

## Density and Temperature Dependencies of Liquid Surface Tension

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*Dedicated to late professor Mohammad-Nabi Sarboluki*

**ABSTRACT:** In this paper the density and temperature dependencies of surface tension are investigated. Using the Lennard-Jones (12,6), as an effective pair interaction potential, a linear expression is derived for isotherms of  $\gamma/\rho^2$  versus  $\rho^2$  for some normal and ChloroFluoroCarbons (CFCs) fluids, where  $\gamma$  is surface tension and  $\rho = 1/v$  is molar density. The linearity behavior of the derived equation is well fitted onto the experimental data of surface tension for monatomic, diatomic, nonpolar, polar, hydrogen-bonded and chlorofluorocarbons. In addition, the temperature dependence of surface tension for 20 different fluids is examined, in which the contributions of both terms of the average effective pair potential to the  $\gamma$  are determined. For all liquids investigated in this work, surface tension increases with density except for water. The surface tension of water for isotherms within 280-300 K decreases with density, whereas increases within the range of 310-320 K.

**KEY WORDS:** Equation of State (EOS), Linear Isotherm Regularity (LIR), Surface tension, Effective pair potential

### INTRODUCTION

The surface tension ( $\gamma$ ) and density ( $\rho$ ) of a liquid are important thermodynamic properties in phenomena such as liquid-liquid extraction, gas absorption, distillation and crystallization, also has been widely used to characterize surface of liquid in chemistry and chemical engineering areas such as the manufacturing of plastics, coatings, textiles and films. Values of gas-liquid interfacial tension are used in studying of liquid-liquid and liquid-solid interfaces. They are also useful for understanding and interpreting the nature of interactions between unlike molecules in a mixture, control the growth of a material on a substrate as well as different phenomena, such as melting, coalescence, evaporation, phase transition, growth of nanoparticles etc. Surface tension is

the physical property of liquids in which exposed surface tendency to contract to the smallest possible area. A liquid that molecules are strongly attracted to each other tends to have higher surface tension and molecular density. Surface tension in dense systems has not been extensively studied. The available experimental data for density and surface tension at some subcritical temperatures are available for some ionic and normal fluids [1]. Surface tension is defined as the ratio of energy needed to bring a molecule from the bulk to surface of a liquid to the increase of the liquid surface area, which is represented by surface free energy per unit surface area in thermodynamics [2]. Although there is a significant source of data for the surface tension for pure

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components, it is difficult to find data for the surface tension of binary systems due to the various composition and temperature ranges of liquid mixtures and the extensive amount of time needed for obtaining such data by measurement using experimental devices [3]. The surface tension of binary systems has been predicted by using a corresponding states model proposed by *Rolo et al.* [4], which is based on only pure component properties such as critical molar volumes, critical temperatures and the acentric factors. *Kahl, Wadewitz & Winkelmann* estimated the surface tension of some binary mixtures using a cubic polynomial regression in terms of mole fraction [5]. *Ramirez-Verduzco et al.* predicted the surface tension of binary systems as a function of concentration and temperature, which relates the surface concentration of each component to the individual activity coefficient and to the molar surface area of each component [6].

Critically reviewed surface tension of pure liquids, ranging from the melting point to critical temperature, is available for a great number of substances [7,8]. The methods for calculating the surface tension of liquid mixtures can be divided into two categories [9]: those based on empirical relations and others are derived from thermodynamics. The former comprises the method of *Macleod-Sugden* and principle of corresponding states. In the latter case there are a variety of equations, such as the *Butler* equation [10], expressions based on gradient theory [11], perturbation theory [12] and the *Kirkwood-Buff* radial distribution function theory [13,14]. Among the thermodynamics-based equations, the *Butler* type equation is widely accepted by engineers and has been extensively developed in different forms such as *Eberhart* equation [15], the *Sprow-Prausnitz* equation [16] and the *Wang-Fu* equation [17]. Those equations based on the gradient theory, perturbation theory, and the *Kirkwood-Buff* theory have not been widely used in practice as a consequence of their complexity and limited accuracy, however.

Measurements of this thermodynamic property are valuable for investigation and interpretation of properties of colloidal systems, interfacial monolayers, and many others. Since intermolecular attraction is the agency underlying interfacial phenomena, the temperature would be expected to have a marked influence on the interfacial tension [18].

Due to recent technological advances there are increased applications for the liquid alkali metals. An accurate knowledge of the physical properties of these fluids is vital in many applications. One such property, surface tension, is a fundamental and most important quantity in theory and practice of material processing (crystal growth, soldering, brazing and sintering) [19]. The surface tension of ionic liquids has been the subject of a relatively small number of studies [19-29].

