Revised Osmotic Pressure Estimation Program

Seung Jae Lim, Shin Hyo Bang, and Taeseon Yoon

***Abstract*—Recently, the Computer Technology advanced profoundly that the application has no limit. Equipped with programming, we wanted to make a program which is related to molecular science. While finding an appropriate adoption of computer programming to molecular science, we thought that estimating osmotic pressure might be the one. Previously, our recent research about Boiling Point Estimation Program [1] was highly recognized by international journal. Generally speaking, cellular membranes are semipermeable which allows osmosis to happen. To some extent, osmosis is explained by Van't Hoff Equation, which assumes solute's movement to be same as that of ideal gas. On this paper, however, we will use the modified version (to explain osmosis of real solution) of Van der Waals Equation, which is the corrected version of ideal gas equation.**

***Index Terms*—Revised, osmotic pressure, van der waals equation, van't hoff equation.**

I. Introduction

In this paper, we are going to suggest a computer related model which estimates osmotic pressure. Molecular Sciences and informatics seem an ill-assorted couple. Molecular Sciences is the scientific study of the structure of substances and of the way that they react with other substances. Informatics, by the way, is a study of the computer and statistics. We cannot discover chemical mechanisms by computer works. A standard, and traditional procedure for researching the field of molecular sciences would be doing experimental works. However, by analyzing the chemical patterns using informatics, we at least expect to demonstrate existing laws, or even gain new ones. The informatics could be used as a tool for molecular sciences.

The importance of computer in the field of Molecular Sciences is increasing; this year, three U.S. scientists won the Nobel chemistry prize on for pioneering work on computer programs. Similarly, we wanted to adopt a computer program into the world of molecules.

II. Experiment Object

A. Osmosis

Osmosis is a type of diffusion. When there is permeable membrane (selectively accept substances to pass through) osmosis can occur. Cell membrane is well-known partially permeable membrane. Fig. 1 shows osmosis very well. In Fig 1, P_{1a} is the high solute concentration solution and P_{2a} is the low solute concentration solution. At initial state, they remain steady with same height of water. At final state, however, water, which represents solvent of solution, rose up because the semi-permeable membrane between P_{1a} and P_{2a} caused osmosis that water from low solute concentration (P_{2a}) move to high solute concentration (P_{1a}). If the cell is submerged in saltwater, water molecules move out; if it is submerged in freshwater, however, water molecules move in; this is called osmosis. The selective cell membrane makes only necessary materials are let into the cell and wastes are left out.

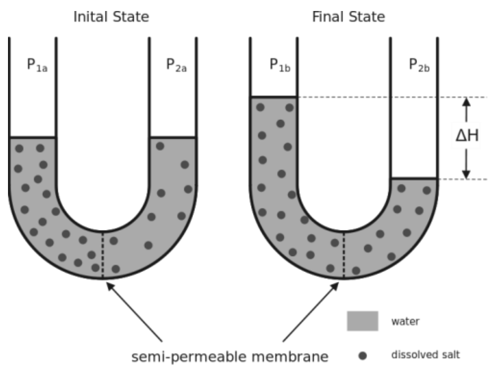

Fig. 1. Osmosis with Semi-permeable Membrane [2].

Osmosis can be explained using the concept of thermodynamic free energy: There are more free energy with low solute concentrated solution. Thus, its solvent molecules try to find a place of lower free energy in order to equalize free energy. Because the semi-permeable membrane selectively allows materials, only solvent molecules can pass through it. As a result, a net flow of water to the side with the higher solute concentrated solution. Let's assume that permeable membrane doesn't broke up. Then, this net flow will slow and finally stop at the equilibrium of the atmosphere pressure and osmotic pressure: this state is called dynamic equilibrium.

B. Ideal Gas Equation and Its Revision

$$PV = nRT \tag{1}$$

Equation (1) is Ideal Gas Equation [3]. The state of gas has always been a big interest for molecular scientists. And they drew the equation so called 'Ideal Gas equation.'

