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# A SECOND ATTEMPT TO ESTABLISH AN ANALYTICAL EXPRESSION TO STEAM-WATER DIPOLE ORIENTATION PARAMETER USING THE BOUBAKER POLYNOMIALS EXPANSION SCHEME

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In this paper, an analytical expression to the steam-water dipole orientation parameter is proposed. The calculations have been carried out under the presumptions that: the electric properties of the water molecules are characterized completely by a permanent dipole moment and a constant scalar polarizability, that translational fluctuations may be neglected, and that the positions are orientation-free. The results have been presented in the form of continuous and integrable expressions which could be easily compared to precedent studies as well as involved in similar analytical models

**K e y w o r d s:** steam-water, BPES; permanent dipole moment, analytical expression.
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Steam-water mixture molecular configuration has been discussed, in the last decades, by several specialists [1—10]. For example, A.D. Chistyakov [1] studied the applicability of several well-known equations describing the dependences of the relative permittivities of liquid water and steam on their densities and temperature. His works yielded original semi-empirical equations which related the permittivity of equilibrium steam to that of the liquid phase and allowed tabulation of the calculated permittivities of water and steam in saturation states.

In the same way, N.M. Putintsev *et al.* [2] applied several polarization theory equations to different states of aggregation of molecular systems in order to calculate the characteristics of water-steam polarization. The same authors have already explained the deformation polarization [3] through steam-water dipoles perturbation.

More recently, Yu.K. Tovbin [4] and S.G. Dyakonov *et al.* [5] used phase equilibria and molecular theory of curved steam-water interphase boundaries in terms of lattice gas models. They considered Laplace equations for the quasi-equilibrium distribution of molecules at the steam-water boundaries taking into account direct correlations between the nearest interacting molecules.

In the present study, a polarization theory is developed in order to describe intermolecular influence inside a given steam-water medium. A particular attention is given to the as-defined dipole orientation parameter *g*.

## THEORY AND EXPERIMENT

Given the following relevant parameters (Table 1) inside a steam-water metastable mixture: and under some presumptions, the steam-water dipole orientation parameter *g* (Eq. 1), evaluates the mean interaction [6—10] between adjacent molecules (nearest neighbourhood):

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*Main prefixed parameters significations, values and units*

| Parameter | Signification | | Value | Unit |
|---|---|---|---|---|
| $\mathbf{p}$ | Molecule dipole moment | | $\|\mathbf{p}\| = 61375$ | $10^{-30}$ C.m |
| $t_m$ | Mean temperature | | 225 | °C |
| $N_A$ | Avogadro constant | | $602 \cdot 10^{23}$ | $\text{mol}^{-1}$ |
| $k_B$ | Boltzmann constant | | $138 \cdot 10^{-23}$ | $\text{J} \cdot \text{K}^{-1}$ |
| $\varepsilon_0$ | Vacuum permittivity | | $8854 \cdot 10^{-12}$ | $\text{F} \cdot \text{m}^{-1}$ |
| $\rho_{sat}$ | | Density | *variable* | $\text{Kg} \cdot \text{m}^{-3}$ |
| $\tilde{n}_D$ | $H_2O$ | Mean refractive index | 1.33 | Dim. less |
| $M$ | | Molar mass | 0.0180 | $\text{Kg} \cdot \text{mol}^{-1}$ |
| $\varepsilon$ | | Relative permittivity | *variable* | Dim. less |

$$g = \frac{18M\varepsilon_0}{N_{Av}\rho_{sat}} \frac{k_B t_m}{\|\mathbf{p}\|^2} \frac{\varepsilon}{(2+n_D^2)^2}. \tag{1}$$

Inside a given temperature range, $t_m$ is accurately known, Equation (1) can be written as

$$g(\varepsilon, \rho_{sat}) = A \frac{\varepsilon}{\rho_{sat}(2+n_D^2(\varepsilon, \rho_{sat}))^2} \tag{2}$$
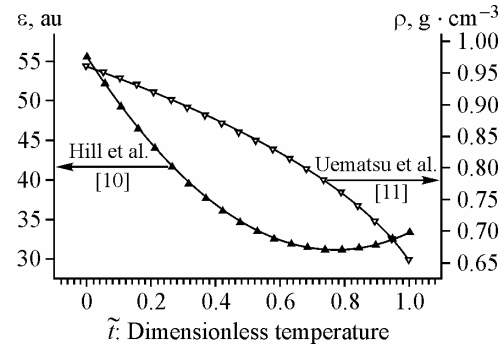
with $A$ constant.

For pure and de-ionised water, a complete set of data concerning the relative permittivity $\varepsilon$ have been recorded by P.G. Hill *et al.* [11], parallel to values of the density at saturation line $\rho_{sat}$, detailed by M. Uematsu *et al.* [12]. An extracted sample of this data is represented in Fig. 1.

