

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

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### INTRODUCTION

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 (Eq. 1). Empirical validation using 90 data set of 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 (Eq. 2). More, causal correlation between these parameters and the normal boiling temperature ( $T_b$ ) of the corresponding fluids leads us to propose two predictive empirical equations one with the activation energy (Eq. 3) and one with the logarithm of pre-exponential factor (Eq. 4). We conclude that the boiling temperature 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 ( $\ln A_s$ ) or ( $E_a$ ). To correct this observation, we will try to suggest in future works, an expression both explicit, the two viscosity Arrhenius parameters  $T_b(E_a, \ln A_s)$  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.

**Key words** Pure liquid · Arrhenius activation energy · Boiling temperature · Arrhenius temperature · Solvents · Correlation

#### Arrhenius-Type Equation

$$\eta = A_s \cdot \exp\left(\frac{E_a}{RT}\right) \quad (1) \quad \ln \eta = \ln A_s + \frac{E_a}{RT} \quad T_b(E_a) = -\frac{E_a}{68 - 4.05 \times E_a^{0.34}} \quad (3)$$

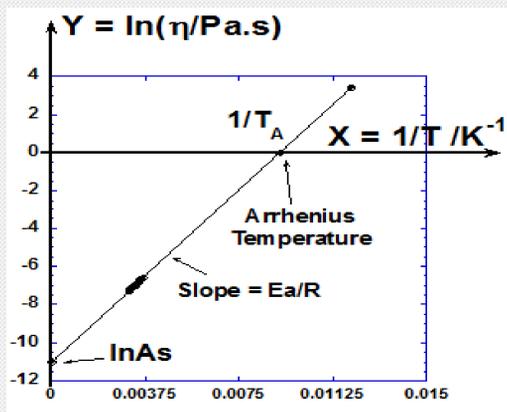


Figure 1 : This plot shows how to determine graphically ( $E_a/R$ ), ( $\ln A_s$ ) and ( $T_A$ ). We have proceeded by extrapolation to reach these two parameters...

$$T_b(\ln A_s) = \frac{(-\ln A_s)^{2.933}}{8.2 + \ln A_s} \quad (4)$$

#### Mutual correlations between Arrhenius parameters and Hajkacem-Ouerfelli equations

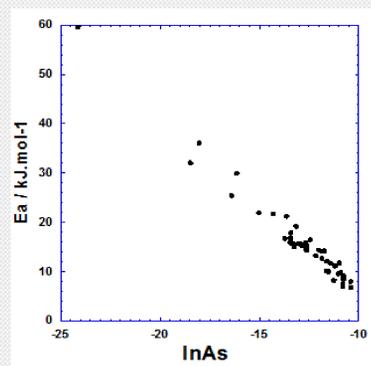


Figure 2 : Correlation between the Arrhenius activation energy  $E_a$  / ( $\text{kJ}\cdot\text{mol}^{-1}$ ), and the logarithm of the entropic factor of Arrhenius  $-\ln(A_s/Pa\cdot s)$  / ( $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ ) for some pure solvents.

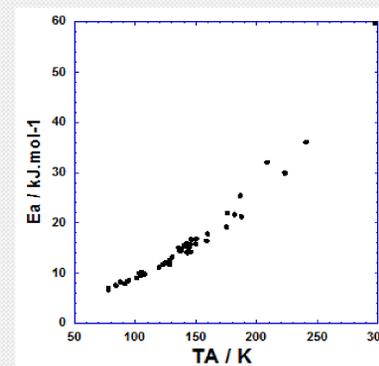


Figure 3 : Correlation between the Arrhenius activation energy  $E_a$  / ( $\text{kJ}\cdot\text{mol}^{-1}$ ), and the Arrhenius temperature  $T_A$  / (K) for some pure solvents.

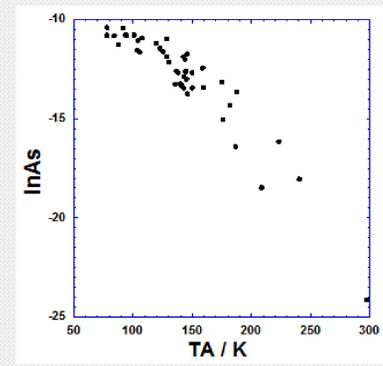


Figure 4 : Correlation between the logarithm of the entropic factor of Arrhenius  $-\ln(A_s/Pa\cdot s)$  / ( $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ ) and the Arrhenius temperature  $T_A$  / (K) for some pure solvents.

