The Application of Shannon's Measure of Information for a Complex Chemical System

F. Safinejad,*,† A. Shafiee,‡ and M. Asghari-Khiavi†

Department of Chemistry, Tarbiat Modares University, P.O.Box 14115-175, Tehran, Iran. Department of Chemistry, Sharif University of Technology, P.O.Box 11365-9516, Tehran, Iran

Received: January 22, 2006; In Final Form: May 3, 2006

Information theory and, specifically, Shannon's measure of information is used to compare the interaction parameters (β) in regular solution theory (RST) and Ingram's model for the mixture of cetyltrimethylammonium bromide (CTAB) and Triton X-100 (TX100). Results show that β values from regular solution theory are more accurate than those of Ingram's model. Additionally, the procedure applied in this paper for the calculation of uncertainties in the continuous case, prevents difficulties concerning differential entropy.

1. Introduction

The number of literature articles investigating simple (physical) systems with information theory are numerous. But the applicability of information theory in complex systems, e.g., chemical systems has a great potential for development.[1−6]

Shannon's measure of information is a powerful measure of information in both classical and quantum domain.[7−10] This is a matter of controversy, however, that if one can extend the applicability of this measure to any new domain of examination.

Surfactants are chemical compounds with special physicochemical properties such as critical micelle concentration (cmc) in which surfactant molecules create some aggregates.

In this paper, we apply information theory to study a complex chemical system consisting of cationic surfactant cetyltrimethylammonium bromide (CTAB) and nonionic surfactant Triton X-100 (TX100). For this purpose, two models for the calculation of interaction parameter (β) were selected, that is, regular solution theory (RST) and Ingram's model. To compare the aforementioned models, we first determine the probability density of β in each model and then we calculate their uncertainties with two methods. Finally, mutual information will be used to assess the calculated uncertainties for interaction parameter and, therefore, the two models as a whole.

Our results in the present work show that regular solution theory is more accurate than Ingram's model.

In this paper, first we introduce some aspects of information theory that are related to this work. Then, two models for the calculation of interaction parameter are explained and we determine the probability density of β in each model. Finally, the uncertainties concerning interaction parameter are compared with each other and with an information−theoretic concept which is represented by the so-called mutual information.

2. Information Theory

Information theory deals with measurement and concept of information. We can attribute its origin to Shannon's paper in 1948[11], in which he investigated the mathematical theory of communication and introduced his well-known measure of information as

$$H = -\sum_{i=1}^{n} p_i \log_2 p_i, \tag{1}$$

where p_i is the probability of event i, n is the total number of events, and H is the measure of information, uncertainty, or entropy.

H satisfies the following three properties (Shannon's postulates):

(1) H is continuous in p_i.

(2) If all the p_i are equal, $p_i = (1/n)$, then H is a monotonic increasing function of n.

(3) If a choice is broken down into two successive choices, the original H is a weighted sum of the individual values of H.

2.1. Entropy of a Continuous Distribution. Relation 1 is the entropy of a discrete set of probabilities p_1, ..., p_n. In an analogous manner we can define the entropy of a continuous distribution as

$$h(X) = -\int_{\Gamma} f(x) \log f(x) dx, \tag{2}$$

where $h(X)$ is the differential entropy of a continuous random variable [Note: In applied statistics discrete random variables assume integer values and are associated with the process of *counting*. In contrast, a continuous random variable which can assume any value along a scale of values, is associated with the process of *measuring*.[12]] X with probability density function $f(x)$ and $x \in \Gamma$. $f(x)$ is greater than or equal to zero for all values of x.

Unfortunately, differential entropy has some conceptual and mathematical difficulties which prevent its application as a continuous measure of entropy:[13]

(1) Differential entropy may be negative.

(2) Differential entropy may become infinite.

(3) Differential entropy may vary under the transformation of the coordinate system.

(4) Despite its analogous form, differential entropy cannot be obtained as a limiting case of discrete entropy.

To overcome some of the above difficulties, some authors prefer to use the Kullback−Leibler entropy [Note: Higher Kullback−Leibler entropy means less uncertainty, in contrast

* Corresponding author e-mail: safinej@modares.ac.ir.

† Department of Chemistry, Tarbiat Modares University.

