Journal of Applied Sciences

ISSN 1812-5654

science alert

ANSInet
an open access publisher
http://ansinet.com

Journal of Applied Sciences 12 (9): 809-821, 2012
ISSN 1812-5654 / DOI: 10.3923/jas.2012.809.821

Computing Density Profile and Square End To End Distance of Protein using MS Visual Studio C++

[1]Ali Khwaldeh, [2]Amani Tahat and [3]Hala Al Edwan
[1]Department of Computer Engineering, Faculty of Engineering, Philadelphia University Amman, Jordan
[2]Department of Physics and Nuclear Engineering, Technical University of Catalonia, Barcelona, Spain
[3]Department of Physics, University of Hail (Girls Branch), Hail, Saudi Arabia

Abstract: This study modified and examined an intensive numerical model adopted from a previous study of the peptide-lipid system to study more complex proteins. The density profile $\rho(z)$ as well as the mean square end to end distance R(z) of the protein near the cell membrane interface have been computed by using the programming language MS Visual Studio C++ based on the Green's function technique. The study discussed the analytical modifications and its corresponding verification, the results and chart discussions were illustrated and compared with those of literature. This study addressed that the asymmetry of the composition plays an important role in determining the character of the behavior of the peptide chain at interfaces, increasing the value of χ makes distribution narrower and vice versa and the statistical weight (G) of this system is proportional to the number of conformations of the protein chain with ends fixed at z and z_0. The model can be used in predicting the experimental results with sufficient accuracy for the same computed values.

Key words: MS Visual Studio C++, GUI, mean square end-to-end R (z), density profile P (z)

INTRODUCTION

Computational modeling (e.g., nuclear and engineering, business...etc) has been rapidly growth within scientific researches and industry. During the process of developments, new circumstances may be come to light (e.g., new problems, areas of application and techniques appearing in modern dynamical processes in physics, chemistry, engineering and economics), (SIAM Working Group on CSE Education, 2001). Developers have produced numerous novel mathematical algorithms aimed at stimulating many complex natural systems. Therefore, to enhance the performance analysis of such computer simulations an innovative ideas and foundational analysis for algorithms are required. Many examples of such algorithms included in mathematical models and computer codes in science and engineering can be found in literature including research of business management (Taiwo, 2007; Mosa *et al*., 2003) can work as a good example industry. In the meantime (Yedjour *et al*., 2011) is a biocomputational as well as neural network example. Furthermore, the new numerical algorithms of (Ponalagusamy, 2008) can be considered as a good example in the field of software engineering. The current study can be considered as good example of computing mathematical methods in biology science based on the use of green's functions (Bayin, 2006).

Cell membranes are multifarious systems, sensitive to various elements such as environmental stress or the presence of other molecules besides containing a rich mixture of lipids. They are able to adjust their shape and fluidity next to another properties as well as a reaction to the new surroundings. Many questions about how the properties of membranes are regulated still have to be answered (Pandhal *et al*., 2008). The main objective of this work was to investigate the effects of interaction between the proteins and the lipid on the conformation and adsorption of the protein. The protein will be modeled as copolymer of specific monomers. The choice of the amino acids sequence distribution of the amino acids along the copolymer chain is to simulate structure of the protein. This amino acids distribution will be used in the numerical modeling. This will be established through:

- Computing the density profile $\rho(z)$ of the protein by using the Green's function technique (Bayin, 2006)
- Computing the mean square end-to-end distance of protein near the cell membrane interface

The theoretical and computational methods of this work are based on the basic theoretical model developed by Khattari (1999). Diblock copolymer system is very important and has been synthesized in several studies (Baimark *et al*., 2008; Baimark and Phromsopha, 2009).

Corresponding Author: Amani Tahat, Department of Physics and Nuclear Engineering, Technical University of Catalonia, Barcelona, Spain

The adsorption behavior of diblock copolymer at interfaces will be extended to study a more complex copolymers or proteins. In particular, we will use the density profiles evaluated in the above reference and the mean square end-to-end distance of the copolymer, for further calculation which describes the adsorption of the protein near the cell membrane. The conclusion and results of Khattari (1999) were important for understanding the properties of the biological macromolecules like protein at penetrable interfaces. Where, such diblock copolymer exhibits stretching or elongation state which is associated with the non-Gaussian behavior so many systems can be derived from the diblock copolymer system by studying the Gaussian behavior and controlling some parameters like) χN (N is the number amino acids of the protein), is the interaction parameter between the polymer and the cell interface), in the limit ($\chi N \to \infty$) (strong segregation regime) the coil is stretched. Such systems can be important in understanding the properties of the effect of synthetic channel forming peptides on the phospholipid bilayer membrane structure at penetrable interfaces.

ANALYTICAL MODIFICATIONS AND ITS CORRESPONDING VERIFICATION

The peptide-membrane interaction, channel forming and ion penetration through the membrane channel can be studied by using the profile density approach p(z). The equations (1, 2, 3, 4 and 5) have been reported by Khattari (1999). The following set of equations present those equations, respectively:

$$p(z) = \frac{1}{\Omega}(p_{-}(z)\theta(-z) + p_{+}(z)\theta(z)) \quad (1)$$

where (p-(z) and (p+(z) are obtained as:

$$p-(z) = I-(z,f)I+(-z,1-f) \quad (2)$$

$$p_{+}(z) = I-(-z,1-f)I_{+}(z,f) \quad (3)$$

$$I-(z,f) = -\mathrm{erf}\left(\frac{z}{\sqrt{12fR_g^2}}\right) + \frac{1}{\pi}\int_0^1 \frac{\exp\left(-\frac{(z/Rg)^2}{12fu} + \chi fN(u-1)\right)}{\sqrt{u(1-u)}}du \quad (4)$$

$$I_{+}(z,f) = \mathrm{erf}\left(\frac{z}{\sqrt{12fR_g^2}}\right) + \frac{1}{\pi}\int_0^1 \frac{\exp\left(-\frac{(z/R_g)^2}{12fu} - \chi fNu\right)}{\sqrt{u(1-u)}} \quad (5)$$

The current updated analytical modifications and its corresponding verification can be started from Eq. 4. It reads the density of the diblock copolymer. Where, the composition, f = NA/ (NA+NB) and the radius of gyration, $R^2_g = Nl^2/6$.

COMPUTATIONAL AND MATHEMATICAL TECHNIQUES

Deriving the peptide-lipid system equations: In this study, the protein will be modeled as copolymer of specific monomers for investigating the effect of protein and lipid interaction on the conformation and adsorption of the protein.

We adopted the amino acids sequence distribution of the amino acids along the peptides chain to simulate the structure of the protein. Denote monomers as (two components A and B) (polypeptide). On the other hand, denote copolymer chain as (multicomponent peptide of portion chain) to simulate the idea of the previous study (Khattari, 1999) with its extension (this study).

Assumptions: To simulate the system let copolymer represents the protein, (copolymer = protein), Monomers (A and B) = Peptides A and B, (polypeptides) where (A and B) are consists of two N = s sequences. Studying the system is depended on (N). N represents the number of amino acids sequence in (A and B) along the portion chain. NA = n1+n2 (2 sequence) NB = n3+n4 (2 sequence), In the meantime N total = n1+n2+n3+n4. (Polypeptide) = multicomponent peptide.

Consider a (multicomponent peptide chain of the protein consists of two components (A and B) each of them has two amino acids sequence of peptide (N = N1+N2+N3+N4) with several junction points (z_0, z_1, z_2, z_3, z_4, z_5, ...z'), as illustrated in Fig. 1. (N) is the number of amino acids sequence in the peptides A and B of the protein chain.