TABLE I: Difference between Ideal Gas & Real Gas

	Ideal Gas	Real Gas
Volume	X	O
Interaction Between Molecules	X	O

However, the ideal gas equation is literally available only

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for ideal gas. Since real gas has its own volume of each molecule and interaction between those, factors in the equation should be revised. The total volume of gas includes the volume of consisting molecules. Assuming the volume of the molecule as b, the total volume taken by molecules is *nb*. So the revised factor of volume should be *V-nb*.

According to the ideal gas equation, 1-mol-gas filling 22.4L-container under 0 degrees Celsius should have a pressure of 1atm. However, the interaction between molecules results in a slightly decreased pressure. Interactions between molecules allow molecules to take less volume, which leads to the slight drop in pressure, which could be expressed as $P = \frac{nRT}{V} - k$. Basic physical rule says that the decreased distance between molecules results in the stronger interaction between those. If the volume increases, the distance between molecules will increase and the interaction will be weakened; the downsizing effect on pressure will decrease. Furthermore, if the number of molecules increases, which means the increased number of interactions, the dropping effect on pressure will increase. Van der Waals experimentally revised the pressure factor as $P - a\frac{n}{V^2}$ (*a* is a distinct value given to each gas).

$$(P - a\frac{n}{V^2})(V - nb) = nRT \tag{2}$$

Equation (2) is Van der Waals Equation (Real Gas Equation). The ideal gas equation is quite reliable under high temperature and low pressure condition, because such conditions make the interaction between molecules to be minimized.

C. State of Ideal Solution

$$\pi = iCRT, (i = 1 + (n-1)\alpha) \tag{3}$$

Equation (3) is Van't Hoff Equation. The Van't Hoff equation is same with the ideal gas equation. The equation explains the state of an ideal solution. The basic hypothesis of this equation is that the ideal solute will act just like ideal gas molecule in the ideal solvent.

A solute sometimes ionizes if it is an electrolyte. So, the number of molecules should be revised. The revision factor *i* depends on the number of ions the solute ionizes into. Also the degree of ionization affects *i*. Researchers found *i* to be $1+(n-1)\alpha$.

III. Induction of Revised Osmotic Pressure Equation

A. Explanation

While real gas has its revised version of equation that explains its state, so called 'Van der Waals Equation,' there is no existing estimation method for real solution. The Van't Hoff equation's hypothesis was that the solutes would act just like ideal gas molecules in ideal solution. Thus, it is thought that by adapting Van der Waals equation to estimate the osmotic pressure of real solutions.

TABLE II: Van der Waals Constants [4]

Name	A (L^2atm/mol^2)	b (L/mol)
Mercury	8.2	0.01696
Neon	0.2135	0.01709
Helium	0.03457	0.0237
Hydrogen	0.2476	0.02661
Nitric oxide	1.358	0.02789
Water	5.536	0.03049
Oxygen	1.378	0.03183
Argon	1.355	0.032
Ammonia	4.225	0.0371
Nitrogen	1.408	0.03913
Krypton	2.349	0.03978
Carbon monoxide	1.505	0.03985
Hydrogen chloride	3.716	0.04081
Carbon dioxide	3.64	0.04267
Methane	2.283	0.04278
Hydrogen sulfide	4.49	0.04287
Nitrous oxide	3.832	0.04415
Nitrogen dioxide	5.354	0.04424
Hydrogen bromide	4.51	0.04431
Hydrogen selenide	5.338	0.04637
Xenon	4.25	0.05105
Phosphine	4.692	0.05156
Acetylene	4.516	0.0522
Fluoromethane	4.692	0.05264
Silicon tetrafluoride	4.251	0.05571
Chlorine	6.579	0.05622
Sulfur dioxide	6.803	0.05636
Silane	4.377	0.05786
Ethane	5.562	0.0638
Chloromethane	7.57	0.06483
Methanol	9.649	0.06702
Cyanogen	7.769	0.06901
Dimethyl ether	8.18	0.07246
Carbon disulfide	11.77	0.07685
Ethanethiol	11.39	0.08098
Ethanol	12.18	0.08407
Ethylamine	10.74	0.08409
Propane	8.779	0.08445
Chloroethane	11.05	0.08651
Dimethyl sulfide	13.04	0.09213
Freon	10.78	0.0998
Acetic acid	17.71	0.1065
Acetone	16.02	0.1124
Benzene	18.24	0.1154
Acetonitrile	17.81	0.1168
Diethyl sulfide	19	0.1214
Butane	14.66	0.1226
Acetic anhydride	20.158	0.1263
Carbon tetrachloride	19.7483	0.1281
Fluorobenzene	20.19	0.1286
Diethyl ether	17.61	0.1344
Ethyl acetate	20.72	0.1412
Cyclohexane	23.11	0.1424
Chlorobenzene	25.77	0.1453
Pentane	19.26	0.146
Toluene	24.38	0.1463
Germanium tetrachloride	22.9	0.1485
Bromobenzene	28.94	0.1539
Tin tetrachloride	27.27	0.1642
Iodobenzene	33.52	0.1656
Hexane	24.71	0.1735