‡ Department of Chemistry, Sharif University of Technology (shafiee@sharif.edu).

10.1021/jp060450z CCC: $33.50
Published on Web 06/03/2006

with Shannon's entropy],

$$H_{KL}(X) = \int_{\Gamma} f(x) \log_2 \frac{f(x)}{m(x)}\, dx \tag{3}$$

for the entropy of a probability density function $f(x)$, $x \in \Gamma$. Here, $m(x)$ is a reference or standard distribution function that must be chosen appropriately.

Yet, the continuous distribution can potentially transfer infinite amounts of information, while the observer can receive information with a bounded accuracy. So, if the receiver has an infinite level of accuracy, it can detect an infinite amounts of information from a continuous distribution. In other words, entropy does not have a unique formula in the continuous case.

Here, we propose another possibility which might be useful in some circumstances. To clarify, consider a one-dimensional random variable X in a well-defined range $[a, b]$ and with a probability density $f(x)$. Suppose we divide the interval between a and b into subintervals Δa_i ($i = 1, 2, ..., n + 1$), with $\Delta a_i = a_i - a_{i-1}$, so that

$$P(a_{i-1} < X < a_i) = \int_{a_{i-1}}^{a_i} f(x)\, dx. \tag{4}$$

By inserting probabilities from relation 4 into relation 1, the entropy of the continuous distribution will be determined. This entropy depends on the number of subintervals and does not have the difficulties indicated about differential entropy. Choosing the number of subintervals depends on the type of problem one encounters and usually could be sufficiently limited.

2.2. Mutual Information. Mutual information or transinformation is a general correlation measure which is based on the information theoretic notion of entropy (relations 1 and 3). Mutual information between variables X and Y can be written as

$$I(X; Y) = H_{KL}(X, Y) - H_{KL}(X) - H_{KL}(Y), \tag{5}$$

where $H_{KL}(X)$ and $H_{KL}(Y)$ are the Kullback−Leibler entropies of the variables X and Y, respectively, and $H_{KL}(X, Y)$ is the joint Kullback−Leibler entropy of the variables X and Y. $I(X; Y)$ which is nonnegative (i.e., $I(X; Y) \geq 0$) and symmetric (i.e., $I(X; Y) = I(Y; X)$) can be interpreted as the part of information that is common to both variables or the information in X about Y. $I(X; Y)$ could be also defined as $H(X) + H(Y) - H(X, Y)$, where each H term is defined in relation 1.

3. Mixed Micelles and Interaction Parameter

The interaction parameter β, which is a dimensionless parameter, characterizes the interaction between two surfactant species in a mixed micelle. A negative value of β indicates an attractive interaction (the more negative the β value, the greater the attraction), a positive value of β implies a repulsion between the two species and $\beta = 0$ indicates that mixed micelle formation is ideal.[14−17]

In the following, we consider two models for the calculation of interaction parameter: Rubingh's regular solution theory and Ingram's Model [Note: In this study, we are interested in the uncertainties concerning β. We chose RST and Ingram's model, because each of these models represents a formula for the determination of β (i.e., relations 6 and 7) and β in each formula is related to the experimentally attainable quantity cmc].

3.1. Rubingh's Regular Solution Theory (RST). A regular solution is one for which $\bar{S}^E = 0$ and $\bar{V}^E = 0$, where $\bar{S}^E$ and $\bar{V}^E$ are molar excess entropy and molar excess volume, respectively.

Regular solution model can be used to investigate the nonideal mixed systems (mixed micellar solutions). According to this theory,[18]

$$\beta = \frac{\ln\left(\frac{y_1 cmc_{12}}{x_1 cmc_1}\right)}{(1 - x_1)^2}, \tag{6}$$

where y_1 is the molar fraction of surfactant 1 (CTAB) in the bulk solution, x_1 is the molar part of surfactant 1 in the mixed micelle, cmc_{12} is the critical micelle concentration of the mixture of surfactants 1 and 2, and cmc_1 is the critical micelle concentration of surfactant 1.