$$(2) \quad E_a = \lambda \cdot R \times (-\ln A_s)^{\alpha_0}$$

$$\ln(E_a/R) = \alpha_1 + \alpha_2 \cdot \ln T_A$$

$$\ln A_s = \left(\frac{\alpha}{T_A - \beta}\right)$$

#### Correlation between Arrhenius parameters and boiling temperature

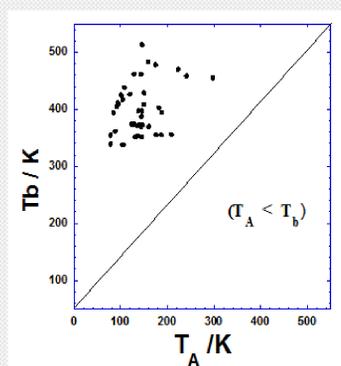


Figure 5 : Correlation between the boiling point  $T_b$  / (K), and the Arrhenius temperature  $T_A$  / (K) for some pure solvents.

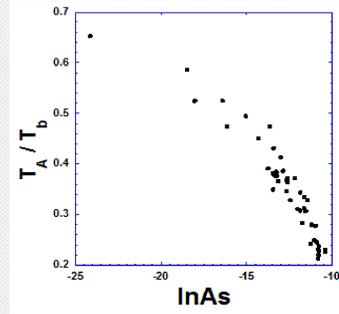


Figure 6 : Correlation between the ratio Arrhenius temperature / boiling point  $T_A/T_b$  and the logarithm of the entropic factor of Arrhenius  $-\ln(A_s/Pa\cdot s)$  / ( $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ ) for some pure solvents

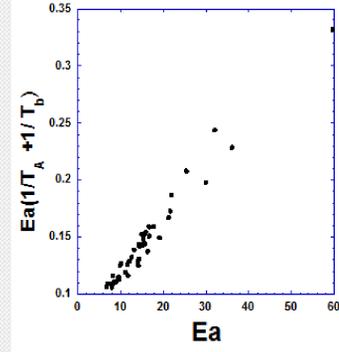


Figure 7 : Correlation between the quantity  $E_a(1/T_A + 1/T_b)$  and the Arrhenius activation energy  $E_a$  / ( $\text{kJ}\cdot\text{mol}^{-1}$ ), for some pure solvents.

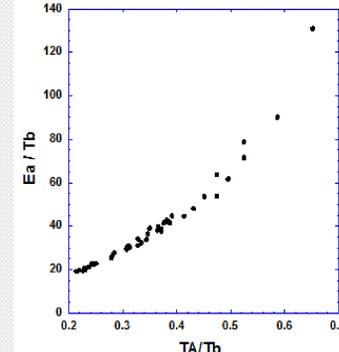


Figure 8 : Correlation between the ratios and Arrhenius activation energy-boiling point ( $E_a/T_b$ ) and the Arrhenius temperature-boiling point ( $T_A/T_b$ ) for some pure solvents.

#### Prediction of boiling point via viscosity Arrhenius parameters

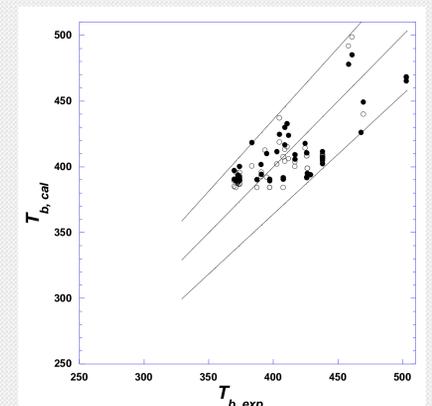


Figure 9 : Correlation between the experimental boiling temperature  $T_{b,exp}$  / K and the calculated boiling temperature ( $T_{b,cal}$ ) / K for some pure liquids studied at previous work [1]; (●): from Eq. 3 and (○): from Eq. 4). (—) around the first bisector ( $Y = +X$  and  $Y = (1 \pm 9\%) \times X$ ) in the present axis system.

### Conclusion

Correlation between Arrhenius parameters reveals interesting Arrhenius temperature which is closely related to the vaporization temperature in the liquid vapor equilibrium and the limiting corresponding partial molar properties can permit us to estimate the boiling points of the pure components. In conclusion, we can ascertain that with more mathematical handlings, we will be able to reveal some physical significances of the viscosity Arrhenius parameters and it definitely develops as well as improves the thermodynamic theories and also to predict some information on liquid-vapor diagram through the study of the viscosity versus temperature and molar fraction only in the liquid phase of binary mixture.

We can add that an additional study on the eventual relationship between the Arrhenius temperature and the properties of great number binary mixtures can prove how the method predicts the properties of other non treated fluid mixtures.

We conclude that the boiling point is in causal correlation with the two viscosity Arrhenius parameters, but also implicitly in correlation with other chemical and physical properties for which there are some ones are common for the two Arrhenius parameters while others are in relationship only for only a single parameter ( $E_a$ ) or ( $\ln A_s$ ).