Khattari (1999) addressed that the statistical weight (G) is proportional to the number of conformations of the diblock copolymer with ends fixed at z and z0. We can implements the same idea in our system, where, the density profile of the system is equal to the number of conformations of the (multicomponent peptide) chain as a function of the position of the joint points of theses conformations (peptides). Suppose that we have two conformations A and B, then the number of conformations (density profile = P (Z)) is given by Eq. 6 adopted from the Greens functions:

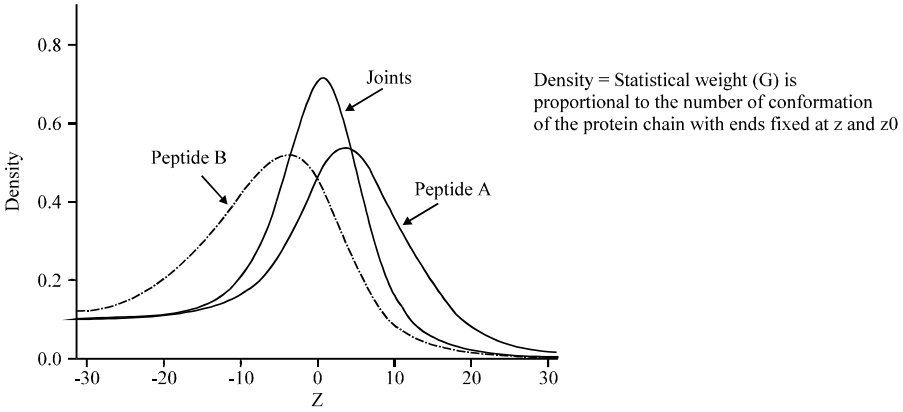


Fig. 1: Peptides (A, B) of the protein chain and its junction points

$$P(z)=\frac{1}{\Omega}\int\int_{-\infty}^{+\infty} G_{\chi}(Z',N_A;Z,0)G_{\chi}(Z,N_B;Z_0,0)dz'dz_0 \quad (6)$$

Where:

$$G_{AB}(z,N;z_0,0)=\int_{-\infty}^{+\infty} G_{\chi}(z,N_A;z')G_{\chi}(z',N_B;z_0,0)dz' \quad (7)$$

The normalization constant (Ω) is given by Eq. 8:

$$\Omega=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} G_{\chi}(z',N_A;z,0)G_{\chi}(z,N_B;z_0,0)dz'dz_0dz \quad (8)$$

where, $N_A = N1+N2$, $N_B = N3+N4$ and $N = N1+N2+N3+N4$ and substituting this into Eq. 6 will lead to Eq. 9:

$$p(z)=\frac{1}{\Omega}\int G_{\chi}(Z',N_1,Z_1,0)G_{\chi}(Z_1,N_2,Z_2)G_{\chi}(Z_2,N_3,Z_3) G_{\chi}(Z_3,N_4,Z_0,0)dz'dz_1dz_3dz_0 \quad (9)$$

Herein, we are searching to get an expression of p (z_2) like the one appears in equation (Eq. 10), to match the following (Khattari, 1999) equations:

$$p(z_2)=\int\int_{-\infty}^{+\infty} G_{\chi}(Z',N_1,Z_1,0)G_{\chi}(Z_1,N_2,Z_2)dz'dz_1p(Z_2,N_1,N_2)$$
$$P(Z_2,N_1,N_2)=P12(Z_2)$$

$$P(Z2)=\int\int_{-\infty}^{+\infty} G_{\chi}(Z_2,N_3,Z_3)G_{\chi}(Z_3,N_4,Z_0,0)dz_3dz_0$$
$$P(Z_2,N_3,N_4)=P_{34}(Z_2)$$

Integrating the above equations with respect to (z', z_1, z_0, z_2, z_3) leads to the required expression of $p(z_2)$ that stands for the density profile of the multicomponents peptide around the junction (z_2) can be written by using Eq. 10:

$$P(z_2)=P_{12}(Z_2,N_1,N_2)\times P_{34}(Z_2,N_3,N_4) \quad (10)$$

On the other hand, for studying the stretching properties of the peptide chain at the interface we calculate the mean square end-to-end distance of the system as a function of the distance to the interface by using the produced data of the computed equation (Eq. 10). Simply the produced density profile will be multiplied by $(Z_2)^2$ as illustrated in equation (Eq. 11):

$$< R^2 >= Z_2^2\times P_{12}(Z_2)P_{34}(Z_2) \quad (11)$$

From now and then we will use P_{12} instead of P_A and P_{34} instead of P_B.

We need to derive an expression for both p_{12} and p_{34} starting from equation (Eq. 1) In order to compute the required density profile p(z) this leads to the following derivations:

- The density profile of p_{12} at $z = z_2$ where, the total numbers of the amino acids in this (peptide) is $N = N1+N2$. Let $N_1 = 1$ and $N_2 = 1$, Eq. 12 appears in appendix 1
- The density profile of p_{34} at $z = z_2$ where the total numbers of amino acids on this peptide is $N = N3+N4$. Let $N3 = 1$ and $N4 = 1$, Eq. 13 appears in appendix 2

Rewriting the above derived equations (Eq. 12 and 13) into a simpler form in order to compute them enables us to get a new equation sets (Eq. 14 and 15) besides which represents the total density profile of the system p (z_2). Theoretical and computational processes of the density profile are listed below:

- Input values:

Ω – ...
Z_2 – ...
f – ... (0 < f < 1)
R_g – ...
χ – ...
N – ...

- Intermediate values:

$$A_1 = \frac{Z_2}{\sqrt{12fR_g^2}} \Rightarrow A_1^2 = \frac{(Z_2/R_g)^2}{12f}$$

$$A_2 = \frac{Z_2}{\sqrt{12(1-f)R_g^2}} \Rightarrow A_2^2 = \frac{(Z_2/R_g)^2}{12(1-f)}$$

$$B_1 = \chi fN \quad B_2 = \chi(1-f)N$$

The following new expressions of p_{12} and p_{34} can be written by substituting the intermediate values in to the derived equations:

$$\rho_{12}(Z_2) = \frac{1}{\Omega}*\left[-\mathrm{erf}(A_1)+\frac{1}{\pi_0^1}\int\frac{\exp\left(-\frac{A_1^2}{u}+B_1(u-1)\right)}{\sqrt{u(1-u)}}du\right]*\left[\mathrm{erf}(-A_2)+\frac{1}{\pi_0^1}\int\frac{\exp\left(-\frac{A_2^2}{u}-B_2u\right)}{\sqrt{u(1-u)}}du\right]*\Theta(-Z_2)$$
$$+\frac{1}{\Omega}*\left[-\mathrm{erf}(-A_2)+\frac{1}{\pi_0^1}\int\frac{\exp\left(-\frac{A_2^2}{u}+B_2(u-1)\right)}{\sqrt{u(1-u)}}du\right]*\left[\mathrm{erf}(A_1)+\frac{1}{\pi_0^1}\int\frac{\exp\left(-\frac{A_1^2}{u}-B_1u\right)}{\sqrt{u(1-u)}}du\right]*\Theta(Z_2) \quad (14)$$