3.2. Ingram's Model. Ingram's model can be considered as a modification of the RST. Here, the interaction parameter β is evaluated by[18]

$$\beta = \frac{\ln\left(\frac{c_1}{x_1 cmc_1}\right)}{(1 - x_1)^2}, \tag{7}$$

where x_1 is the molar fraction of surfactant 1 (CTAB) in the mixed micelle, cmc_1 is the critical micelle concentration of surfactant 1, and c_1 is the monomer concentration of surfactant 1 in the bulk solution ($c_1 = y_1 c_t$, in which c_t is the total molar concentration of the two surfactants).

4. The Probability Density of β

Consider a set of (continuous) random variables X_1, ..., X_n and their joint probability density. We may be interested in finding the probability density of a random variable $Y = u(X_1, ..., X_n)$. This means that the values of Y are related to those of the X's by

$$y = u(x_1, ..., x_n). \tag{8}$$

Distribution function technique is a straightforward method to obtain the probability density of a function of continuous random variables. This technique consists of first finding the distribution function of Y and then its probability density by differentiation. So, the probability density of $Y = u(X_1, ..., X_n)$ can be obtained by[19]

$$f(y) = \frac{dF(y)}{dy} \tag{9}$$

where $F(y)$ is the value of the distribution function of Y at y and is given by

$$F(y) = P(Y \leq y) = P[u(X_1, ..., X_n) \leq y]. \tag{10}$$

Using the above procedure for β in RST, relation 6, we found $f(\beta)$, the probability density of β in the form

$$f(\beta) = \frac{d}{d\beta}\left[\frac{1}{2\sqrt{2\pi}} \int_{\frac{-\mu_1}{\sigma_1}}^{5} e^{\frac{-z_1^2}{2}} (\mathrm{erf}\,(\theta_1) + \mathrm{erf}\,(\theta_2))dz_1\right] \qquad -2.5 < \beta < 0 \tag{11}$$

with

$$z_1 = \frac{cmc_1 - \mu_1}{\sigma_1} \quad cmc_1 > 0 \tag{12a}$$

$$\theta_1 = \frac{1}{\sqrt{2}y_1\sigma_{12}}(x_1 z_1 \sigma_1 e^{\beta(1-x_1)^2} + x_1\mu_1 e^{\beta(1-x_1)^2} - \mu_{12}y_1) \tag{12b}$$

$$\theta_2 = \frac{\mu_{12}}{\sqrt{2}\sigma_{12}}. \tag{12c}$$

Here, μ_1, σ_1 are the mean and standard deviation of cmc_1 distribution and μ_{12}, σ_{12} are the mean and standard deviation of cmc_{12} distribution (cmc_1 and cmc_{12} have normal probability density). All the calculations were performed using Mathcad 12.

For CTAB/TX100 mixture, the quantities $y_1 = 0.5$ and $x_1 = 0.2937$ were obtained from ref 20 and $\mu_1 = 0.00099$ mol dm^{-3} and $\mu_{12} = 0.000312$ mol dm^{-3} from ref 21. $\sigma_1 = 0.0001$ mol dm^{-3} and $\sigma_{12} = 0.00004$ mol dm^{-3} were suggested according to the values of cmc_1 and cmc_{12}, respectively.

Similarly, we found $g(\beta)$, the probability density of β in Ingram's model, relation 7, as

$$g(\beta) = \frac{d}{d\beta}\left[\frac{1}{2} + \frac{1}{2}\,\mathrm{erf}\left(\frac{-c_1 e^{-\beta(1-x_1)^2} + x_1\mu_1}{\sqrt{2}x_1\sigma_1}\right)\right] \quad -1.9 < \beta < -0.4 \tag{13}$$

For CTAB/TX100 system, the quantities $c_1 = (1/2)(0.000312)$ mol dm^{-3} and $x_1 = 0.2937$ were obtained from ref 20 and $\mu_1 = 0.00099$ mol dm^{-3} from ref 21. $\sigma_1 = 0.0001$ mol dm^{-3} was suggested according to the values of cmc_1 ($c_1 = y_1 c_t$ is considered as a constant, since for the measurement of critical micelle concentration, y_1 and c_t are predetermined.).

5. Calculation of Uncertainties

We want to calculate $H(cmc_1)$, uncertainty of cmc_1 in mixed micelle; $H(cmc_2)$, uncertainty of cmc_2 in mixed micelle; $H(cmc_1, cmc_2)$, joint entropy of cmc_1 and cmc_2; $H(\beta)_{RST}$, uncertainty of β in RST and $H(\beta)_{Ing}$, uncertainty of β in Ingram's model with two methods.