B. Induction

According to Van't Hoff Equation, osmotic pressure is described as multiple of Van't Hoff's factor (*i*), molar concentration of solute (*C*), gas constant (*R*) and absolute temperature (*T*).

$$\pi = iCRT \tag{4}$$

Equation (4) which is a Van't Hoff Equation, concentration of solute (*C*) is same as mol of solute per volume of solution ($\frac{n_s}{v}$, n_s : mole of solute, *V*: volume of solution).

$$\pi V = in_s RT \tag{5}$$

By adapting (4), (5) is induced. According to Van't Hoff equation, osmotic pressure in solution and ideal gas' pressure are known to be the same. In other words, P, which represents pressure of ideal gas according to ideal gas equation, and π, which represents osmotic pressure are same. So, Van der Waals equation can be used to correct and revise Van't Hoff equation to be more appropriate for estimating real solution's osmotic pressure. But, there are a few things to be corrected before adapting it. *V*, which is the volume of solution replaced with $V - in_s b$, has difference with Van der Waals equation's modified volume $(V - nb)$, because in solution, factor *i* exists, which depends on whether solute is electrolyte or not. In ideal gas, it should be considered with gas molecules' own volume. However, in solution, it should be considered with increased volume effect due to ionization if it is electrolyte. So, factor *i* is added to describe increased mol of solute. Similarly, π, which is the pressure of solute (same as gas), has difference with Van der Waals equation's revised pressure $(P - a\frac{n^2}{V^2})$. Factor *i* should be added contingently considering whether the solute is electrolyte or not.

$$(\pi - a(\frac{(in_s)^2}{V^2})(V - in_s b) = in_s RT \tag{6}$$

Using these facts, (6) which is revised Van't Hoff equation with Van der Waals equation, subsequently induced after (5).

$$\pi_r = \frac{\{1+(n-1)\alpha\}n_s RT}{V - \{1+(n-1)\alpha\}n_s b} + a\frac{[\{1+(n-1)\alpha\}n_s]^2}{V^2} \tag{7}$$

Lastly, by organizing equation and changing factor *i* with specific equation $(i = 1 + (n-1)\alpha)$, (7) which is revised osmotic pressure equation (Lim's Equation) induced. Additionally, specific equation of factor *i*, *n* represents for the number of ionized ion per one chemical species and *α* represents for degree of ionization.

