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BOOKLET

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Title: Surface tension OF O2-Ar, N2-Ar AND O2-N2-Ar Mixtures

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Introduction

The troposphere is the atmosphere layer nearest to the ground and it is also where most all weather conditions take place.

The air in such layer is composed of 78% nitrogen and 21% oxygen and the remaining part, it means, 1% is composed of argon, water vapor and carbon dioxide.

We determine the numerical values of the Lennard-Jones parameters for argon that reproduce the experimental surface tension as a pure fluid.

The surface tension of the binary mixtures oxygen-argon and nitrogen-argon has been estimated by molecular dynamics simulations. This interfacial property was estimated at T = 83.85K for all mixtures, in order to compare with theoretical and experimental data previously obtained. As a result we found a good agreement.

Introduction

The surface tension of the ternary mixture oxygen-nitrogen-argon was calculated by molecular dynamics simulations for several temperatures.
mixture 1: χ_{O2}=70.4%, χ_{N2}=11.6% y χ_{Ar}=18%.
mixture 2: χ_{O2}=21%, χ_{N2}=78% y χ_{Ar}=1%.

We assume that it is necessary to have good force fields for pure components to calculate accurate data for binary and ternary mixtures. To the best of our knowledge, there is no benchmark of such interfacial property for a wide range of temperatures.

An immediate extension of the present work is the analysis of the influence of the air in the measurement of the apparent surface tension of the aqueous solution of hydrophilic solutes. In case of sugars, experimentally measured of surface tension did not correspond to theoretical data.

Methodology

Molecular dynamics simulations were performed in a canonical ensemble. N = 8000 molecules were placed in a cubic crystalline arrangement centered on the faces, which forms a liquid plate that is surrounded by vacuum, forming a parallelepiped cell. The free GROMACS-5.2.1 software was used for all our simulations.

The interaction law among molecules is the superposition of Lennard-Jones and Coulomb potentials and it is writen as follows

$$u=4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right]+\frac{1}{4\pi\varepsilon_0}\frac{q_i q_j}{r}$$

The Surface tension was estimated as a difference between normal and tangential pressure, respect to the interfacial area

$$\gamma=\frac{L_z}{2}\left[\langle P_{ZZ}\rangle-\frac{1}{2}\langle P_{XX}+P_{YY}\rangle\right]$$

The pressure components were estimated by using the following expression

$$VP_{\alpha\beta}=\sum m_i\,(v_i)_\alpha(v_i)_\beta+\sum\sum\left(r_{ij}\right)_\alpha\left(f_{ij}\right)_\beta$$

The partial charges associated to each atom was determined by means a simple relationship with the experimental quadrupole moment

$$\Theta=\frac{L}{2}q$$

All the potential parameters were collected in Table I

Átomo	σ(A)	ε(kJ/mol)	L(A)	q_i(e)
O	3.11	0.4015	1.23	-0.1101
N	3.375	0.29508	1.098	-0.482
Ar	3.484	0.9556		0