The variables cmc_1 ($\mu_1 = 0.00063$ mol dm^{-3},[21] $\sigma_1 = 0.0001$ mol dm^{-3}) and cmc_2 ($\mu_2 = 0.000312$ mol dm^{-3},[21] $\sigma_2 = 0.00004$ mol dm^{-3}) have normal distributions [Note: The well-defined range for cmc values is $[-5\sigma + \mu, 5\sigma + \mu]$. In fact, integration can be restricted to this interval because the tails of the distributions do not contribute so much]. The joint probability density of cmc_1 and cmc_2 is a bivariate normal distribution with correlation coefficient $cor = 0.9$ obtained from data in the literature[21] for the mixture of CTAB/TX100 (see Table 1).

The mutual information I between variables cmc_1 and cmc_2 is

$$I(cmc_1; cmc_2) = H(cmc_1) + H(cmc_2) - H(cmc_1, cmc_2). \tag{14}$$

We apply mutual information as a criterion to decide which model (RST or Ingram) is more appropriate, since I is a correlation measure between two quantities concerning two surfactants CTAB and TX100 (that is, cmc_1 and cmc_2) and β is an interaction parameter between two surfactants CTAB and TX100 in mixed micelle. So, the concept of mutual information is similar to the concept of $H(\beta)_{RST}$ and $H(\beta)_{Ing}$ and can be used for their evaluation.

TABLE 1: The Values of cmc_1 and cmc_2 (in mol dm^{-3}) in Mixed Micelle[21]

y_1	cmc_1	cmc_2
0.8	0.00084	0.000366
0.75	0.00079	0.000341
0.67	0.00072	0.000336
0.5	0.00063	0.000312
0.33	0.00044	0.000297
0.25	0.00038	0.00028
0.2	0.00034	0.000275

5.1. First Method for the Calculation of Uncertainties. In the first method we use relation 3, in which $m(x)$ is selected in a way that the argument of the logarithm becomes dimensionless.

According to relation 3 we can determine $H_{KL}(cmc_1)$, $H_{KL}(cmc_2)$, $H_{KL}(cmc_1, cmc_2)$, $H_{KL}(\beta)_{RST}$, and $H_{KL}(\beta)_{Ing}$ as follows:

$$H_{KL}(cmc_1) = H_{KL}(X_1) = \int_{-5\sigma_1+\mu_1}^{5\sigma_1+\mu_1} p(x_1)\log_2[10\sigma_1 p(x_1)]\,dx_1 = 1.275 \text{ bits} \tag{15}$$

$$H_{KL}(cmc_2) = H_{KL}(X_2) = \int_{-5\sigma_2+\mu_2}^{5\sigma_2+\mu_2} q(x_2)\log_2[10\sigma_2 q(x_2)]\,dx_2 = 1.275 \text{ bits} \tag{16}$$

$$H_{KL}(cmc_1, cmc_2) = H_{KL}(X_1, X_2) = \int_{-5\sigma_2+\mu_2}^{5\sigma_2+\mu_2}\int_{-5\sigma_1+\mu_1}^{5\sigma_1+\mu_1} (x_1, x_2)s \log_2[100\sigma_1\sigma_2 s(x_1, x_2)]dx_1 dx_2 = 3.748 \text{ bits} \tag{17}$$

where $(1/10\sigma_1)$, $(1/10\sigma_2)$, and $(1/100\sigma_1\sigma_2)$ are reference normalized distributions in relations 15, 16 and 17, respectively. Also,

$$p(x_1) \equiv \frac{1}{\sigma_1\sqrt{2\pi}}\exp\left[\frac{-(x_1-\mu_1)^2}{2{\sigma_1}^2}\right], \tag{18}$$

$$q(x_2) \equiv \frac{1}{\sigma_2\sqrt{2\pi}}\exp\left[\frac{-(x_2-\mu_2)^2}{2{\sigma_2}^2}\right] \tag{19}$$

are the probability densities of cmc_1 and cmc_2, respectively and

$$s(x_1, x_2) \equiv \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-cor^2}}\exp\left[\frac{-z}{2(1-cor^2)}\right] \tag{20}$$

is the joint probability density of cmc_1 and cmc_2 in mixed micelle, in which

$$z \equiv \frac{(x_1-\mu_1)^2}{{\sigma_1}^2} - \frac{2cor(x_1-\mu_1)(x_2-\mu_2)}{\sigma_1\sigma_2} + \frac{(x_2-\mu_2)^2}{{\sigma_2}^2}. \tag{21}$$

Now, applying relations 14−17 we find

$$I(cmc_1; cmc_2) = 1.198 \text{ bits} \tag{22}$$

which we have used the relation 5 to obtain the above result.