A general regularity has been applied for dense fluids, both compressed liquids and dense supercritical fluids, namely that  $(Z-1)v^2$  varies linearly with respect to  $\rho^2$  for each isotherm, where  $Z = P/\rho RT$  is the compression factor and  $\rho = 1/v$  is the molar density. The regularity was originally tested with experimental data for 13 fluids (Ar, N<sub>2</sub>, O<sub>2</sub>, CO, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>6</sub>H<sub>6</sub>, CH<sub>3</sub>OH, NH<sub>3</sub>, H<sub>2</sub>). It was shown to be compatible with an equation of state based on statistical-mechanical theory, although the latter do not predict as great a range of linearity as was suggested by experiment. The regularity holds experimentally for densities greater than the *Boyle* density ( $\rho_B \approx 1.8\rho_C$ ) and for temperatures below about twice the *Boyle* temperature ( $T_B \approx 2.5-2.7T_C$ ), where  $\rho_C$  and  $T_C$  are critical density and temperature, respectively [30].

The ratio of surface area to volume of any system changes substantially with size. The same is true for energy and other properties. As a result the interfacial region is always different from the bulk region. Interfacial effects, resulting from the existence of surface, can frequently be neglected for large bulky systems while in finally divided systems their properties depend practically only on the interfacial regions properties. When we consider properties of individual atoms or molecules, knowing their atomic or molecular constants, we know that they do not allow directly describe the bulk properties build from the mentioned elements. Each bulk phase has, however, a characteristic material constants, only when the bond lengths between atoms and molecules are very small in comparison with their distance from the interface. The lengths are usually very small in comparison with their distance from the interface. The interfacial material constant (imc) becomes essential when this condition is not fulfilled. In reference [31]

nanometrically dispersed systems and their properties which depend on the imc values are discussed.

The aim of this work is to obtain analytical expression for the surface tension of subcritical fluids as a function of density. To do such task, we have introduced a simple model to calculate both changes in energy and surface area by transferring a molecule from bulk to surface. Owing to the fact that the measurement of surface tension can be done only when liquid is in equilibrium with its vapor, i.e. there is only one measurement for each isotherm, one is not able to evaluate the derived expression, directly, by using experimental data. However, the experimental data for liquid viscosity are used for the indirect evaluation. Also, we have used the derived expression to predict the contributions of both terms of the effective pair potential to the surface tension of a liquid.

#### LINEAR ISOTHERM REGULARITY (LIR)

Using the Lennard-Jones (12,6) potential as the effective near neighbor pair potential, in which the medium and longer range interactions are included, the Linear Isothermal Regularity (LIR) was derived from the exact thermodynamic relations as [30].

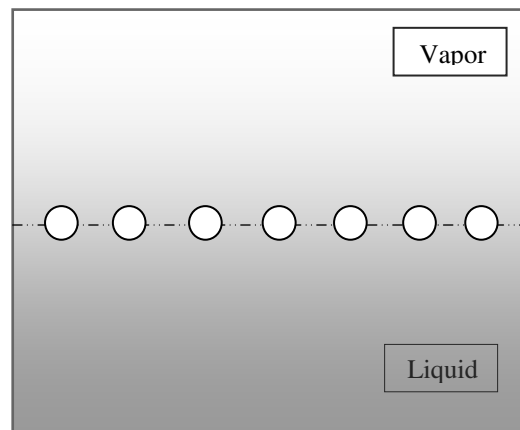
$$(Z-1)v^2 = A + B\rho^2 \quad (1)$$

where  $A$  and  $B$  are the temperature dependent parameters. It was experimentally found that the regularity holds for all types of dense fluids, including nonpolar, polar, hydrogen bonded, and quantum fluids, for densities greater than the Boyle density ( $\rho_B \approx 1.8\rho_C$ , where  $\rho_C$  is the critical density) and temperatures less than twice the Boyle temperature, the temperature at which the second virial coefficient is zero. On the basis of a simple model, the temperature dependencies of the LIR parameters are found to be [30]:

$$A = A_2 - \frac{A_1}{RT} \quad (2)$$

$$B = \frac{B_1}{RT} \quad (3)$$

where  $A_1$  and  $B_1$  are related to the attraction and repulsion terms of the average effective pair potential and  $A_2$  is related to the nonideal thermal pressure.