$$\rho_{34}(Z_2) = \frac{1}{\Omega}\left[-\mathrm{erf}(A_1)+\frac{1}{\pi_0^1}\int\frac{\exp\left(-\frac{A_1^2}{u}+B_1(u-1)\right)}{\sqrt{u(1-u)}}du\right]*\left[\mathrm{erf}(-A_2)+\frac{1}{\pi_0^1}\int\frac{\exp\left(-\frac{A_2^2}{u}-B_2u\right)}{\sqrt{u(1-u)}}du\right]*\Theta(-Z_2)$$
$$+\frac{1}{\Omega}\left[-\mathrm{erf}(-A_2)+\frac{1}{\pi_0^1}\int\frac{\exp\left(-\frac{A_2^2}{u}+B_2(u-1)\right)}{\sqrt{u(1-u)}}du\right]*\left[\mathrm{erf}(A_1)+\frac{1}{\pi_0^1}\int\frac{\exp\left(-\frac{A_1^2}{u}-B_1u\right)}{\sqrt{u(1-u)}}du\right]*\Theta(Z_2) \quad (15)$$

$$\text{Denote: } \mathrm{fIntegral}(a,b,m) = \frac{1}{\pi}\int_0^1\frac{\exp\left(-\frac{a}{u}+b(u-m)\right)}{\sqrt{u(1-u)}}du = \frac{\exp(-bm)}{\pi}\int_0^1\frac{\exp\left(-\frac{a}{u}+bu\right)}{\sqrt{u(1-u)}}du$$

Then:

$$\rho_{12}(Z_2) = \frac{1}{\Omega}*\begin{cases}\left[-\mathrm{erf}(A_1)+\mathrm{fIntegral}(A_1^2,B_1,1)\right]*\left[\mathrm{erf}(-A_2)+\mathrm{fIntegral}(A_2^2,-B_2,0)\right] & ,Z_2 \le 0\\ \left[-\mathrm{erf}(-A_2)+\mathrm{fIntegral}(A_2^2,B_2,1)\right]*\left[\mathrm{erf}(A_1)+\mathrm{fIntegral}(A_1^2,-B_1,0)\right] & ,Z_2 > 0\end{cases}$$

$$\rho_{12}(Z_2) = \frac{1}{\Omega}*\begin{cases}\left[\mathrm{fIntegral}(A_1^2,B_1,1)-\mathrm{erf}(A_1)\right]*\left[\mathrm{fIntegral}(A_2^2,-B_2,0)-\mathrm{erf}(A_2)\right] & ,Z_2 \le 0\\ \left[\mathrm{fIntegral}(A_1^2,-B_1,0)+\mathrm{erf}(A_1)\right]*\left[\mathrm{fIntegral}(A_2^2,B_2,1)+\mathrm{erf}(A_2)\right] & ,Z_2 > 0\end{cases}$$

Knowing that p_{12} and p_{34} have the same expressions by following (Eq. 14 and 15) equations. As well they may have the same value when N1 = N2 = N3 = N4 = 1. This means that we can rewrite Eq. 11 by using p_{12} instead of p_{34}, thus, P (total) = P (z_2) = (P_{12}) 2, But changing the values of N = s will generate different values of p_{12}, p_{34} and p (total), respectively. Consequently the values of p(z) will be different for different compositions (F). On other words the statistical weight (G) of this system is proportional to the number of conformations (amino acids) of the peptide with ends fixed at z and z0, Fig. 1.

Program over viewing: This program is namely called (Ro calculation); it provides a graphical user interface (GUI), works under the operating system (windows). It produced tabulated data files. Appendix 3 defines the class behaviors for the application. However, this program makes it easy to specify the input file in order to schedule the computation processes, besides viewing and saving the output data, therefore, it allows typical calculations to be carried out far away from the deeply understanding of the theoretical physics of this topic. The program has a source file written in the programming language C++. Moreover, user has two options to run the program, each option has a different set of input parameters that allows studying the density profile under several preconditions related to the specified case study via the suitable interface. Section three presents such case studies. Figures 2 and 3 present the two GUI interfaces of the program.

Selecting the first interface allows user to calculate the density profile ($p(Z_2)$, p_{12} ,p_{34}) beside calculating the intermediate values by inserting six parameters (Ω, Z_2, f, Rg, X, N),in this case user has to set these parameters by following his specified case study , almost it is a general case depended on (N) total (the total number of amino

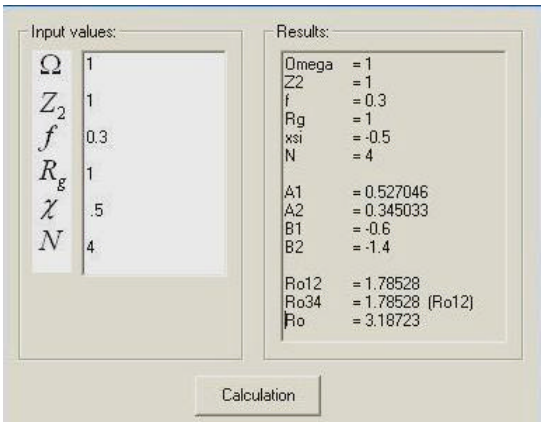
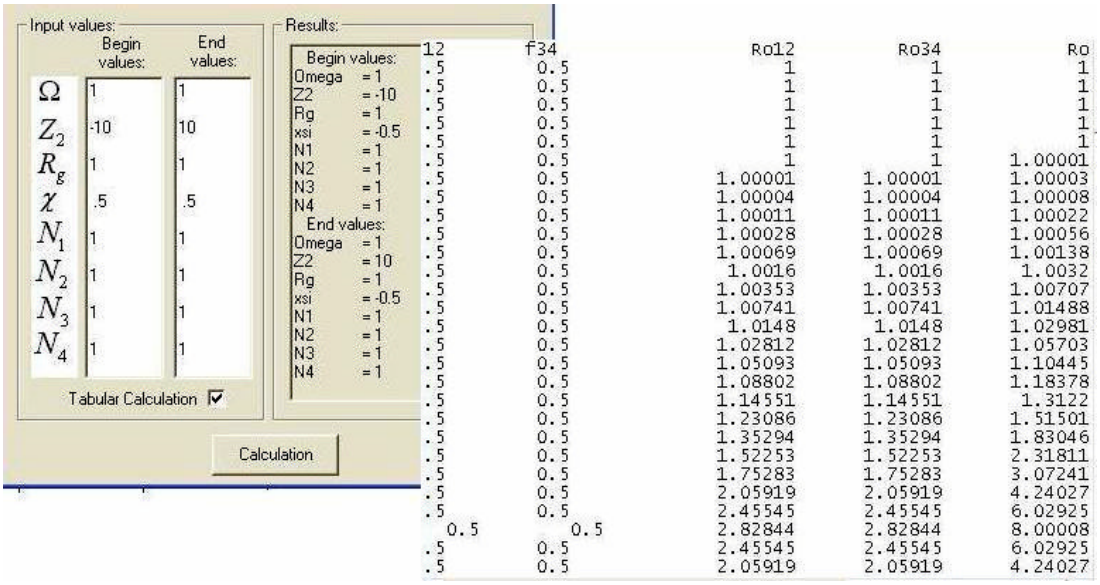


Fig. 2: The main screen of the first option (general case)