TABLE 2: The Values of $H(cmc_1) = H(cmc_2)$, $H(cmc_1, cmc_2)$ and Mutual Information (I) in Several Divisions (n) for CTAB/TX100 Mixture (All the Values in Columns 2−4 Are in bits)

n	$H(cmc_1)$	$H(cmc_1, cmc_2)$	I
5	1.2412	1.9836	0.4987
10	2.1048	3.3621	0.8476
15	2.6583	4.3073	1.0093
20	3.0620	5.0406	1.0833
40	4.0508	6.9348	1.1668
60	4.6337	8.0835	1.1839
80	5.0480	8.9060	1.1900
100	5.3696	9.5464	1.1929
120	5.6325	10.0705	1.1944
140	5.8547	10.5141	1.1953
160	6.0473	10.8987	1.1960
180	6.2172	11.2380	1.1964
200	6.3692	11.5416	1.1967
250	6.6910	12.1849	1.1971
300	6.9540	12.7107	1.1974
350	7.1764	13.1553	1.1975
400	7.3690	13.5405	1.1976
450	7.5390	13.8802	1.1977
500	7.6910	14.1842	1.1977
1000	8.6909	16.1840	1.1979

TABLE 3: The Values of $H(\beta)_{RST}$ and $H(\beta)_{Ing}$ and Their Differences in Several Divisions (n) for CTAB/TX100 Mixture (All the Values in Columns 2−4 Are in bits)

n	$H(\beta)_{RST}$	$H(\beta)_{Ing}$	$H(\beta)_{Ing} - H(\beta)_{RST}$
5	1.5780	1.6056	0.0277
10	2.4868	2.5153	0.0285
15	3.0532	3.0821	0.0289
20	3.4615	3.4905	0.0290
40	4.4547	4.4839	0.0292
60	5.0382	5.0675	0.0293
80	5.4526	5.4819	0.0294
100	5.7742	5.8036	0.0294
120	6.0370	6.0664	0.0294
140	6.2592	6.2886	0.0295
160	6.4517	6.4812	0.0295
180	6.6215	6.6510	0.0295
200	6.7734	6.8029	0.0295
250	7.0951	7.1247	0.0296
300	7.3580	7.3876	0.0296
350	7.5803	7.6099	0.0296
400	7.7728	7.8025	0.0296
450	7.9427	7.9723	0.0296
500	8.0946	8.1243	0.0297
1000	9.0941	9.1239	0.0298

Furthermore, we can determine I directly as

$$I(cmc_1;cmc_2) = I(X_1;X_2) = \int_{-5\sigma_2+\mu_2}^{5\sigma_2+\mu_2}\int_{-5\sigma_1+\mu_1}^{5\sigma_1+\mu_1} s(x_1, x_2) \log_2\frac{s(x_1, x_2)}{p(x_1)q(x_2)}dx_1dx_2 = 1.198 \text{ bits} \quad (23)$$

The argument of the logarithm in relation 23 is dimensionless and so it does not need any correction. This shows that if the reference function in relation 3 is $m(x_1)$ for $H_{KL}(X_1)$ and $m(x_2)$ for $H_{KL}(X_2)$, then the reference function for $H_{KL}(X_1, X_2)$ should be $m(x_1)m(x_2)$. Therefore, the choice of $m(x)$ in relation 3 is arbitrary.