*Fig. 1: Simple hypothetical model for a two-phase system. The liquid surface is shown by the dashed line. One half of each surface molecule is assumed to be in liquid phase and the remaining in the vapor phase.*

#### DRIVING AN ANALYTICAL EXPRESSION FOR SURFACE TENSION USING A SIMPLE MODEL

We simply imagine that the liquid surface as a flat surface, macroscopically, and one-half of each spherical surface molecule is within the bulk and its other half in the vapor phase as shown in Fig. 1. It is shown that the interaction potential energy of a fluid can be presented in terms of a simple effective pair potential (originally called the average effective pair potential) which is the interaction energy of a given pair, to which the medium effect and long range interactions are added [32]. Such an effective pair potential was used to derive a regularity for many kind of dense normal fluids, known as Linear Isotherm Regularity (LIR) [30]. We shall use the concept of effective pair potential, along with the simple model shown in Fig. 1, to derive an analytical expression for the surface tension.

Considering a general form of Lennard-Jones ( $n, m$ ) potential function as the effective pair potential:

$$u(r) = \frac{C_n}{\bar{r}^n} - \frac{C_m}{\bar{r}^m} \quad (4)$$

where  $\bar{r}$  is the average nearest neighbor molecular separation in the fluid.

According to definition, surface tension ( $\gamma$ ) is the ratio of energy change to surface change:

$$\gamma = \frac{du(r)}{d\sigma} \quad (5)$$

Based on the model, the number of neighboring molecules for a surface molecule is one half of that for a molecule in the bulk (ignoring its insignificant interactions with gaseous molecules). Therefore, when a molecule within the liquid bulk is transferred to the surface, its potential energy will change from  $Zu(r)$  to  $Zu(r)/2$ , where  $Z$  is the number of neighboring molecules for a molecule in the bulk. Such transferring will increase the liquid surface by  $\frac{1}{2}(4\pi\sigma^2) = 2\pi\sigma^2$ , where  $\sigma$  is molecular diameter. Hence, surface tension may be given as:

$$\gamma = \frac{\left(\frac{Z}{2} - Z\right)u(r)}{2\pi\sigma^2} = -\frac{Zu(r)}{4\pi\sigma^2} \quad (6)$$

Substitution of  $u(r)$  from Eq. (4) in Eq. (6) resulted in:

$$\gamma = -\frac{Z\left[\frac{C_n}{\bar{r}^n} + \frac{C_m}{\bar{r}^m}\right]}{4\pi\sigma^2} \quad (7)$$

or

$$\gamma = \frac{\frac{k_n}{\bar{r}^n} + \frac{k_m}{\bar{r}^m}}{4\pi\sigma^2} = \frac{k_n\rho^{\frac{n}{3}} + k_m\rho^{\frac{m}{3}}}{4\pi\sigma^2} \quad (8)$$

(Note that  $\bar{r}\propto\rho^{-\frac{1}{3}}$ , where  $\rho$  is the fluid density)

The surface tension may then be simply expressed as:

$$\frac{\gamma}{\rho^2} = C\rho^{\frac{n-6}{3}} + D\rho^{\frac{m-6}{3}} \quad (9)$$

Since it is shown that the effective pair interaction potential can be satisfactory presented by a LJ (12,6) [30], we may take  $n=12$  and  $m=6$  to find the density dependence of  $\gamma$  as,

$$\frac{\gamma}{\rho^2} = C\rho^2 + D \quad (10)$$

where the parameters  $C$  and  $D$  are obviously related to the repulsive ( $k_n$ ) and attractive ( $k_m$ ) parameters of effective pair potential, respectively.

### Experimental Test

To examine the accuracy of Eq. (10) we need the value of surface tension ( $\gamma$ ) for different densities of

an isotherm. However, experimentally, its value is available only at the liquid-vapor equilibrium at each temperature. We may use *Marshall* equation, in which surface tension is expressed in terms of fluid viscosity as [33],

$$\gamma^{-\frac{1}{4}} = \gamma_0 + \frac{\gamma-1}{\eta} \quad (11)$$

Based on Marshall equation, we may use experimental data of  $\gamma$  and viscosity ( $\eta$ ) of liquid for different temperatures to plot  $\gamma^{-1/4}$  against reverse of viscosity ( $1/\eta$ ) to obtain  $\gamma_0$  and  $\gamma_1$  parameters for the liquid. We have used the data given in reference 34 to plot Fig. 2 for water, xenon and propane. The values of intercept ( $\gamma_0$ ) and slope ( $\gamma_1$ ) for each fluid are given in Table 1. Similar results obtained for 17 other liquids are summarized in this table, along with their coefficient of determination ( $R^2$ ).

