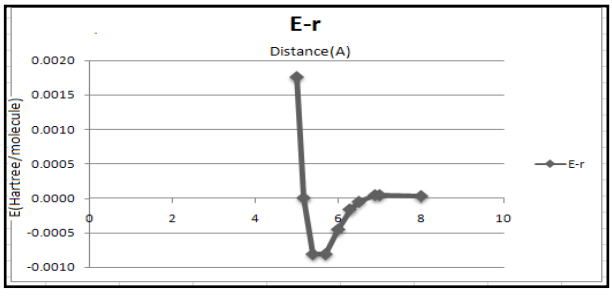

Fig. 6. Intermolecular potential energy Versace distance for normal paraffin c_{27}

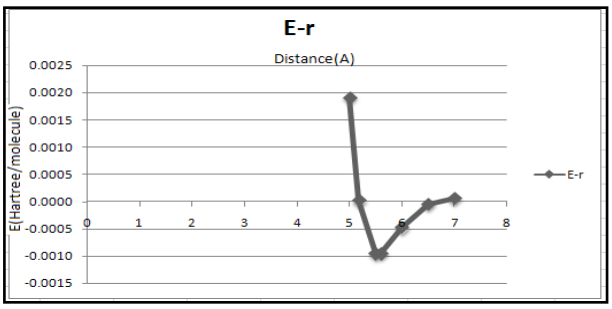

Fig. 7. Intermolecular potential energy Versace distance for normal paraffin c_{29}

Table 2. Second virial coefficient for C_{20}, C_{21}, C_{23}, C_{24}, C_{25}, C_{27}, C_{29}

	C_{20}	C_{21}	C_{23}	C_{24}	C_{25}	C_{27}	C_{29}
$B_2(\frac{cm^3}{mole})$	-226.3	-249.3	-296.7	-321.4	-344.1	-397.7	-451.8

Second virial coefficient is a function of temperature. For 300K following amounts have been achieved, as shown in Table 2.

As it is shown in Figure 8, Second virial coefficient has decreasing trend by increasing temperature. These results were fitted using an exponential model ($B_2(T)=c\ e^{dT}$) with the values: c= -1485.87 and d= -0.00628 for C_{20}. C and d constants were also obtained for other molecules.

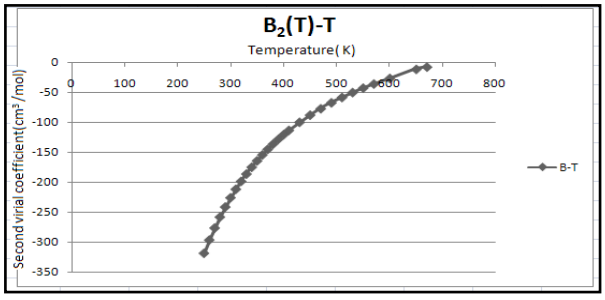

Fig. 8. Second virial coefficient of C_{20} Versace temperature

CONCLUSION

Quantum mechanics and statistical thermodynamics have been used to obtain intermolecular potential energy and its graphs have been drawn. Lennard-Jonse parameters have been obtained. Second virial coefficients have been calculated. Base on Figure 8, second virial coefficient decreases by increasing temperature. Finally SRK and PR equation of states parameters have been calculated based on Lennard-Jonse parameters for further studies.

Symbols

$E(C_{20}\text{-}C_{20})$: potential energy of C_{20}-C_{20}
$E(C_{20})$: potential energy of C_{20}
ε: maximum energy of attraction between a pair of molecules
σ: collision diameter
B_2: second virial coefficient
a: van der Waals´ equation constant
b: van der Waals´ equation constant
R: gas universal constant

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