Also, using relation 3 we can obtain

$$H_{KL}(\beta)_{RST} = \int_{-2.5}^{0} f(\beta) \log_2[2.5\, f(\beta)]\, d\beta = 0.867 \text{ bit} \quad (24)$$

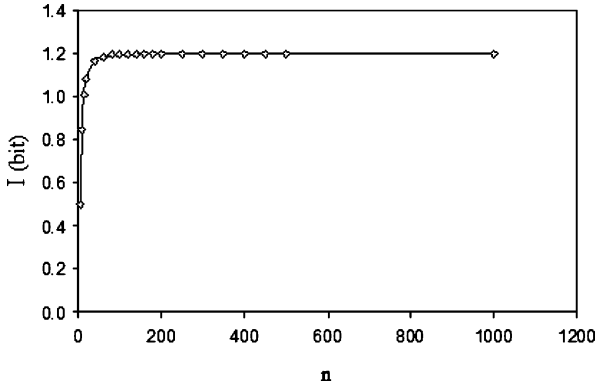

Figure 1. Plot of mutual information (I) versus divisions (n).

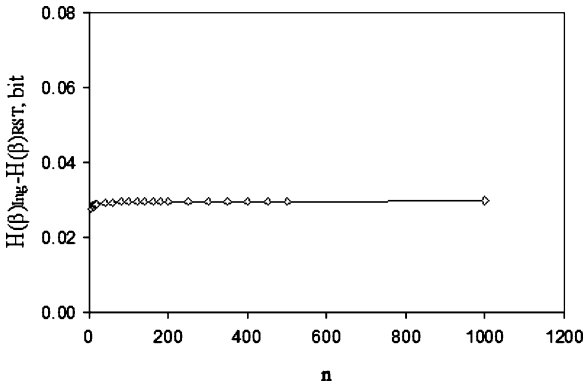

Figure 2. Plot of $H(\beta)_{Ing} - H(\beta)_{RST}$ versus divisions (n).

and

$$H_{KL}(\beta)_{Ing} = \int_{-1.9}^{-0.4} g(\beta) \log_2 [1.5g(\beta)]d\beta = 0.838 \text{ bit} \quad (25)$$

where $f(\beta)$ and $g(\beta)$ were substituted from relations 11 and 13, respectively.

Relations 24 and 25 show that $H_{KL}(\beta)_{RST} > H_{KL}(\beta)_{Ing}$, i.e., RST distribution is sharper than Ingram distribution. Moreover, the difference between $H_{KL}(\beta)_{RST}$ and $H_{KL}(\beta)_{Ing}$ is 0.029 bit.

5.2. Second Method for the Calculation of Uncertainties. In the second method we use relations 4 and 1 for different divisions, n to obtain the entropies (each division consists of equal subintervals. Dividing into equal subintervals is inevitable for the calculation of probabilities in this work, since here we want to compare the entropies.) subintervals). Results are shown in Tables 2 and 3.

Table 2 shows that $H(cmc_1)$, $H(cmc_2)$, and $H(cmc_1, cmc_2)$ increase with increasing the number of divisions (n), while I approaches the same value of 1.198 bits, according to relation 14 (see relation 22 and Figure 1) which is a great evidence for the correctness of our calculations.

Also, results in table 3 show that $H(\beta)_{RST}$ and $H(\beta)_{Ing}$ increase with increasing the number of divisions (n) and $H(\beta)_{Ing} - H(\beta)_{RST}$ approaches the constant value of 0.029 bit similar to the corresponding result in section 5.1 (see relations 24, 25 and Figure 2).

According to data in Tables 2 and 3, uncertainties $H(cmc_1)$, $H(cmc_2)$, $H(cmc_1, cmc_2)$, $H(\beta)_{RST}$, and $H(\beta)_{Ing}$ do not approach a constant value, indicating that we cannot find a unique $m(x)$ in relation 3.

A comparison between the values of $H(\beta)_{RST}$ and $H(\beta)_{Ing}$ shows that the uncertainty in RST is less than that of Ingram's model for a specific division and since we expect a model with less uncertainties, so β values in RST are more accurate than

those of Ingram's model. This fact can also be confirmed by the comparison between $H(\beta)_{RST} - I$ and $H(\beta)_{Ing} - I$, since $H(\beta)_{RST} - I < H(\beta)_{Ing} - I$ for each division.

Finally, the large difference between I and $H(\beta)$ (in both models), especially when n becomes large, can be attributed to the existence of auxiliary assumptions in the basis of these two models.