By having  $\gamma$  at any desire temperature for a liquid, we may use its experimental PVT data [34] to plot  $\gamma/\rho^2$  versus  $\rho^2$  for that isotherm, to investigate the validity of Eq. (10). The results of such investigation are shown for one isotherm of water, xenon and propane in Fig. 3. As shown in this figure, the coefficient of determination is larger or equal to 0.999 for each liquid. Similar investigation is carried out for 17 other liquids, for which the results are summarized in Table 2.

### Temperature dependencies of parameters of equation (10)

Unlike the parameters of the isolated pair interaction potential, it is well known that the parameters of effective pair potential depend on temperature [35]. In the case of effective LJ (12,6) used to derive LIR, it is shown that the density dependencies of the parameters are negligible for densities greater than Boyle density for which the LIR is valid. However, the parameter  $\sigma$ , the separation at which the potential is zero, increases with  $T$  while the depth of the potential well decreases [32]. For this reason we may expect that the parameters of  $C$  and  $D$  of Eq. (10) are temperature dependent. To examine such expectation, we have plotted  $\gamma/\rho^2$  versus  $\rho^2$  for a few isotherms of nitrogen and water, which are shown in Fig. 4. Similar investigation are carried out for some isotherms of some other liquids, for which value of the parameters are presented in Table 3. In accordance with our prediction, the parameters of Eq. (10) are temperature dependent.

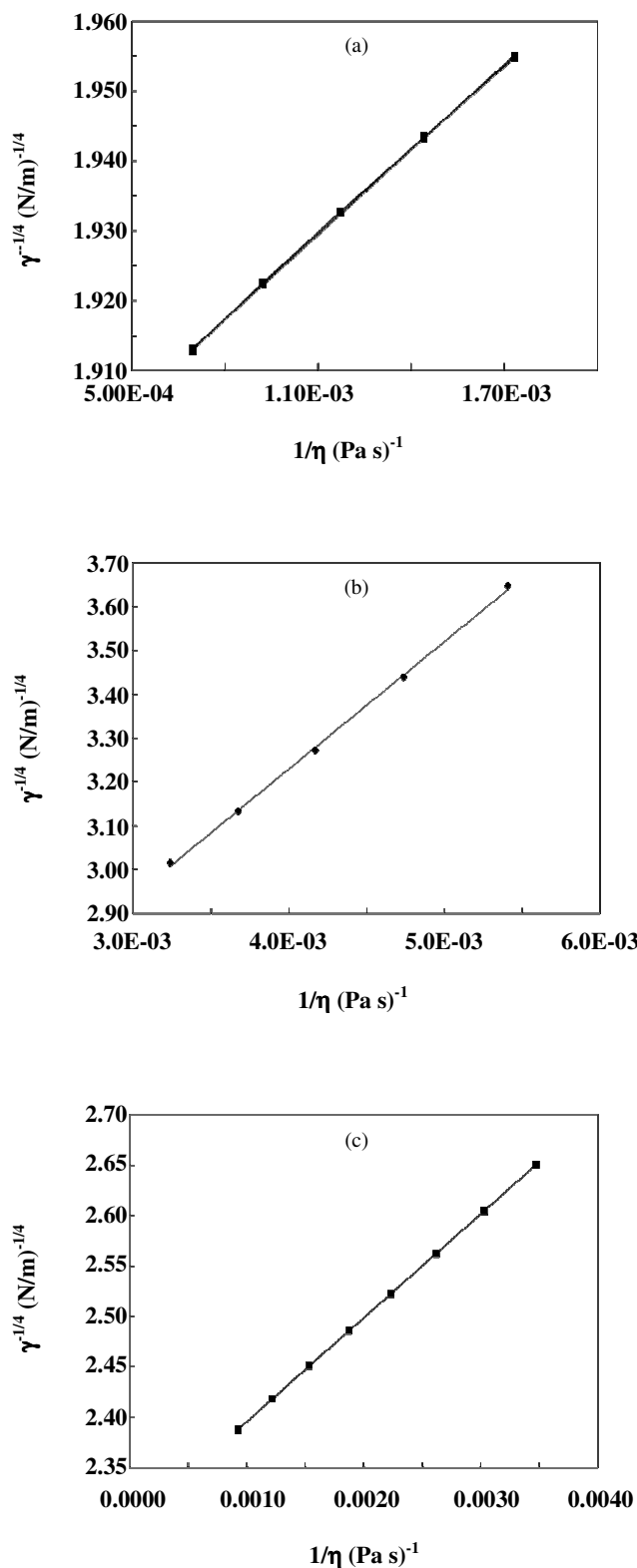


Fig. 2: linearity of  $\gamma^{-1/4}$  versus  $1/\eta$  for (a) water within 280-320 K, (b) xenon within 200-240 K, (c) propane within 130-200 K.