12	f34	Ro12	Ro34	Ro
.5	0.5	1	1	1
.5	0.5	1	1	1
.5	0.5	1	1	1
.5	0.5	1	1	1
.5	0.5	1	1	1
.5	0.5	1	1	1
.5	0.5	1.00001	1.00001	1.00003
.5	0.5	1.00004	1.00004	1.00008
.5	0.5	1.00011	1.00011	1.00022
.5	0.5	1.00028	1.00028	1.00056
.5	0.5	1.00069	1.00069	1.00138
.5	0.5	1.0016	1.0016	1.0032
.5	0.5	1.00353	1.00353	1.00707
.5	0.5	1.00741	1.00741	1.01488
.5	0.5	1.0148	1.0148	1.02981
.5	0.5	1.02812	1.02812	1.05703
.5	0.5	1.05093	1.05093	1.10445
.5	0.5	1.08802	1.08802	1.18378
.5	0.5	1.14551	1.14551	1.3122
.5	0.5	1.23086	1.23086	1.51501
.5	0.5	1.35294	1.35294	1.83046
.5	0.5	1.52253	1.52253	2.31811
.5	0.5	1.75283	1.75283	3.07241
.5	0.5	2.05919	2.05919	4.24027
.5	0.5	2.45545	2.45545	6.02925
0.5	0.5	2.82844	2.82844	8.00008
.5	0.5	2.45545	2.45545	6.02925
.5	0.5	2.05919	2.05919	4.24027

Fig. 3: The main screen plus the tabulated output file of the second option

acids in the multicomponents peptide chain (polypeptide) so that user can set the parameter (f) to any value where 0< f <1. Selecting this option means that user can get one output value for each density profile ($p(Z_2)$, p_{12} ,p_{34}) then by using the technique of (copy and paste) user can compose his own output data to be plotted elsewhere . On the other hand Fig. 3 presents the main screen of the second interface of the program which allows studying the effect of changing the parameters (N1, N2, N3, N4) instead of studying the effect of N (total) alone, where, N = N1+N2+N3+N4. Herein, the values of (f) will be changed following the values of N1, N2, beside N3+N4 which affect the value of p12 and p34, respectively. The input values panel is consists of two parts (begin values and end values) in order to determine the interval of changing them. For example if user need to calculate the values of (P_{12}, P_{34} , P (total)) when -10 ≤Z2≤ 10 he can set the begin value to -10 and the end value to 10, after filling all other required fields and pressing the button (calculation) the output file window will be opened automatically to show the tabulated data. This file can be saved and imported to excel, origin or any related program to be plotted. Next section includes more descriptions.

Program verifying and data validity: Here, we will generate data by using the produced program all data and charts will be compared with those of (Khattari, 1999). The produced data will be used for studying the interfacial properties of the multicomponents peptide of the protein chain by calculating the density profile (of the unit 10-6 mole cm^{-3}) for several cases beside calculating the mean square end-to-end distance for studying the stretching properties of the protein chain for several cases. This was established through:

Table 1: The data are generated by using the currently program (the first interface of it)

Z2	P(f =0.3, x = 0.54)	p(f = 0.5, x = 0.54)	p(f = 0.7, x = 0.54)
-1	5.22E+11	4.26E+11	5.56E+11
0	1.31497E+12	1.05124E+12	1.31497E+12
1	5.56E+11	4.26E+11	5.22E+11

- Calculating the density profile for different values of (f) for the same value of (χ = 0.54) and different values of (χ) for f = 0.5
- Calculating the mean square end-to-end distance for different values of (f) for the same value of (χ = 0.54) and different values of (χ) for (f = 0.5)
- Calculating the density profile for different values of (f) at the same value of x

Case one: Table 1 shows the data are generated by using the currently program (the first interface of it), (Fig. 2).

Calculating the density profile as a function of the distance from the interface z, where, z = -1, 0, 1 the density distribution of the system is shown for different values of f (f = 0.3, 0.5, 0.7) for χ = 0.54, the case f = 0.5 is

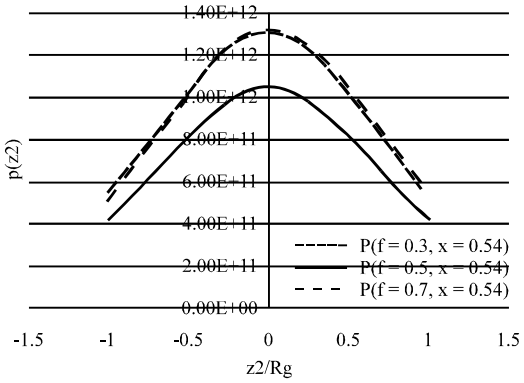


Fig. 4: The density profile as a function of the distance from the interface z by using the currently program

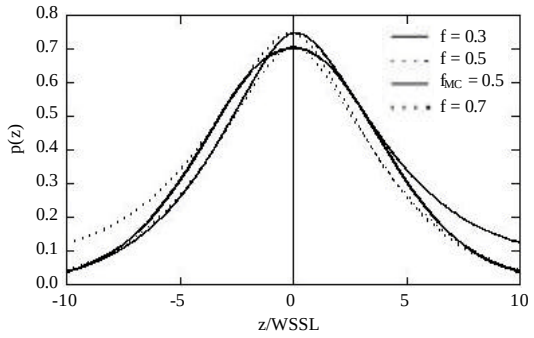


Fig. 5: The density profile as a function of the distance from the interface z, for different values of f(0.3, 0.5, 0.7) where χ = 0.54 and N = 32, as adopted from Khattari (1999)

compared with the MC results. The values N = 32, Rg = 1, Ω = 1 are used in obtaining the density profiles. Table 1 and Fig. 4 presents the results.

Data analysis: From Table 1 and Fig. 4, we can study the density distribution of the protein chain around z = 0, for different compositions f. (0.3, .0.5, 0.7). The density profile is symmetric for f = 0.50 with respect to the position of the interface z = 0, asymmetric and it is asymmetric for compositions f = 0.30 or 0.70.

Data validity: Figure 5 presents the density profile as a function of the distance from the interface z, for different compositions f (0.3, .0.5, 0.7) it has been adopted from (Khattari, 1999). Generally our results show a very good agreement with both Khattari (1999) and the prediction of Monte Carlo Simulations (MCS) Matsen and Bates (1997) results. We verified this fact by comparing the density profiles results of Fig. 4 with density profiles results of Fig. 5. It is as expected, the density profile is symmetric for f = 0.50 with respect to the position of the interface z = 0 and it is asymmetric for compositions f = 0.30 or 0.70 in the Fig. 4 and 5. in the most transparent symmetric case a comparison with the prediction of MCS shows a very good agreement with our generated data as appeared in Table 1 when f = 0.5, (χ) = 0.54 around z = 0. Because the Monte Carlo Simulations (MCS) predicts that the density profile in this status at the same conditions where, f = 0.5 must be symmetric for composition f = 0.5. Figure 4 and 5 illustrate the same behavior of the relation between p (z) and z/Rg, so that Leads to the same curve when plotting (p (z) versus z/Rg) but not the same values of p (z) because (Khattari, 1999) has dealt with the density profile as a function of the distance from the interface z, in units of wSSL where the radius of gyration in these units is Rg = 4.2 wSSL. Whereas, Rg = 1 in all of our calculation. (Khattari, 1999) also presented a comparison for the density profile with the Monte Carlo Simulations (MCS) for the case f = 0.5 this comparison was in a good agreement with our results.

Case two: Calculating the density profile as a function of the distance from the interface z, where, z = (-10, 0, 10). The density distribution of the (p total, $p_{12,}$ $p_{34)}$ is shown for different values of f (f = 0.001, 0.5, 0.999), respectively. Thus, for χ = 0.54, N = 32, Rg = 1, Ω = 1. Table 2 and Fig. 6, show the results.

Table 2 show the data of case 2, generated by using the (first interface of the program) (Fig. 1).

Data analysis: Figure 6 shows the density profiles of p_{12} and p_{34} for the strongly asymmetric composition (f = 0:999 or 0:001) and the density profile of P (total) with symmetric composition (f = 0:50).

