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DEVELOPING A NOVEL ALGORITHM FOR THE COMPUTATION OF POISSON'S RATIO USING MOLECULAR DYNAMICS FOR POLYMERS

Sunita Andreea MOGA[1], Nicolae GOGA[2], Anton HADAR[3]

This article presents a method for the computation of Poisson's ratio for an elastic material using molecular dynamic theory, based on an original algorithm and implemented in GROMACS environment. An overview of the theoretical approach (algorithm, computation formulas) is presented and also the simulation results. The simulation results for the chosen system (expanded polystyrene) are in agreement with the experimental results.

Keywords: molecular dynamics, polymers, Poisson's ratio, GROMACS

1. Introduction

In this century of technological development and research, molecular dynamics is becoming increasingly popular for the study of dynamical properties of molecular systems [1]. The ability to predict different properties of polymers from molecular simulations is of great value in the design of new polymeric materials.

It should be noted that the authors have already developed several methods [2-5, 13] based on molecular dynamics theory for the computation of elastic and mechanical properties of polymers.

The goal of this article is to present a new method for the computation of Poisson's ratio (Poison's coefficient), and also, to describe the simulation results obtained by the application of the new method using molecular dynamics. The system chosen for our simulation experiments is expanded polystyrene (EPS). This type of polystyrene is a rigid and tough plastic which is found in a multitude of shapes and applications (trays, plates, fish boxes). EPS is usually white and is obtained from oil, as schematically suggested in Fig. 1 [6].

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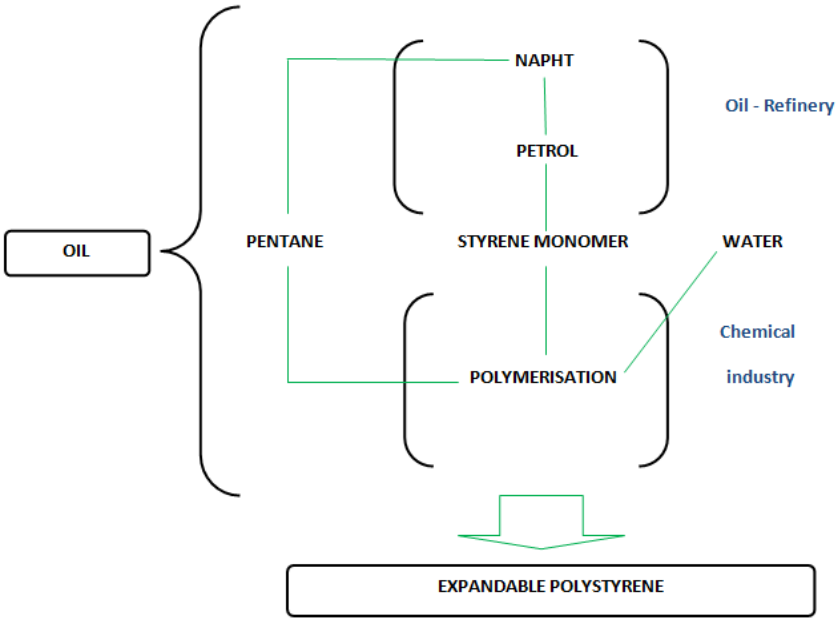


Fig. 1. EPS diagram [7-8]

All the simulations were done in GROMACS environment [9], one of the most used open sources available in the molecular dynamics domain. This software package is a collection of programs and libraries that was primary developed at the University of Groningen, the Netherland, in the Department of Biophysical Chemistry, but now is maintained and improved by researchers from all around the world [10-11]. GROMACS is a complex package that simulates the Newtonian equation of motion for different systems including polymers.

Although its primary target are biological molecules with complex bonded interaction, the very effective implementation of non-bonded force calculation makes GROMACS suitable for all kinds of molecular dynamics simulation based on pair potentials.

Instead of normal potential function (Lennard-Jones, Buckingham, Columb) it is possible to use arbitrary forms of interaction - such as spline-interpolate tables [12].

The next section will describe the theoretical content, followed by the simulation results. The last section discusses the conclusions and some future directions of development.

2. Theoretical content

This section will describe the theory of the new approach for the computation of Poisson ratio γ.

Theoretically, Poisson ratio, is the contraction in "y" or "z"- direction after elongation in the "x"- direction. Both expressed as a fraction or percentage, the ration is dimensionless. It is related to the bulk modulus, "K", which is the inverse of compressibility, β. For isotropic incompressible materials (zero β, infinite K), Poisson's ratio equals 0.5. For compressible isotropic materials, Poisson's ratio equals (3K-E)/6K, where E is Young's modulus. Fig. 2 present a schematic overview of the main algorithm for the computation of Poisson's ratio.