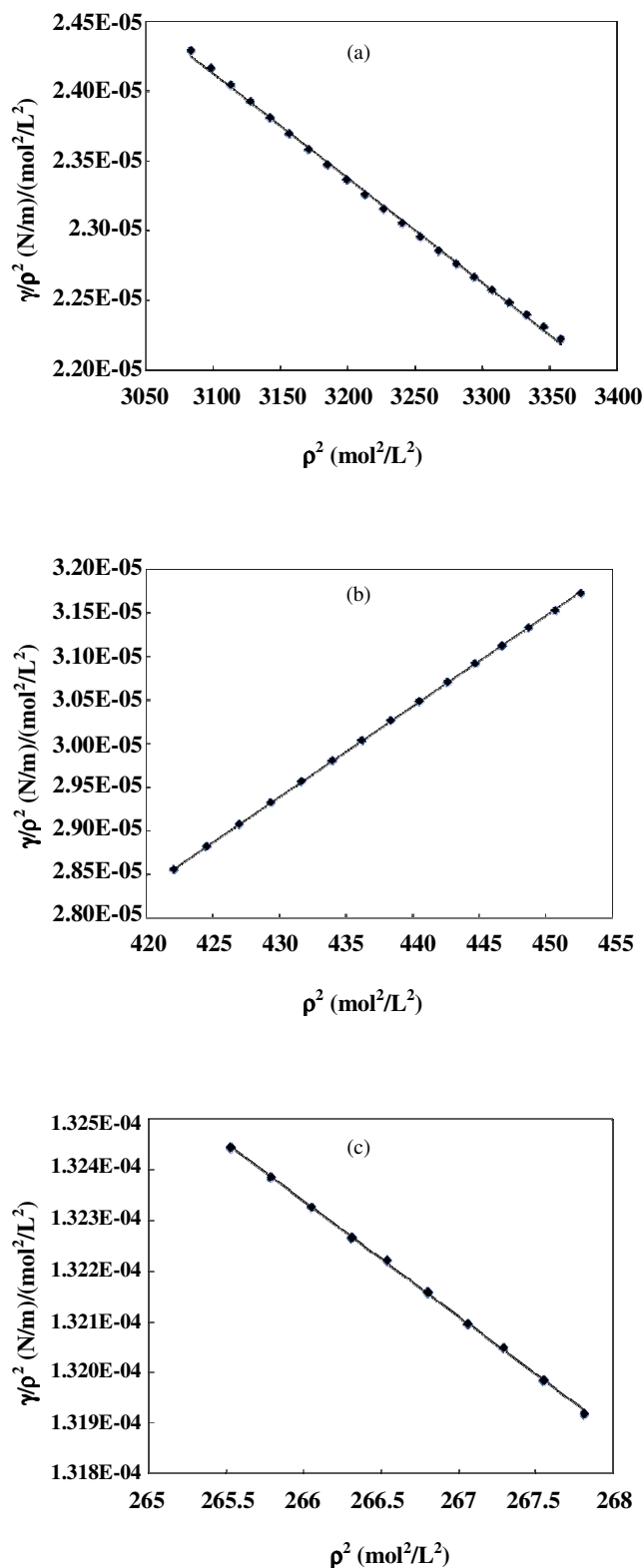


Fig. 3: searching for validity of equation (10) obtained on the bases of the simple model for (a) water at 280 K, (b) xenon at 200 K and (c) propane at 100 K.

**Table 1: Intercept ( $\gamma_0$ ), slope ( $\gamma_1$ ) and coefficient of determination ( $R^2$ ) of equation (11) for given fluids.**

Fluid	$\Delta T(K)$	$\gamma_0 (N/m)^{-1/4}$	$\gamma_1 (N/m)^{-1/4} \cdot (Pa.s)$	$R^2$
Water*	280-320	1.88500	40.4590	0.999
Water*	330-370	1.88236	41.3295	0.999
Xenon*	200-240	2.06837	290.326	0.999
Propane*	130-200	2.29280	102.970	0.999
Octane*	245-285	2.36952	129.497	0.999
Octafluoropropane*	190-220	2.57677	240.598	0.999
Krypton*	145-165	2.27903	197.468	0.998
Methane*	91-101	2.3850	64.6200	1.000
Neon*	29-37	2.69175	129.675	0.998
Nitrogen*	85-100	2.56125	105.152	0.998
Argon*	90-105	2.49687	131.659	0.999
Ammonia*	245-280	1.81593	90.5229	0.999
Butane*	265-355	2.19000	135.000	0.998
Carbon dioxide*	250-260	2.11370	163.516	0.998
Carbon monoxide*	110-120	1.09997	274.877	0.998
Heptane*	190-430	2.31818	132.557	0.999
Hexane*	180-380	2.31451	125.913	0.999
Nonane*	220-430	2.35951	148.132	0.999
Pentane*	150-300	2.31382	112.800	0.999
1,2 dichloro-1,1,2,2,tetrafluoroethane*	290-340	2.34979	204.321	0.999
Ethane 1,1,1,2-tetrafluoro*	225-265	2.34878	185.331	0.999

\*) Data are taken from Reference 34.