argon surface tension

Results

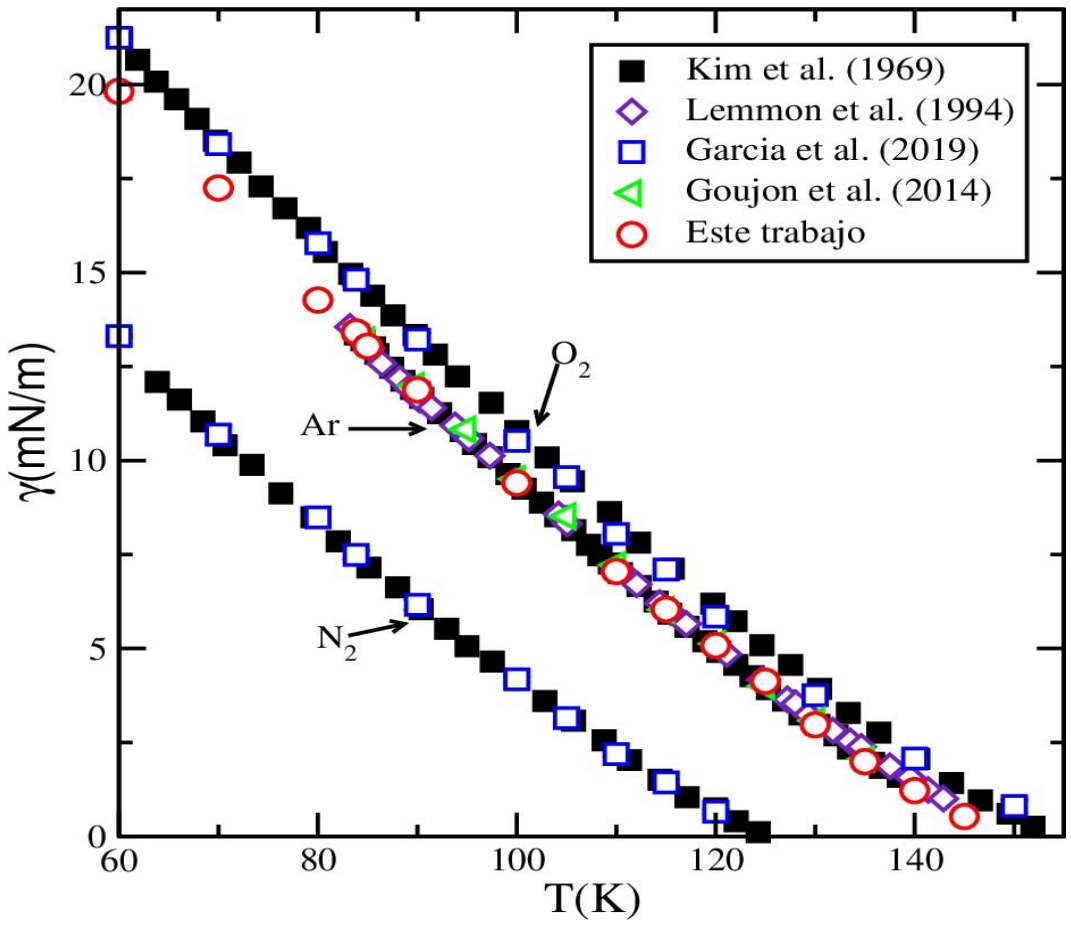

Figure 1. The surface tension of argon as a function of temperature was calculated using the parameters ε = 0.9556kJ / mol and σ = 0.3484nm to reproduce the experimental data. The Goujon et al. (2014) data were included for comparison, and it can be seen that the agreement is excellent. The surface tension of both pure fluids, oxygen and nitrogen was also included, these data were taken from the García et al. (2019) work.