Data validity: The Fig. 7 show that the asymmetry of the composition plays an important role in determining the character of the behavior of the peptide chain at interfaces. In the meantime that the protein chain prefers the region where, the concentration of one kind of the amino acid is rich. As a consequence of this rearrangement of the amino acids, the peak of the distribution no more coincides with the interface position at z = 0. For example, in the regime of strongly asymmetric composition the longer part of the protein chain affects the density profile dramatically. In this case, the whole profile appears to be very similar to a profile of a pure homopolymer chain. Our results present a very good agreement with those of (Khattari, 1999) as appeared in Fig. 6. Another comparison of the symmetric case

Table 2: The data of case 2, generated by using the (first interface of the program), (Fig. 1)

Z2	P_{12} (f = 0.001, χ = 0.54)	P (total) (f = 0.5, χ = 0.54)	P_{34} (f = 0.999, χ = 0.54)
-10	7.98E-01	4.26E+11	0.01
0	1.30E-01	1.25E+13	1.30E-01
10	1.11E-02	4.26E+11	0.93421

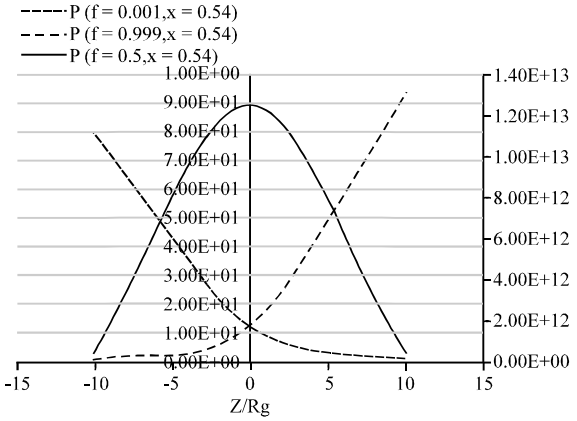


Fig. 6: The density profile of (P (total), p_{12}, p_{34}) as a function of the distance from the interface z

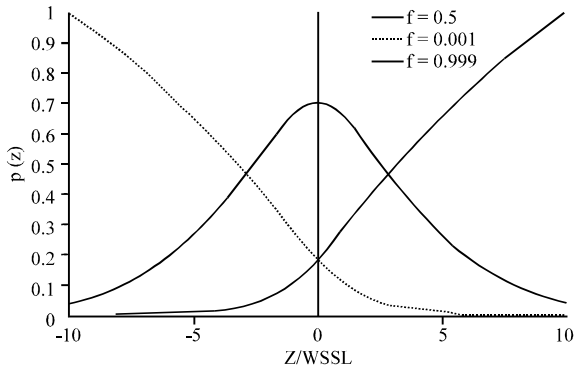


Fig. 7: The density profile of the whole system plus the subsystems density profiles as a function of the distance from the interface z, in units of wSSL, adopted from Khattari (1999), χ = 0.54, f = 0.5, 0.001, 0.999., N=32, Ω = 1

between our numerical evaluations and those of (Khattari, 1999) is illustrated in Fig. 7.

Case 3: This case depends on generating data with respect to several conditions in order to study the effect of changing the parameter (f). The generated data are illustrated in Fig. 8-11 besides Table 3 and 4.

By comparing our figures with those of (Khattari, 1999), we found that the density profiles of the MCS are slightly broader than the other density profile, nevertheless the agreement is very good. The density

Table 3: Data of Fig. 10 generated by using the second part of the program (Fig. 3)

z	p_{12} (f =0.4)	p_{34} (f =0.4)	pt (f =0.4)	p_{12} (f =0.5)	p_{34} (f =0.5)	pt (f =0.5)	p_{12} (f =0.6)	p_{34} (f =0.6)	p (=0.6)
-10	0.010	0.0001	0.010	0.100	0.100	0.001	0.023	0.001	0.000023
-3.2	0.300	0.002	0.310	0.480	0.480	0.230	0.400	0.001	0.420
0	0.100	0.100	0.395	0.532	0.531	0.282	0.100	0.100	0.490
3.2	0.001	0.300	0.310	0.480	0.480	0.230	0.001	0.400	0.420
10	0.000	0.010	0.010	0.100	0.100	0.001	0.001	0.023	0.000023

Table 4: P (total), at different values of, f = 0.5, N = 32, Rg = 1, Ω = 1

z	P (total, χ = 0.54)	p (total, χ = 0.75)	p (total, χ = 0.85)
-10	1.00006	1.0016	1.00767
0	1.05124E+12	1.68874E+23	1.22E+23
10	1.00006	1.0016	1.00767

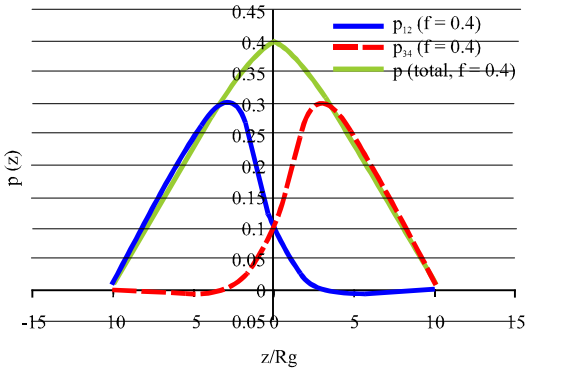


Fig. 8: The density profile of the whole protein chain as well as the individual peptides (p_{12}, p_{34}) in the symmetric case for =.54, Rg=1, Ω = 1, N=32

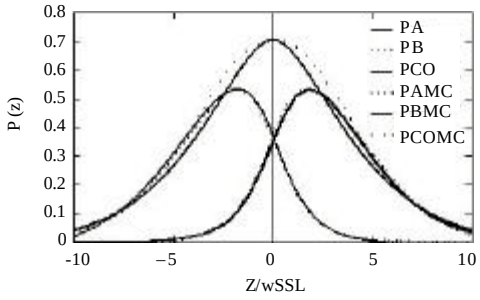


Fig. 9: The density profile as a function of the distance from the interface z, in units of wSSL, the density distribution of the whole system (PAB) are shown as well as the individual subsystems (PA and PB) and compared with the predications of the MC results for the symmetric case for = 0.54. Adopted from Khattari (1999)

profiles of the whole system (p (total) = p_{12}*p_{34}) and of the individual profiles (p_{12}, p_{34}) for different compositions (f = 0:50, 0:40 and 0:60) are shown in Fig. 8.

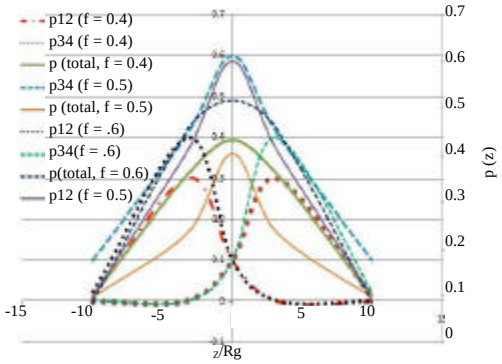


Fig. 10: The density distribution of the whole system and the individual subsystems for f=0:5, 0:4 and 0:6 for = 0:54, Rg=1, N=32, Ω = 1(Table 3)

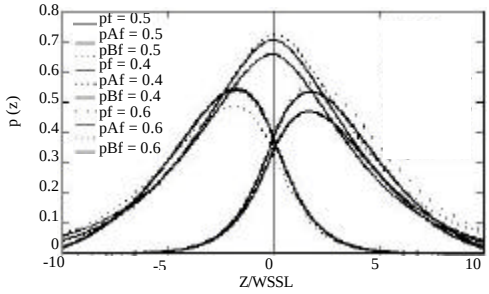


Fig. 11: The density profile as a function of the distance from the interface z, in units of wSSL, the density distribution of the whole system and the individual subsystems for f = 0:5, 0.4 and 0.6 for x = 0.54. Adopted from Khattari (1999)

The Fig. 11 show that the asymmetry of the composition plays an important role in determining the character of the behavior of the peptide chain at interfaces.