IV. Programming and Application

A. Source Code

1) PHP[5]

```
if ($sec1=="Electrolyte")
  $numbers=(((1+($g8-1)*$g7)*$g5*0.082*$g2)/(($g1-(1+$g8-1)*$g7)*$g5*$g4))+($g3*(((1+($g8-1)*$g7)*$g5)*((1+($g8-1)*$g7)*$g5))/($g1*$g1));
  else
    $numbers=((1*$g5*0.082*$g2)/(($g1-1)*$g5*$g4))+($g3*((1*$g5)*(1*$g5))/($g1*$g1));
```

2) HTML[6]

```
<p>Volume (V) : <font color="black"><input type=text name=g1 size=4></font> L</p>
<p>Temperature(T) :<font color="black"><input type=text name=g2 size=4></font> K</p>
<p>a : <font color="black"><input type=text name=g3 size=4></font> L2atm/mol2    </p>
<p>b : <font color="black"><input type=text name=g4 size=4></font>L/mol</p>
<p>Mole of Solute(ns) :<font color="black"><input type=text name=g5 size="12"></font> mol</p>
<p>R=0.082atm.L/mol.k</p>
<p>Degree of Ionization (alpha) :<font color="black"><input type=text name=g7 size=4></font></p>
<p>Number of Ions (n) :<font color="black"><input type=text name=g8 size=4></font></p>
```

The program is made with php language. The code shown above is the most essential part of the entire source code. The required variations in Revised Van't Hoff Equation are named gN. If the user selects the solute as 'electrolyte,' the shown program implements. The internet address for this program is http://125.247.90.14/~osmotic/.

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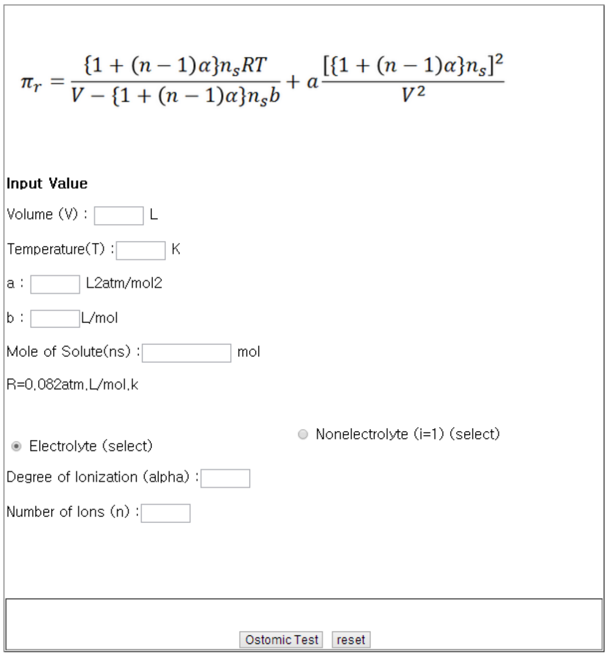

V. Experiments

A. Real Osmotic Pressure

The solution used in the experiment was made by adding

5.945g NaCl (approximately 0.1 mol) into 1.315L of water. The solution was extracted into twenty 100μL samples using micro pipet. These 20 samples' osmotic pressure was measured by Osmomat Auto (HWASHIN Instrument co.). The average osmotic pressure of solution was 3.49atm.

B. Program Based Osmotic Pressure

According to the revised osmotic pressure estimation program, the osmotic pressure should be approximately 3.48atm. On the other hand, the osmotic pressure calculated by Van't Hoff equation was 3.46atm. The observational error of using Van't Hoff equation was 0.03atm and using revised osmotic pressure equation was 0.01atm. Thus, revised osmotic pressure equation significantly fits with real state solution even more than Van't Hoff equation.

VI. Conclusion

A. Results

This research gained a formula which efficiently accounts for the osmotic pressure of real solutions. Furthermore, building a computer related program shows the potential of informatics that could be applied to chemistry

B. Expectations

There exists a revised equation for the state of gas, but none for solutions. Inspired by Van der Waals equation, authors revised osmotic pressure equation and made an estimation program. The result of experiment was successful which means that revised osmotic pressure equation fits well in real state.

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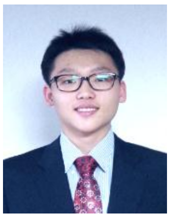

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