nitrogen-argon surface tension

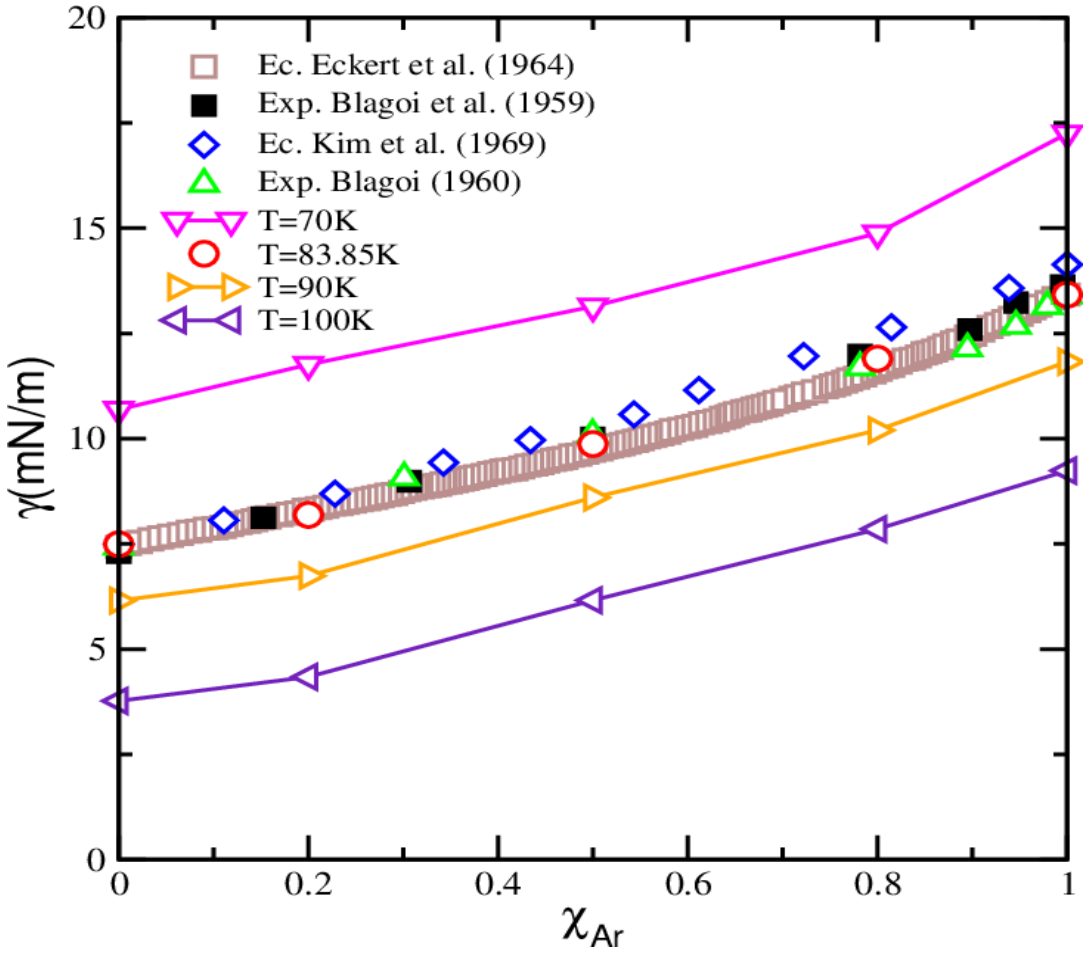

Figure 2. Surface tension of the binary nitrogen-argon mixture as a function of argon mol fraction, at different temperatures. The experimental and theoretical data were obtained at T = 83.85K. The symbols that identify all data are explained in the inset. The empty circles at T = 83.85K are results of this work, as well as the data shown for temperatures 70K, 90K and 100K.

oxygen-argon surface tension

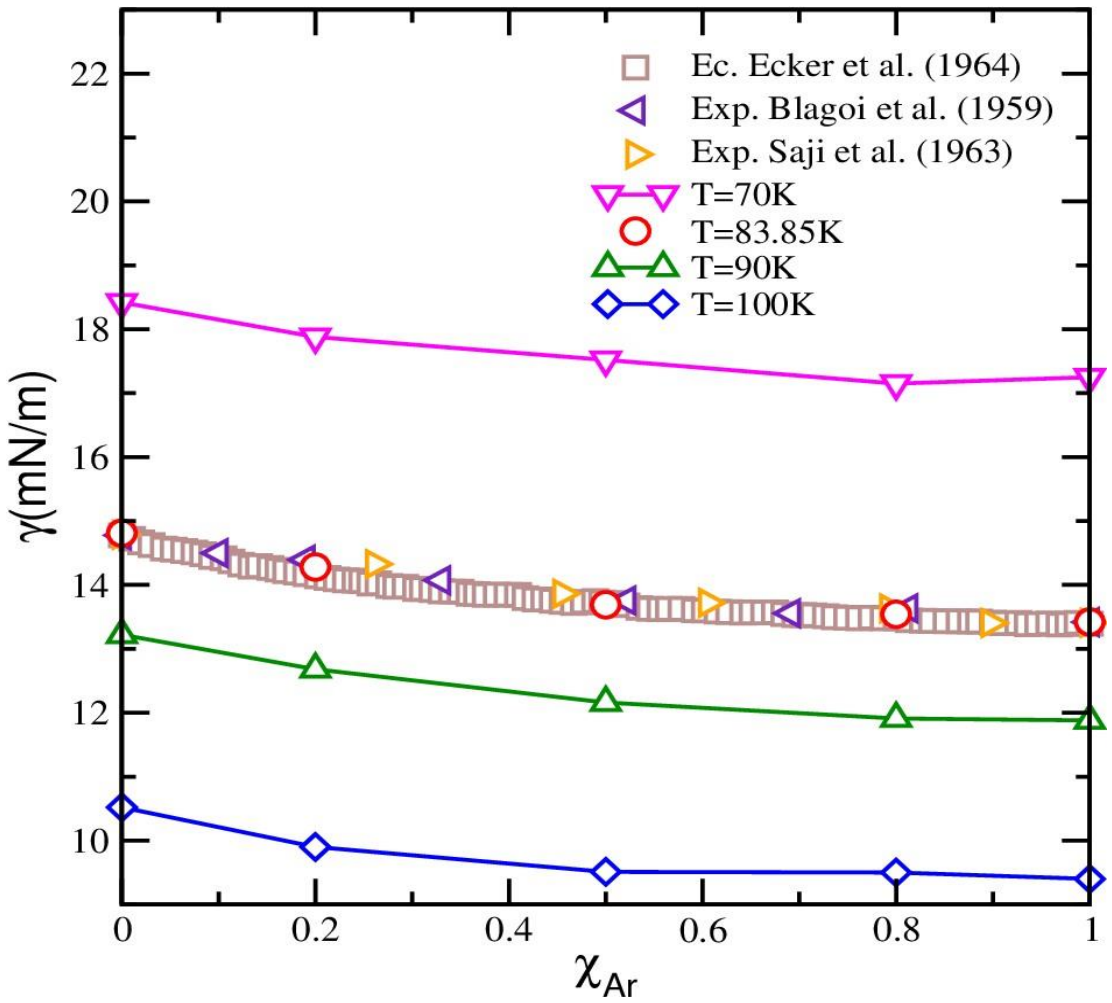

Figure 3. Surface tension of oxygen-argon at different temperatures. The symbols are identified in the inset. Empty circles are data generated in this work at T = 83.85K. Curves corresponding to temperatures 70K, 90K and 100K were also generated in this work.