Like showed in Fig. 2, the method of the computation of Poisson's ratio has several steps:

I. Start with an equilibrated constant - pressure box, zero isotropic pressure (or 1 bar).
II. Then switch to constant volume. Run the system, monitor the pressure tensor, all components should be fluctuating around zero.
III. Then elongate the box a few percent in x-direction only, from *Lx* to $Lx + \Delta Lx$, scaling all *x*-coordinates proportionally.
IV. Monitor the pressure tensor. Let the system run such that the sudden change equilibrate.
V. witch to constant - pressure simulation, with pressures:

$$P_{xx} = \langle P_{xx} \rangle \tag{1}$$

from step 5 of Young's modulus determination [13]
(*Pxx* is negative);

$$P_{yy} = P_{zz} = 0 \tag{2}$$

Run the system and monitor the box size*: Lx, Ly, Lz*.
VI. Look for linear drift, if necessary, subtract the drift.
VII. Determine <*Lx*>, <*Ly*>, <*Lz*>. If the polymer has not rearranged significantly,
VIII.

$$\langle L_x \rangle - L_x = -L_x * \frac{P_{xx}}{E} \tag{3}$$

That is, Lx should not really change very much. *Ly* and *Lz* will equilibrate to the values given by Poisson's ratio.

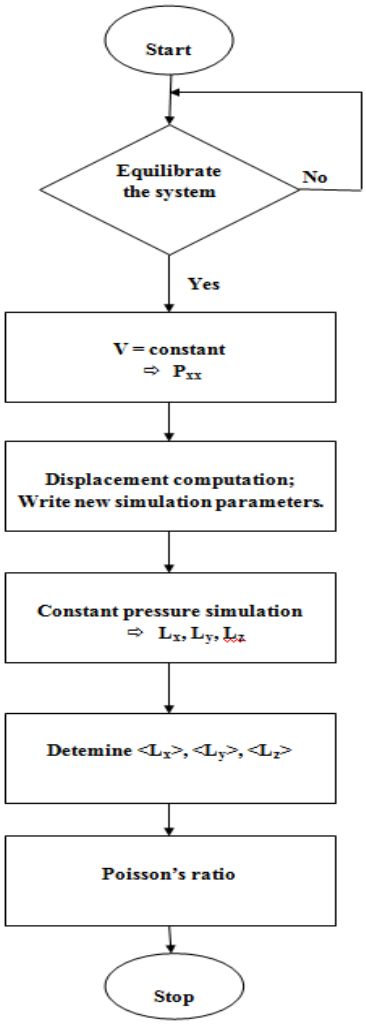


Fig. 2. Poisson's ratio - method of computation

Poisson's ratio is:

$$\gamma = -0{,}5 * \frac{\left(\frac{\langle L_y \rangle}{L_y} - 1\right) + \left(\frac{\langle L_z \rangle}{L_z} - 1\right)}{\left(\frac{\langle L_x \rangle}{L_x} - 1\right)} \tag{4}$$

with L_x, L_y and L_z the original box lengths. The lengths in step V are time - depending: $L_x(t)$, $L_y(t)$ and $L_z(t)$ with averages $<L_x>$, $<L_y>$ and $<L_z>$.

3. Simulations details and results

All the molecular simulation were made in GROMACS. The system chosen for the test was expanded polystyrene (EPS) with 400 atoms.

During the simulation the molecules were represented by groups of particles of Course Grain (CG) type. This specific model is named MARTINI [14] and is highly used in this domain. In all the simulation, the integrator used was "md" and the time step was of 0.0040.

We took into account different values for the reference temperature: 320K, 360K and 400K. The simulation time varies from 1000 steps to 50000 steps.

Table 1

Poisson's ratio for EPS

	320K	360K	400K
Poisson's ratio	0.3785	0.3810	0.3868

The density for simulation system at different temperature was in the range of 16 - 237 kg/m^3 which correspond to the one reported in literature for EPS which varies between 16 - 640 kg/m^3 [15]. Poisson's ratio is computed by using the pressure of the system. This was analyzed by a tool integrated in GROMACS package – *g_energy*. This tool examine the information from a energy file (.edr file), that contains all the energy terms that are saved during a simulation, and prints the output to an data formatted for import into the Grace 2-D plotting program so that it's ready for further analyze and plotting[9]. Grace 2-D is a plotting tool that runs on any version of Unix OS as well as, VMS, OS/2 and Win9*/NT/2000/XP (although in the last some minor functionality may be missing).

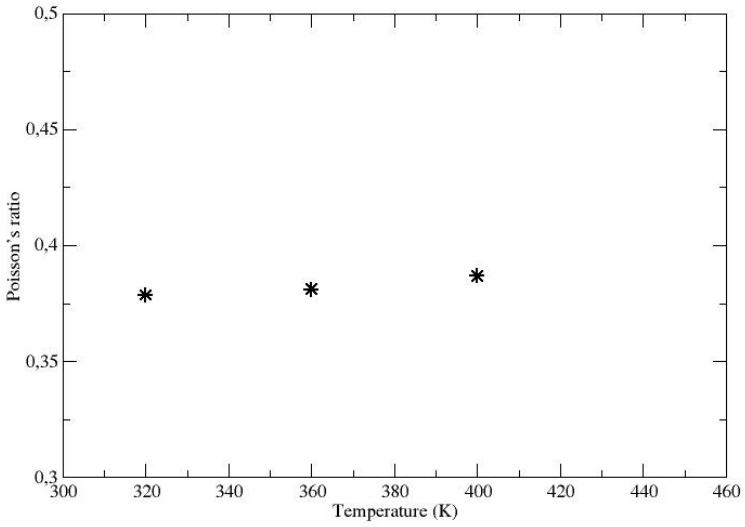
Table 1 presents the values for the Poisson's ratio for different temperatures.

