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Statistical estimation of the boiling point of some pure fluids through the Arrhenius viscosity parameters

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Knowledge and estimation of transport properties of fluids are necessary for mass flow and heat transfer. Viscosity is one of the main properties which are sensitive to temperature and pressure variation. In the present work, based on the use of statistical techniques for regression analysis and correlation tests, we propose an original equation modeling the relationship between the two parameters of viscosity Arrhenius-type equation

$$\boldsymbol{ln\eta = lnAs + \frac{Ea}{RT}}$$

Empirical validation using 76 data set of pure fluids provided from the literature and studied at different temperature ranges gives excellent statistical results which allow us to redefine the Arrhenius-type equation using a single parameter instead of two ones.

$$E_a = \lambda \cdot R \times (-lnA_s)^{\alpha_0}$$

More, causal correlation between these parameters and the normal boiling temperature (Tb) of the corresponding fluids leads us to propose two predictive empirical equations one with the activation energy,

$$T_b(E_a) = -\frac{E_a}{68 - 4.05 \times Ea^{0.34}}$$

and one with the logarithm of pre-exponential factor,

$$T_b(lnA_s) = \frac{(-lnA_s)^{2.933}}{8.2 + lnA_s}$$

We conclude that the boiling point is in causal correlation with the two Arrhenius parameters, but with other physical and chemical properties implicitly for which there are some ones are common for the two Arrhenius parameters while others are in relationship only for a single parameter (*lnAs*) or (*Ea*). To reform this observation, we will try to propose in future works, an expression both explicit, the two viscosity Arrhenius parameters Tb(*Ea*,ln*As*) alternatively in the numerator and in the denominator. Note that this equation is tested to some heavy oils with reliable agreement for which we can conclude that it can be useful for petroleum chemistry.

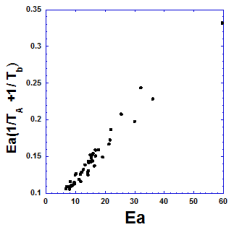

Figure 1 : Correlation between the product Ea.($1/T_A + 1/T_b$) and the Arrhenius activation energy Ea / (kJ•mol^{-1}) for some pure solvents

Biography

Noureddine Ouerfelli has a PhD and Habilitation in Chemistry; he is a head of research project in the Laboratory of Biophysics and Medical Technologies. Published papers are more than 60 in reputed journals on modeling of physicochemical properties in solution.

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