**Table 2: the results of fitting equation (10) onto experimental data for one isotherm of given liquids.**

Fluid	T (K)	C (N/m)(L/mol) <sup>4</sup>	D (N/m)(L/mol) <sup>2</sup>	$R^2$
Water*	280	-7.0E-9	5.0E- 5	0.9991
Xenon*	200	1.0E-7	-2.0E-5	1.0000
Propane*	100	-2.0E-7	2.0E-4	0.9996
Octane*	250	-3.0E-6	8.0E-4	0.9993
Octafluoro propane*	190	-2.0E-6	0.0004	1.0000
Krypton*	150	3.0E-8	-2.0E-6	0.9999
Methane*	100	3.0E-8	-2.0E-7	0.9996
Neon*	30	7.E-10	-1.0E-6	0.9945
Nitrogen*	100	2.0E-8	-4.0E-6	0.9999
Argon*	100	1.0E-8	-3.0E-6	0.9998
Butane*	300	2.E-06	-7.0E-05	0.9999
Carbon dioxide*	250	6.0E-8	-2.0E-5	1.0000
Carbon monoxide*	110	-2.E-08	2.0E-05	0.9999
Heptane*	300	2.E-05	-0.0005	0.9999
Hexane*	300	1.0E-5	-0.0005	0.9999
Nonane*	400	2.0E-5	-8.0E-05	1.0000
Pentane*	300	6.E-06	-0.0003	1.0000
Ammonia*	250	9.0E-9	2.0E-5	0.9997
1,1,1,2-tetrafluoro Ethane*	290	4.0E-7	3.0E-5	0.9999
1,2 dichloro- 1,1,2,2,tetrafluoroethane*	250	4.0E-6	-2.0E-4	1.0000

\*) Data are taken from Reference 34.

Table 3: Results of searching for temperature dependencies of parameters of the equation (10).

Fluid	T/K	$10^8 \times C \text{ (N/m)(L/mol)}^4$	$10^6 \times D \text{ (N/m)(L/mol)}^2$	$R^2$
Argon	90	0.49870	4.04708	0.999
	95	0.612431	2.36624	0.999
	100	0.708049	1.03243	0.999
	105	0.784541	0.02584	0.999
Octane	250	2.35284	5.24318	0.999
	260	3.87177	4.54348	0.997
	270	5.27133	3.90714	0.999
	280	6.48768	3.35818	1.000
Propane	150	1.42992	5.99607	0.999
	170	1.97817	4.24699	0.998
	190	2.35270	3.06229	0.999
	200	2.52689	2.53715	0.999
Nonane	110	-9.56088	1.21183	0.999
	114	-5.01030	0.83752	0.999
	118	-1.45039	0.55546	1.000
	120	0.01014	0.44286	0.967
Nitrogen	85	1.55924	- 2.21323	0.999
	90	1.52288	-2.22123	1.000
	95	1.48635	- 2.16616	0.999
	100	1.41843	- 1.84957	0.999
Ammonia	250	1.97044	-3.83459	0.999
	260	1.99315	- 4.42993	0.999
	270	1.97739	-4.36566	0.999
	280	1.93719	-3.90725	0.999
1,2 dichloro-1,1,2,2,tetraflouroEthane	290	3.68338	- 1.17631	1.000
	300	3.66613	- 1.15173	0.999
	320	3.57969	- 1.06343	0.999
	330	3.51042	- 1.00227	0.999
Krypton	145	2.50928	- 2.30667	0.999
	150	2.48157	- 2.36987	0.999
	155	2.43423	- 2.26316	1.000
	160	2.38302	- 2.10397	1.000
Neon	27	7.22095	- 1.24938	1.000
	30	6.95218	- 1.25730	0.994
	33	6.00541	- 0.98833	0.990
	39	4.05481	- 0.44718	0.991

Table 3 (continue)