In Table 4, p(total), at different values of, f = 0.5, N = 32, Rg = 1, Ω = 1

Figure 12 p(total) versus z/Rg, where, Rg =1, Ω =1, f = 0.5

Calculating the Density Profile for Different Values of (χ) at the Same Value of (f): The dependence of the interfacial profile on the interaction parameter χ is illustrated in Fig. 12-13 and Table 4. The profiles are shown for χ = 0.54, 0.75 and 0.85 at symmetric composition f = 0.50. It shows how the distribution profile of the protein chain is affected by the variation of the interaction between the peptides and interface.

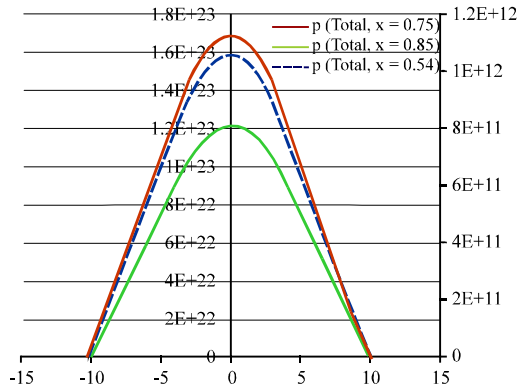


Fig. 12: P (total) versus z/Rg, where, Rg =1, Ω =1, f = 0.5

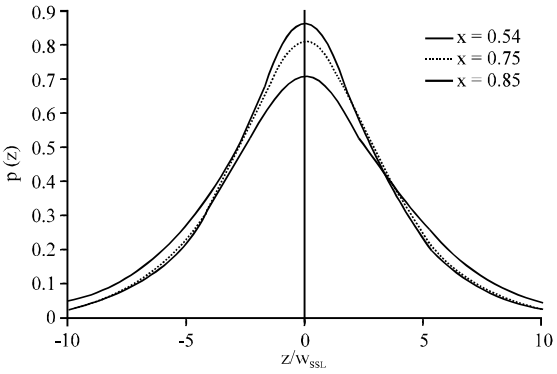


Fig. 13: The density profile as a function of the distance from the interface z, in units of wSSL, the density distribution of different values of x, for f = 0.5, adopted from Khattari (1999)

From the Fig. 12 and 13 we can noted that increasing the value of χ makes distribution narrower and vice versa. This can be interpreted due to the effect of localization of the peptide_protien at the interface. A common feature of all the above profiles is that the peaks of the distributions are broader than the gyration radius Rg. The above results agree with the experiments of Dai *et al.* (1994) and Russell *et al.* (1991) and with the simulations of Werner *et al.* (1996) plus the mean field theory of Noolandi and Hong (1982).

The stretching properties of the peptide chain: In this section, we consider the stretching properties of the protein chain (peptides+amino acids). Figure 14 and 15, illustrate the chain stretching in the direction perpendicular to the interface. This Fig. 14 and 15 shows the z-component of the mean square end-to-end distance obtained by using Eq. 11 after computing the

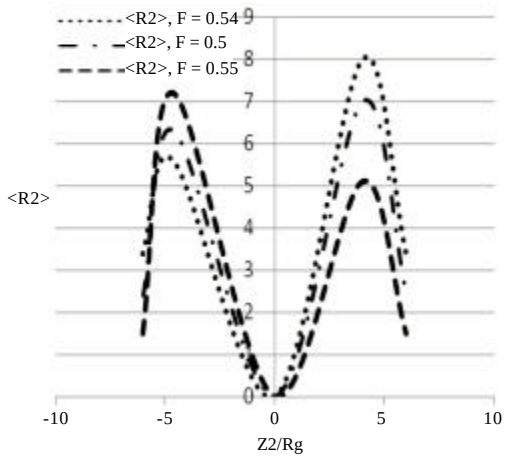


Fig. 14: The mean square end-to-end distance by using the current program, for χ = 0.54, different values of f (0.54, 0.5, 0.55), Rg = 1, N = 32.Ω = 1

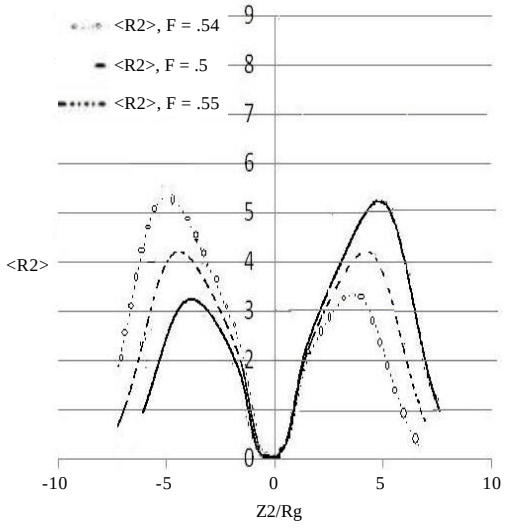


Fig. 15: The mean square end-to-end distance obtained by using the current program (second interface), for χ = 0.54, different values of f (0.54, 0.5, 0.55). Rg = 1, N = 32 but N1 = 8, N2 = 8, N3 = 8, N4 = 8, Ω=1

density profile for different compositions (f = 0.50, 0.45 and 0.55). The figures are shown a good agreement with Fig. 16 that was adopted from Khattari (1999). Moreover, this picture was confirmed in many previous investigations such the experiments of Sommer and Daoud (1995) and by simulations Sommer *et al*. (1996), in addition to the study of Werner *et al*. (1996). The effect of the stretching is very strong for those peptides that

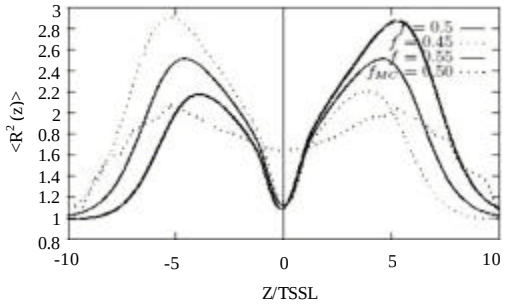


Fig. 16: The mean square end-to-end distance in unites of a2N = 3, plotted vs. z=wSSL. The results are shown for different values of f for χ = 0.54, the symmetric case is compared with the MC results. Adopted from, Khattari (1999)

centered at about two to three gyration radii away form the interface but it almost disappears for the peptides that centered at the interface.

The mean square end-to-end distance by using the current program, for = 0.54, different values of f (0.54, 0.5, 0.55). Rg = 1, N = 32, Ω = 1 (Fig. 14).

The mean square end-to-end distance obtained by using the current program (second interface), for = 0.54, different values of f (0.54, 0.5, 0.55). Rg =1, N = 32 but N1 = 8, N2 = 8 ,N3 = 8 ,N4 = 8, Ω =1 (Fig. 15).

The mean square end-to-end distance in unites of a2N = 3, plotted vs. z = wSSL (Fig. 16). The results are shown for different values of f for = 0:54, the symmetric case is compared with the MC results. Adopted from, Khattari (1999).