This sample has been subjected, along with Eq. (1), to the Boubaker Polynomials Expansion Scheme (BPES) [13—22]. The BPES is a resolution protocol which has been extensively proposed in many mathematical and engineering fields to yield meaningful results for both numerical and analytical problems. This scheme has been successfully applied in several recent applied physic studies [17, 21, 22]. Its main expansion $f(x)$:

$$f(x) = \frac{1}{2N_0} \sum_{q=1}^{N_0} a_q \times B_{4q}(\beta_q x), \tag{3}$$

where $B_{4q}$ are the $4q$-order Boubaker polynomials; $\beta_q$ are $B_{4q}$ minimal positive roots; $N_0$ is a prefixed integer; $a_q\big|_{q=1\ldots N_0}$ are real coefficients coefficients, has been demonstrated [15, 21] to be the unique solution of the system (4):



*Fig. 1.* Variations of $\varepsilon$ and $\rho$ versus dimensionless temperature

$$\begin{cases} \sum_{q=1}^{N} B_{4q}(x \times \beta_q) \Big|_{x=0} = -2N \neq 0 \\[2mm] \sum_{q=1}^{N} B_{4q}(x \times \beta_q) \Big|_{x=1} = 0 \\[2mm] \sum_{q=1}^{N} \frac{dB_{4q}(x \times \beta_q)}{dx} \Big|_{x=0} = 0 \\[2mm] \sum_{q=1}^{N} \frac{dB_{4q}(x \times \beta_q)}{dx} \Big|_{x=1} = \sum_{q=1}^{N} H_q \\[2mm] \sum_{q=1}^{N} \frac{d^2 B_{4q}(x \times \beta_q)}{dx^2} \Big|_{x=0} = \frac{8}{3}(N(N^2-1)) \\[2mm] \sum_{q=1}^{N} \frac{d^2 B_{4q}(x \times \beta_q)}{dx^2} \Big|_{x=1} = \sum_{q=1}^{N} G_q, \end{cases} \tag{4}$$

where $H_q = \dfrac{dB_{4q}(x)}{dx}\Big|_{x=\beta_q} = \left( \dfrac{4\beta_q[2-\beta_q^2] \times \sum_{j=1}^{q} B_{4j}^2(\beta_q)}{B_{4(q+1)}(\beta_q)} + 4\beta_q^3 \right)$

and $G_q = \dfrac{d^2 B_{4q}(x)}{dx^2}\Big|_{x=\beta_q} = \dfrac{3\beta_q(4q\beta_q^2 + 12q - 2)H_q - 8q(24q^2\beta_q^2 + 8q^2 - 2q + 4)}{(\beta_q^2 - 1)(12q\beta_q^2 + 4q - 2)}.$

According to the BPES protocol, the two $t$-dependent variables are expressed in the range $[t_0; t_1]$, as a function of the normalised variable $\tilde{t}$:

$$\begin{cases} \tilde{t} = \dfrac{1}{\Delta t}(t - t_0); \qquad t \in [t_0; t_1], \\[2mm] \Delta t = t_1 - t_0, \end{cases} \tag{5}$$

The proposed expressions of $\rho_{sat}(t)$ and $\varepsilon(t)$ are

$$\begin{cases} \rho_{sat}(t) = \dfrac{1}{2N_0} \sum_{q=1}^{N_0} \xi_q \times B_{4q}(\beta_q \tilde{t}), \\[2mm] \varepsilon(t) = \dfrac{1}{2N_0} \sum_{q=1}^{N_0} \xi'_q \times B_{4q}(\beta_q \tilde{t}), \end{cases} \tag{6}$$

where $\xi_q\big|_{q=1\ldots N_0}$ and $\xi'_q\big|_{q=1\ldots N_0}$ are coefficients whose values minimize the Minimum Square functions $\Delta_{MS_1}$ and $\Delta_{MS_2}$, respectively.

$$\Delta_{MS_1} = \sum_{k=1}^{M_0} \left( \varepsilon_k - \frac{1}{2N_0} \sum_{q=1}^{N_0} \xi_q \cdot B_{4q}(\beta_q \tilde{t}_k) \right)^2, \tag{7}$$

$$\Delta_{MS_2} = \sum_{k=1}^{M_0} \left( \rho_{sat_k} - \frac{1}{2N_0} \sum_{q=1}^{N_0} \xi'_q \cdot B_{4q}(\beta_q \tilde{t}_k) \right)^2. \tag{8}$$