Fluid	T/K	$10^8 \times C \text{ (N/m)}(\text{L/mol})^4$	$10^6 \times D \text{ (N/m)}(\text{L/mol})^2$	$R^2$
Butane	280	1.94080	- 6.72951	0.999
	300	1.95078	- 6.93244	0.999
	320	1.89935	- 6.45970	0.999
	340	1.80412	- 5.58888	0.999
Carbon dioxide	250	3.99374	- 6.25388	1.000
	254	3.94755	- 6.13515	1.000
	258	3.88341	- 5.90614	0.999
	260	3.84987	- 5.78010	0.998
Xenon	200	0.10023	- 1.31722	0.999
	210	0.10033	- 1.36977	1.000
	220	9.90718	- 1.35519	1.000
	230	9.65201	- 1.28424	0.999
Heptane	250	75.3944	1.100590	0.998
	300	1.15461	-0. 96449	0.999
	350	1.24955	- 1.40992	0.999
	400	1.17631	- 1.12025	1.000
Methane	95	2.77878	1.33995	0.999
	100	2.93427	- 0.23030	0.999
	110	3.10923	- 2.12081	0.999
	140	3.02643	- 2.47449	0.999
	160	2.73944	- 0.91866	1.000
Hexane	200	2.58481	2.07973	0.999
	250	6.67507	- 0.78345	0.999
	300	8.22464	- 1.66669	0.999
	350	8.09893	- 1.48851	1.000
1,1,1,2-tetrafluoro Ethane	230	4.22634	9.95040	0.999
	240	4.44306	4.59493	1.000
	250	4.66512	- 5.71022	0.999
	260	4.78985	- 3.68824	1.000
Octafluoropropane	190	1.59807	3.70141	0.999
	200	1.93360	6.84337	1.000
	210	2.22480	- 1.82138	0.999
	220	2.46753	- 3.81326	0.999
Pentane	150	-0.82511	3.86655	0.999
	200	1.66077	1.11895	0.999
	250	2.96023	- 0.11598	1.000
	300	3.51598	- 0.49730	1.000



Table 3 (continue)

Fluid	T/K	$10^8 \times C$ (N/m)(L/mol) <sup>4</sup>	$10^6 \times D$ (N/m)(L/mol) <sup>2</sup>	R <sup>2</sup>
Water	280	-7.48432	4.73250	0.999
	320	-6.45481	4.21313	0.999
	350	-5.49053	3.75710	0.999
	400	-4.00865	3.07804	0.999
	450	-3.09812	2.64720	0.999
Carbon monoxide	110	-9.56088	1.21183	0.999
	114	-5.01030	0.83752	0.999
	118	-1.45039	0.555459	1.000
	120	0.01014	0.442865	0.967

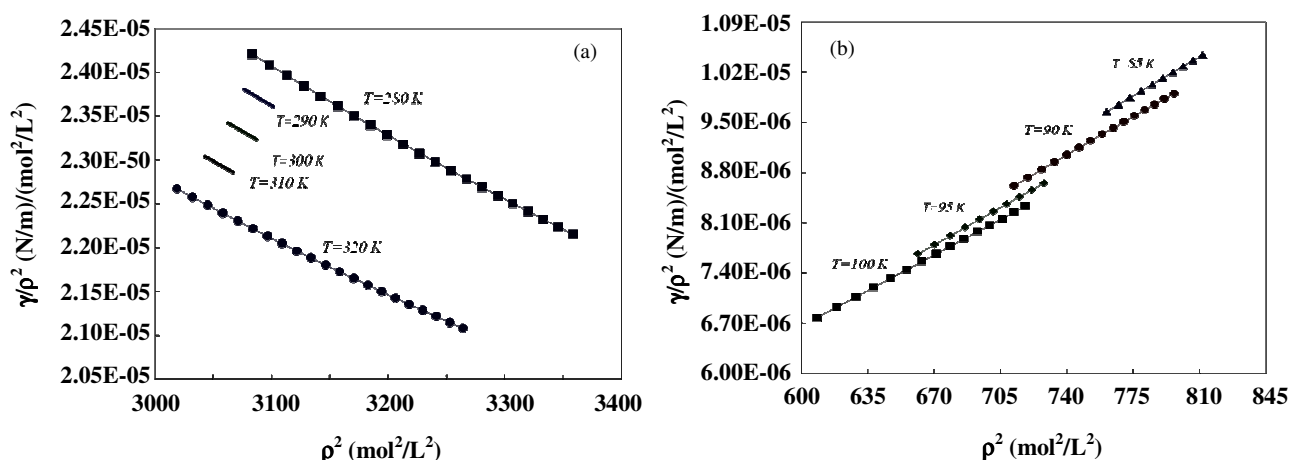


Fig. 4: Searching for temperature dependencies of parameters of equation (10) for given isotherms of (a) nitrogen and (b) water.