6. Conclusions

Information theory can be applied to study systems with different levels of complexity, like complex chemical systems. Here, the Shannon's measure of information was used for the comparison of β values in RST and Ingram's model. Results show that β values from RST are more reliable than those of Ingram's model.

More appropriateness of RST with respect to Ingram's model can also be explained with physical evidences. To calculate β in RST, we encounter two variables, cmc_{12} and cmc_1 (formula 6). In fact, the role of mixing is introduced directly in the formula of β due to cmc_{12}. But to calculate β in Ingram's model, we have one variable, that is, cmc_1 (formula 7). This difference also leads to different entropies in two models.

Relation 3 has some advantages over differential entropy (e.g., it does not change under the transformation of the coordinate system) but in some cases it may become infinite.

The strategy applied in this paper for the calculation of entropies or uncertainties in the continuous case (section 5.2), prevents the difficulties concerning differential entropy. We believe uncertainty in the continuous case has a relative interpretation and it depends on the way we look the problem (that is, on the number of divisions). But, relation 2 has an absolute interpretation (i.e., it refers to infinite number of divisions). So, we prefer to use directly the probabilities in relation 1 which are discrete, to avoid difficulties mentioned about differential entropy.

The regularity in results for the complex chemical compounds CTAB/TX100 (Tables 2 and 3), rather than simple physical systems, is remarkable and its repeatability for other complex systems is an open problem that must be examined in additional studies.

Our results endorse the appropriateness of the Shannon entropy as a criterion for the credibility of a model relative to another model even for complex compounds in chemical systems.

Acknowledgment. We acknowledge an anonymous referee of this journal for many helpful comments. We also thank Dr. N. L. Hadipour from Tarbiat Modares University.

References and Notes

(1) Hobson, A. *J. Chem. Phys.* **1966**, *45*, 1352.
(2) Bernstein, R. B.; Levine, R. D. *J. Chem. Phys.* **1972**, *57*, 434.
(3) Ben-Shaul, A.; Levine, R. D.; Bernstein, R. B. *J. Chem. Phys.* **1972**, *57*, 5427.
(4) Alhassid, Y.; Levine, R. D. *J. Chem. Phys.* **1977**, *67*, 4321.
(5) Levine, R. D. *Annu. Rev. Phys. Chem.* **1978**, *29*, 59.
(6) Fonseca, A. F.; Mesquita, M. V.; Vasconcellos, A. R.; Luzzi, R. *J. Chem. Phys.* **2000**, *112*, 3967.
(7) Duwell, A. *Stud. Hist. Philos. Mod. Phys.* **2003**, *34*, 479.
(8) Timpson, C. G. *Stud. Hist. Philos. Mod. Phys.* **2003**, *34*, 441.
(9) Mana, P. G. L. *Phys. Rev. A* **2004**, *69*, 062108.
(10) Shafiee, A.; Safinejad, F.; Naqsh, F. *Found. Phys. Lett.* **2006**, *19*, 1, e-print arXiv:quant-ph/0407198.
(11) Shannon, C. E. *Bell Syst. Technol. J.* **1948**, *27*, 379.
(12) Kazmier, L. J. *Basic Statistics for Business and Economics;* McGraw-Hill: Auckland, 1979.
(13) Reza, F. M. *An Introduction to Information Theory;* McGraw-Hill: New York, 1961.
(14) Bastiat, G.; Grassl, B.; Khoukh, A.; François, J. *Langmuir* **2004**, *20*, 5759.
(15) Carnero Ruiz, C.; Aguiar, J. *Langmuir* **2000**, *16*, 7946.
(16) Joshi, T.; Mata, J.; Bahadur, P. *Colloids Surf. A* **2005**, *260*, 209.
(17) Zhang, R.; Zhang, L.; Somasundaran, P. *J. Colloid Interface Sci.* **2004**, *278*, 453.
(18) Angarska, J. K.; Tachev, K. D.; Denkov, N. D. *Colloids Surf. A* **2004**, *233*, 193.
(19) Miller, I.; Miller, M. *John E. Freund's Mathematical Statistics;* Prentice Hall: New York, 1999.
(20) Razavizadeh, B. M. Ph.D. Thesis, Tarbiat Modares University, 2000.
(21) Gharibi, H.; Razavizadeh, B. M.; Hashemianzaheh, M. *Colloids Surf. A* **2000**, *174*, 375.