The effect of the interaction of the peptide components with the interface is illustrated in Fig. 17, the data of mean square end-to-end distance was generated by using Eq. 11 after computing the density profile of this case for three different values of the interaction parameter χ = 0:54, 0:65 and 0:75 for two compositions f = 0:50 and 0:40. Our results show a good agreement with Khattari (1999) results that is illustrated in Fig. 18. It is understandable from Fig. 18, that the central region and the wings of the protein chain density profiles (p_{12}, p_{34}) are hardly affected by increasing the value of the interaction parameter between the peptide parts and the interface. On the other hand the amount of the peptides located at about two to three gyration radii is more affected by this variation of the interaction parameter. Increasing the value of (χ) results in stretching the protein chain coil in its rich phase. From these results we can say that peptide chain behaves as it would be

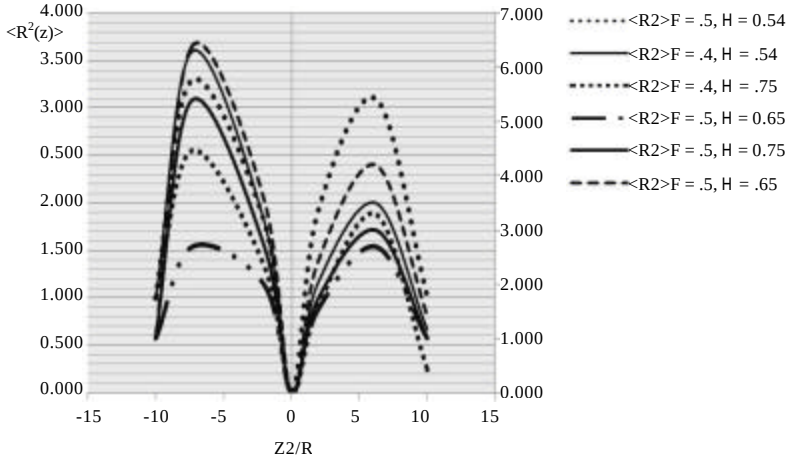


Fig. 17: The mean square end-to-end distance the results are shown for different values of χ for f = 0.5 and 0.4. by using the currently program

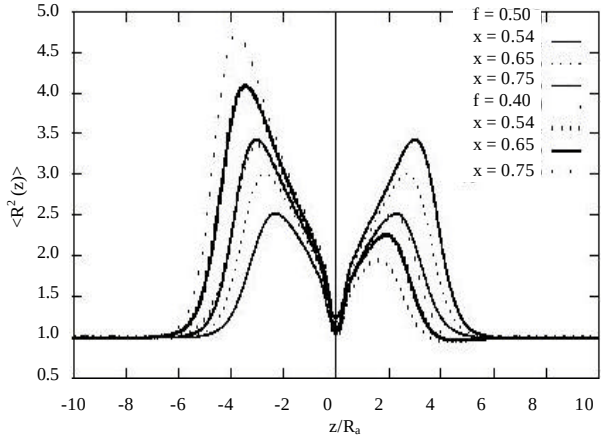


Fig. 18: The mean square end-to-end distance in unites of a2N = 3, plotted vs. z = wSSL. The results are shown for different values of x for f = 0.5 and 0.4, adopted from Khattari (1999)

composed of two independent parts that associated with the non-Gaussian behavior when stretching. However, this is associated with the chain stretching. The existence of the chain stretching is clear hint that the system exhibits a crossover from the weak segregation to the strong segregation regimes. In the weak segregation regime, where it is assumed that the chain is Gaussian coil, the structure is not affected by the parameter χN (N is the number amino acids of the protein, χ is the interaction parameter between the polymer and the cell interface) in contrast, in the limit ($\chi N \rightarrow \infty$) (strong segregation regime) the coil is stretched. Such systems can be important in understanding the properties of the biological macromolecules like protein at penetrable interfaces (Muller and Schmid, 1998).

DISCUSSION

The density profile $\rho(z)$ and mean square end-to-end distance R(z) of the protein near the cell membrane interface have been effectively computed by using the programming language C++ (MS VS) based on the Green's function technique adopted from Khattari (1999). The modified model has been successfully used in generating data easily. The analytical modifications and its corresponding verification has been discussed, results and charts were illustrated and compared with those of literate. The program allowed a rapid processing and viewing of the calculated data for all density profiles ($p(z_2)$, p_{12}, p_{34}), in addition to all intermediate parameters that might be used in the calculations. In order to

determine the accuracy of the calculations and enable testing the results with respect to several preconditions, the program provided an access to many parameters such as (N, Rg, Ω, (χ), Z, f, N_1, N_2, N_3) . Input parameters can be easily entered through a friendly graphical user interface (GUI), however, the model has two different interfaces and each one has its own function for saving user time and verifying the output data. Outputs data has two types a single value of each density profile (p_{12},p_{34},p(z_2)) and a set of values for each density profile following the specified rang of the input parameters (e.g., -10≤0≤10) .The scope of the future work is to add some other models(e.g., protein chain may consist of (A, B, C, D…) component (peptides). In general, the generated data showed a very good agreement with both Khattari (1999) and the prediction of Monte Carlo Simulations (MCS) Matsen and Bates (1997) results.

The current study addressed the following results:

- Changing the values of N's (amino acids) will generate different values of p_{12} , p_{34} as well as p (total), respectively. Consequently the values of p (z) will be different for different compositions (f). In other words the statistical weight (G) of this system is proportional to the number of conformations of the protein chain with ends fixed at z and z_0
- The asymmetry of the composition played an important role in determining the character of the behavior of the peptide chain at interfaces. Also the protein chain (peptide+amino acid) preferred the region where the concentration of one kind of the amino acids is rich. As a consequence of this rearrangement of the amino acids, the peak of the distribution no more coincides with the interface position at z = 0
- As a result of studying the effect of changing χ increasing the value of χ makes distribution narrower and vice versa. This can be interpreted due to the effect of localization of the peptide at the interface. A common feature of all tested profiles was that the peaks of the distributions are broader than the gyration radius Rg

Finally, the program Ro calculation should be useful in rapidly providing large amount of data for modeling peptide_ lipid system.

CONCLUSION

The current study has been successfully investigated the effects of interaction between the proteins and the lipid on the conformation and adsorption of the protein by using a MS Visual Studio C++ computer program that has been computed based on using the same mathematical techniques of a literature model of interfacial properties of diblock copolymers at penetrable interfaces but with diffident assumptions. To study system more complex proteins the new model can be expanded to include larger systems of more than two amino acids for (N = N_A+N_B+N_C+N_DYYNN); where, N > N_1+N_2+N_3+N_4.