#### Contributions of individual terms of effective pair potential to surface tension

Due to the fact that the  $C_n/\bar{r}^n$  and  $C_m/\bar{r}^m$  terms of the effective pair potential contribute in surface tension of Eq. (10), as  $C\rho^4$  and  $D\rho^2$ , respectively, we may calculate their contributions in  $\gamma$  separately. To do so, we simply need the values of  $C$  and  $D$  parameters given in Table 3, at any desire temperature and liquid density. The results of such calculation are presented in Table 4. As one may expect the contributions are larger for water and heavier molecules, because of their significant intermolecular interactions.

#### CONCLUSIONS

We have introduced a simple hypothetical model for the liquid surface, according to which the surface is

macroscopically flat and one half of each surface molecule is in the liquid phase and the remaining in the vapor phase. We have also assumed that the liquid density is much large than that of the vapor phase, so that the interactions of a surface molecule with molecules within the vapor phase are negligible, compared to its interactions with molecules in the liquid phase. Such an assumptions is reasonable expect nearby the critical point. Therefore, only the interactions of a surface molecule with molecules within liquid phase are taken into account.

In order to include both the medium effect and long range interactions, the effective pair potential is considered. It was shown that LJ (12,6) function is appropriate for the pair interaction in a simple normal fluids [30]. However, this function is inaccurate for long chain molecules [36], metallic materials [37] and for

**Table 4: Contributions of attraction and repulsion to the surface tension and their summation for isotherm(s) of given fluids.**

Fluid	T (K)	$\rho$ (mol/L)	$10^{12} \times C\rho^4$ (N/m)(L/mol) <sup>4</sup>	$10^8 \times D\rho^2$ (N/m)(L/mol) <sup>2</sup>	$\gamma$ (N/m)
Argon	90	34.656	71.937	48.61	0.01205
		34.951	74.418	49.44	0.01238
		35.160	76.214	50.03	0.01262
Butane	280	10.229	212.48	-70.41	0.01420
		10.320	220.14	-71.67	0.01485
		10.425	229.24	-73.13	0.01560
Heptane	250	7.1888	201.36	56.88	0.02582
		7.2167	204.50	57.32	0.02619
		7.2502	208.32	57.85	0.02661
	400	5.8668	1.394	-38.56	0.01008
		5.9526	1.477	-39.69	0.01080
		6.0454	1.571	-40.94	0.01161
Octafluoropropane	190	9.4909	129.67	33.34	0.01630
		9.5442	132.60	33.71	0.01664
		9.6067	136.11	34.15	0.01702
	210	9.1152	153.59	-15.13	0.01384
		9.1826	158.19	-15.36	0.01429
		9.2601	163.59	-15.62	0.01479
Pentane	150	10.488	-99.841	42.53	0.032548
		10.511	-10.076	42.72	0.032649
		10.540	-10.184	42.95	0.032769
	300	8.5958	191.95	-3.674	0.015516
		8.6652	198.22	-3.734	0.016093
		8.7452	205.65	-3.803	0.016757
Water	280	55.528	-70819.9	145.33	0.07463
		57.161	-79525.5	154.01	0.07443
		57.952	-84019.7	158.30	0.07440
	320	54.943	-58980.1	127.34	0.06844
		56.414	-65554.7	134.25	0.06866
		57.132	-68956.3	137.69	0.06881
Carbon monoxide	110	23.114	-2729.0	64.74	0.00374
		24.047	-3197.0	70.07	0.00382
		24.911	-3681.9	75.20	0.00384
	118	21.099	-287.43	24.72	0.00218
		22.354	-362.16	27.76	0.00243
		23.545	-445.74	30.79	0.00262
	120	20.513	1.795	7841.30	0.00191
		21.881	2.324	10151.7	0.00213
		23.185	2.930	12796.6	0.00247

substances with significance long range interactions, like water [38]. A new generalized effective pair potential has recently been introduced [35]. The concave deviation of  $\gamma/\rho^2$  versus  $\rho^2$  for 280 K isotherm of water (Fig. 3a), and significant deviation for 120 K isotherm of nonane (Table 3) may be due to inaccurate effective potential of LJ (12, 6) for these liquids. Also  $\gamma/\rho^2$  versus  $\rho^2$  shows a significant deviation for some isotherms of neon (see Table 3). Again, by using long range density data of both solid and fluid neon, discloses that the LJ (12, 6) is inaccurate function for the effective pair potential of neon.

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