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*Obtained values along with values given in the related literature*

| $t$ (°C) | $g$ (dimensionless) ±4 % | | | | | $t$ (°C) | $g$ (dimensionless) ±4 % | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
|  | BPES | Ref. [ 22 ] | Error* | Ref. [ 23 ] | Error** |  | BPES | Ref. [ 22 ] | Error* | Ref. [ 23 ] | Error** |
| 100 | 2.71 | 2.71 | 0 | 2.70 | 0.0001 | 250 | 2.44 | 2.50 | 0.0036 | 2.30 | 0.0196 |
| 125 | 2.57 | 2.58 | 0.0001 | 2.51 | 0.0036 | 275 | 2.39 | 2.27 | 0.0144 | 2.48 | 0.0081 |
| 150 | 2.54 | 2.55 | 0.0001 | 2.44 | 0.01 | 300 | 2.35 | 2.22 | 0.0169 | 2.43 | 0.0064 |
| 175 | 2.53 | 2.54 | 0.0001 | 2.40 | 0.0169 | 325 | 2.23 | 2.14 | 0.0081 | 2.37 | 0.0196 |
| 200 | 2.51 | 2.37 | 0.0196 | 2.52 | 0.0001 | 350 | 2.11 | 2.09 | 0.0004 | 2.26 | 0.0225 |
| 225 | 2.48 | 2.34 | 0.0196 | 2.51 | 0.0009 |  |  |  |  |  |  |

 * Quadratic error (BPES/Ref 22, Heger *et al.*).
** Quadratic error (BPES/Ref 23, Marcus).

The optimal values $\xi_q\big|_{q=1\ldots N_0}$ and $\xi'_q\big|_{q=1\ldots N_0}$ are equivalent to those which solve the linear $N_0 \times N_0$-sized systems which has the same coefficients array:

$$\left|\sum_{q=1}^{N_0}\left(\frac{1}{2N_0}\sum_{k=1}^{M_0}B_{4q}(\beta_q\tilde{t}_k)B_{4j}(\nu_j\tilde{t}_k)\right)\xi_q\right|_{j=1,2,\ldots,N_0} = \left|\sum_{k=1}^{M_0}\varepsilon_k B_{4j}(\beta_j\tilde{t}_k)\right|_{j=1,2,\ldots,N_0} \tag{9}$$

and

$$\left|\sum_{q=1}^{N_0}\left(\frac{1}{2N_0}\sum_{k=1}^{M_0}B_{4q}(\beta_q\tilde{t}_k)B_{4j}(\beta_j\tilde{t}_k)\right)\xi'_q\right|_{j=1,2,\ldots,N_0} = \left|\sum_{k=1}^{M_0}\rho_{sat_k} B_{4j}(\beta_j\tilde{t}_k)\right|_{j=1,2,\ldots,N_0}, \tag{10}$$

respectively.

### RESULTS AND DISCUSSION

By introducing the solutions of Eq. (9)—(10) in Eq. (6), and considering a mean value of the refractive index $\tilde{n}_D$, final analytical *t*-dependent expression of the dipole orientation parameter *g* is:

$$g = \frac{18 M \varepsilon_0}{N_{Av}(2+\tilde{n}_D^2)^2}\frac{k_B T_m}{\|\mathbf{p}\|^2}\frac{\displaystyle\sum_{q=1}^{N_0}\xi_q \times B_{4q}(\nu_q\tilde{t})}{\displaystyle\sum_{q=1}^{N_0}\xi'_q \times B_{4q}(\nu_q\tilde{t})}. \tag{11}$$

The obtained results for the given parameters (table 1), are presented in Table 2, along with precedent values published by K. Heger *et al.* [ 22 ] and Y. Marcus [ 23 ].

The values of the dipole orientation parameter *g* have been truncated to $10^{-2}$, while errors were monitored with three significant digits, for accuracy purposes.

Comparison with existent results [ 22, 23 ] has been made on the basis of absolute quadratic errors, gathered in Fig. 2.

*Fig. 2.* Quadratic errors (BPES versus Ref 22 (Heger *et al.*) and Ref 23 (Marcus))
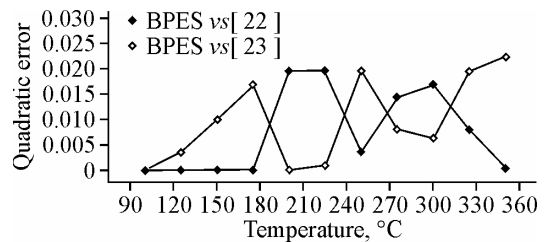
## CONCLUSION

In this paper, data deduced from molecular dynamics simulations permitted the establishment of an analytical expression of the water-steam dipole orientation parameter, albeit for a system with a limited number of water molecules. The used calculation protocol (BPES) produced results presented in the form of continuous and integrable expressions which could be easily compared to precedent studies as well as involved in similar analytical models. Error analyses confirmed that the obtained values are in good agreement with those existing in the related literature.

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