FUTURE WORK

- Add plotting capabilities to the excitants numerical model
- Extend the model to include larger systems that may include more than two amino acids for N = N_A+N_B+N_C+N_D……NN where, N > N_1+N_2+N_3+N_4

APPENDIX

Appendix 1: Equation (Eq. 12)

$$\frac{1}{\Omega}*\left[\left[-\mathrm{erf}\left(\frac{Z_2}{\sqrt{12fR_g^2}}\right)+\frac{1}{\pi}\int_0^1\frac{\exp\left(-\left(Z_2/R_g\right)^2/12fu+\chi fN(u-1)\right)}{\sqrt{u(1-u)}}du\right]*\left[\mathrm{erf}\left(-Z_2/\sqrt{12(1-f)R_g^2}\right)+\frac{1}{\pi}\int_0^1\frac{\exp\left(-\left(-Z_2/R_g\right)^2/12(1-f)u-\chi(1-f)Nu\right)}{\sqrt{u(1-u)}}du\right]\right]*\Theta(-Z_2) \quad (12)$$

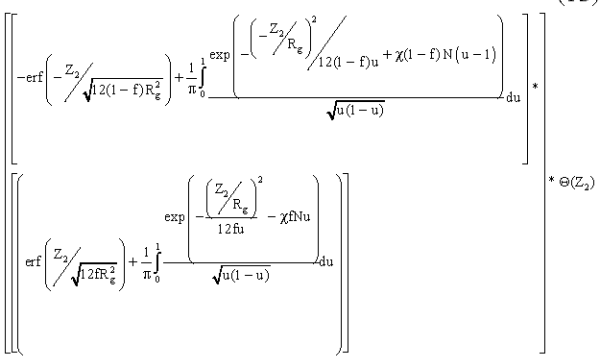
p_{12} (N_1, N_2, Z_2)

$$\frac{1}{\Omega}*\left[\left[-\mathrm{erf}\left(-Z_2/\sqrt{12(1-f)R_g^2}\right)+\frac{1}{\pi}\int_0^1\frac{\exp\left(-\left(-Z_2/R_g\right)^2/12(1-f)u+\chi(1-f)N(u-1)\right)}{\sqrt{u(1-u)}}du\right]*\left[\mathrm{erf}\left(Z_2/\sqrt{12fR_g^2}\right)+\frac{1}{\pi}\int_0^1\frac{\exp\left(-\left(Z_2/R_g\right)^2/12fu-\chi fNu\right)}{\sqrt{u(1-u)}}du\right]\right]*\Theta(Z_2)$$

Appendix 2: Equation (Eq. 13)

$$\frac{1}{\Omega}\left[\left[-\mathrm{erf}\left(Z_2/\sqrt{12fR_g^2}\right)+\frac{1}{\pi}\int_0^1\frac{\exp\left(-\left(Z_2/R_g\right)^2/12fu+\chi fN(u-1)\right)}{\sqrt{u(1-u)}}du\right]*\left[\mathrm{erf}\left(-Z_2/\sqrt{12(1-f)R_g^2}\right)+\frac{1}{\pi}\int_0^1\frac{\exp\left(-\left(-Z_2/R_g\right)^2/12(1-f)u-\chi(1-f)Nu\right)}{\sqrt{u(1-u)}}du\right]\right]*\Theta(-Z_2)+\frac{1}{\Omega}*$$

(13)



$p_{34}(N_1, N_2, Z_2)$

Appendix 3

```
// Ro Calculation. cpp : Defines the class behaviors for the application.

//

#include "stdafx.h"
#include "RoCalculation.h"
#include "RoCalculationDlg.h"

#ifdef _DEBUG
#define new DEBUG_NEW
#undef THIS_FILE
static char THIS_FILE[] = __FILE__;
#endif

/////////////////////////////////////////////////////////////////////////////
// CRoCalculationApp

BEGIN_MESSAGE_MAP(CRoCalculationApp, CWinApp)
	//{{AFX_MSG_MAP(CRoCalculationApp)
	//}}AFX_MSG
	ON_COMMAND(ID_HELP, CWinApp::OnHelp)
END_MESSAGE_MAP()

/////////////////////////////////////////////////////////////////////////////
// CRoCalculationApp construction

CRoCalculationApp::CRoCalculationApp()
{
}

/////////////////////////////////////////////////////////////////////////////
// The one and only CRoCalculationApp object

CRoCalculationApp theApp;

/////////////////////////////////////////////////////////////////////////////
// CRoCalculationApp initialization

BOOL CRoCalculationApp::InitInstance()
{
	// Standard initialization

#ifdef _AFXDLL
	Enable3dControls();  // Call this when using MFC in a shared DLL
#else
	Enable3dControlsStatic();  // Call this when linking to MFC statically
#endif

	CRoCalculationDlg dlg;
	m_pMainWnd = anddlg;
	int nResponse = dlg.DoModal();
	if (nResponse == IDOK)
	{
	}
	else if (nResponse == IDCANCEL)
	{
	}

	// Since the dialog has been closed, return FALSE so that we exit the
	// application, rather than start the application's message pump.
	return FALSE;
}
```

REFERENCES

Baimark, Y. and T. Phromsopha, 2009. Methoxy poly ethylene glycol-b-poly (D, L-lactide-co-glycolide) films as drug delivery systems for ibuprofen. Asian J. Sci. Res., 2: 87-95.

Baimark, Y., Y. Srisuwan, N. Kotsaeng and P. Threeprom, 2008. Preparation of surfactant-free and core-shell type nanoparticles of methoxy poly(ethylene glycol)-b-poly e-caprolactone-co-D, L-lactide diblock copolymers. Asian J. Applied Sci., 1: 237-245.

Bayin, S.S., 2006. Mathematical Methods in Science and Engineering. John Wiley and Sons, New York, USA., ISBN-13: 9780470041420, Pages: 679.

Dai, C.A., B.J. Dair, K.H. Dai, C.K. Ober and E.J. Kramer, 1994. Reinforcement of polymer interfaces with random copolymers. Phys. Rev. Lett., 73: 2472-2475.

Khattari, Z.Y., 1999. Behavior of diblock-copolymers and semi-flexible polymers at interfaces. Ph.D. Thesis, University of Halle, Germany.

Matsen, M.W. and F.S. Bates, 1997. Block copolymer microstructures in the intermediate-segregation regime. J. Chem. Phys., 106: 2436-2448.

Mosa, M., Z. Yuqun and A. Yattara, 2003. Development and simulation of an absorber for small-size Libr-H2O absorption refrigeration machines. J. Applied Sci., 3: 305-316.

Muller, M. and F. Schmid, 1998. Monte Carlo simulations of interfaces in polymer blends. http://arxiv.org/abs/cond-mat/9803111

Noolandi, J. and K.M. Hong, 1982. Theory of polymeric alloys. Polymer Bull., 7: 561-566.

Pandhal, J., P.C. Wright and C.A. Biggs, 2008. Proteomics with a pinch of salt: A cyanobacterial perspective. Saline Syst., Vol. 4, 10.1186/1746-1448-4-1.

Ponalagusamy, R., 2008. A novel and efficient computational algorithm of STWS for generalized linear non-singular/singular time varying systems. J. Software Eng., 2: 1-9.

Russell, T.P., S.H. Anastasiadis, A. Menelle, G.P. Felcher and S.K. Satija, 1991. Segment density distribution of symmetric diblock copolymers at the interface between two homopolymers as revealed by neutron reflectivity. Marcromolecules, 24: 1575-1582.

SIAM Working Group on CSE Education, 2001. Graduate education in computational science and engineering. SIAM Rev., 43: 163-177.

Sommer, J.U. and M. Daoud, 1995. Copolymers at selective interfaces. Europhys. Lett., 32: 407-412.

Sommer, J.U., G. Peng and A. Blumen, 1996. Copolymers at interfaces: Scaling and Monte Carlo studies. J. Phys. II, 6: 1061-1066.

Taiwo, A.S., 2007. Determination of the optimal manpower size using linear programming model. Res. J. Bus. Manage., 1: 30-36.

Werner, A., F. Schmid and K. Binder, 1996. Diblock copolymers at a homopolymer-homopolymer interface: A Monte Carlo simulation. Macromolecules, 29: 8241-8248.

Yedjour, D., H. Yedjour and A. Benyettou, 2011. Combining quine mc-cluskey and genetic algorithms for extracting rules from trained neural networks. Asian J. Applied Sci., 4: 72-80.