Table 2

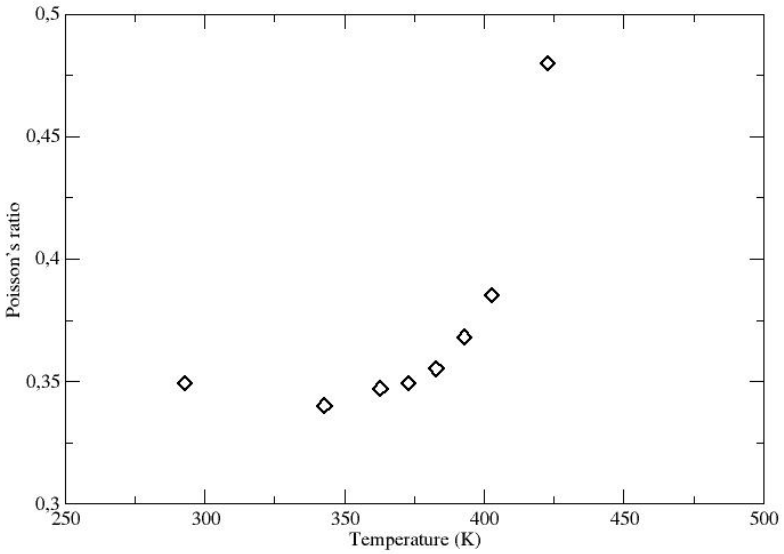
Poisson's ratio for EPS in literature [16 - 17]

	Yamanaka, et. al. (1991)	Negussey and Sun (1996)	Ooa, et. al. (1996)	Sanders (1996)	Momoi and Kokusyo (1996)	Duskov et. al. (1998)	GeoTech (1999)
Poisson's ratio	0.075	0.09 & 0.33	0.08	0.05 - 0.2	0.5	0.1	0.05

From Table 1 and 2 we can conclude that the Poisson's ratio computed using molecular dynamics and GROAMCS is quite close to the results found in literature (Table 2). In Fig. 3 and Fig. 4 we show the Poisson's ratio as reported in literature [18] and from our simulation result.



a. Poisson's ratio simulation results



b. Poisson's ratio literature [18]

Fig. 3. Poisson's ratio

As shown in Fig. 3 and 4, it can be concluded, that the computed Poisson's ratio approaches similar values as the theoretical ones for a range of temperatures (320K - 400 K) corresponding to a equilibrated state of the system.

Our measurements are around 10% off from the experimental values reported in the literature [18] for a range of temperatures between 320K to 360K. For a temperature of 400K the values for the simulation and the ones from literature are almost the same.

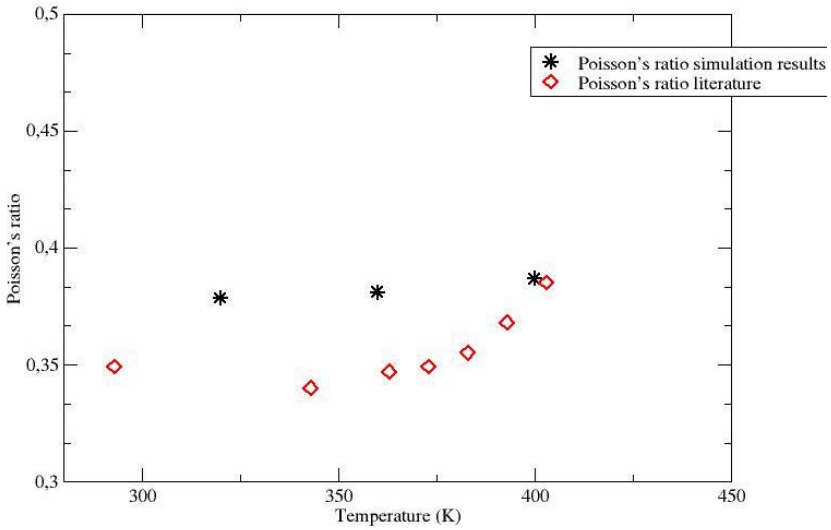


Fig. 4 Poisson's ratio

The differences between simulated system and the experimental are due to numerical approximations in molecular dynamics parameterizations and simulation. In general it can be concluded that computed values are in agreement with the experimental values from the literature

4. Conclusions

This article presents an overview of a new algorithm for the computation of Poisson's ratio using molecular dynamics. In introduction, a short description of the molecular dynamics field is presented. The subsequent part presents the algorithm for the computation of the Poisson's ratio and the results obtained through the simulation of EPS.

It can be observed that in general the computed Potion's ratio approaches similar values with the experimental values for a range of temperature between 320 K and 400K. This method can be used is several interesting applications such as designing new materials (polymers) at molecular level. Future work includes testing the method on others systems, and bench making with results obtained in the laboratory (experimental).

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