oxygen-nitrogen-argon surface tension

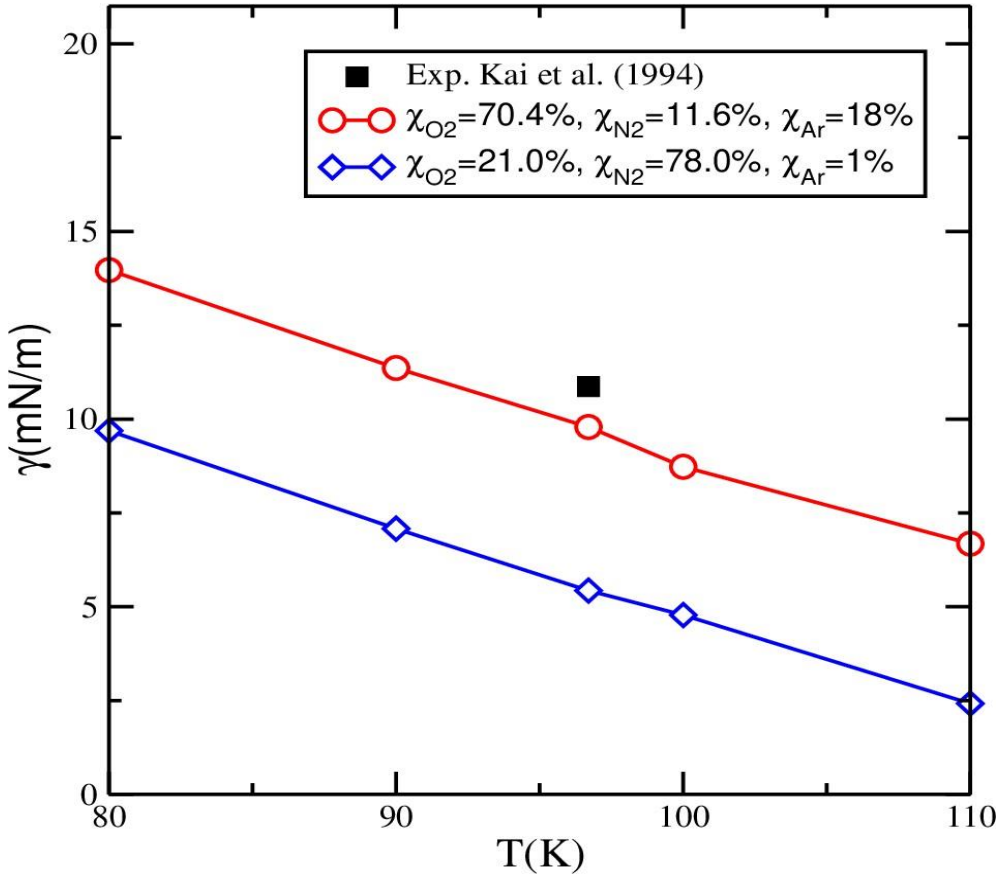

Figure 4. Surface tension of the oxygen-nitrogen-argon ternary mixture at different temperatures. Concentration of the different species χ_{O2} = 70.4%, χ_{N2} = 11.6% and χ_{Ar} = 18%, the full squares are experimental data and the empty circles are data generated in this work.
Empty diamonds are data generated in this work for the concentration χ_{O2} = 21%, χ_{N2} = 78% and χ_{Ar} = 1%.

Conclusions

- Lennard-Jones potential parameters were determined in order to reproduce the experimental argon surface tension curve.
- The surface tension curve of the ternary mixture (N2-O2-Ar) is shown as a function of the temperature. This mixture can be considered as an initial or controlled model of air.
- The force fields that reproduce the surface tension of pure fluids provide the opportunity to obtain good results in binary and ternary mixtures. In addition, surface tension curves of binary and ternary mixtures at temperatures where we have not found experimental data were calculated and shown.
- Some mixtures are difficult to model because cross interactions introduce inaccuracies. This is the case of the oxygen-argon mixture where the cross term of both combination rules had to be modified. Computer simulation is a useful tool for generating reference data where there is no existing data.
- We believe that a simple air model will allow a good analysis of its influence on the apparent surface tension of aqueous solutions of hydrophilic components.

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