New Tools for Teaching Chemical Engineering Thermodynamics

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Abstract. The teaching toolbox described by Elliott and Lira (2000) has been expanded to include three new tools: molecular simulation, ConcepTesting, and a simplified version of the MOSCED model. The previous list of tools included: detailed derivations (e.g. Maxwell's relations), computational tools (calculator and xls), projects, homework, analogies, examples, tours, tests (including samples from past years), quizzes, and help sessions. Students were surveyed to rank these tools from "most instructive" to "least." The new tools are described briefly and the survey assessments are presented. The molecular simulation tool focuses on applets posted at: http://rheneas.eng.buffalo.edu/wiki/DMD. These applets provide visualization of molecular dynamics for ideal gases, hard spheres, and square-well spheres. The students are guided through several homework assignments in which they learn about temperature, energy, pressure, and system size. Further details are available online, so the remainder of this abstract focuses on the Simplified Separation of Cohesive Energy Density (SSCED). In the current work, the acidity and basicity parameters are adopted directly from the latest literature, but the polarity and dispersion parameters are lumped together and the total of all contributions is constrained to match the original Scatchard-Hildebrand solubility parameter. Three composition-dependent parameters of the MOSCED model are set to constants. In this way, the contrast between the physical interactions and the chemical interactions is more readily apparent and the model can be applied directly at all compositions in a self-consistent manner. Examples are given of in-class and exam assessments, along with homework assignments. The simplified model is intended to make the key concepts of hydrogen bonding accessible to any college student, including freshmen. ConcepTesting is demonstrated with in-class assessments of the SSCED model. ConcepTesting refers to an interactive form of class engagement especially as it applies to the use of student response "clickers." Students are prompted with multiple choice questions and their responses are instantly collected and displayed electronically. Students are encouraged to work in small groups (~3) in developing their responses. A strict interpretation of ConcepTesting would limit questions to abstract conceptual content. In our implementation, we integrate conceptual content with more conventional examples and problem solving. This leads to a class that is continuously engaged.

Keywords: Activity coefficient, ConcepTesting, MOSCED, molecular dynamics.

1. Introduction

It seems that the freshmen are onto me. As part of our freshman "Chemical Engineering Computations" course, the students can choose speakers for four half-lectures. Last Spring, they chose me to give a presentation about hydrogen bonding. Rumor has it that they heard of a fanatic professor who was particularly fanatic about thermodynamics, with a soft spot for the

topic of hydrogen bonding. Their strategy was two-fold: first, to butter this guy up by asking him to ramble on about his favorite subject and second, to scout the demon of this dangerous domain called thermodynamics. In my turn, I saw this as a teachable moment. If I made the presentation sufficiently accessible, they might accidentally learn something about thermodynamics.

But what computational model can be accessible to freshmen in 25 minutes and explain hydrogen bonding and its role in chemical engineering? A little scouting of my own revealed that they were already performing flash computations. So they knew about $K_i = y_i/x_i$, but the only solution model they had was Raoult's Law ($K_i = P_i^{sat}/P$). This was my way in. According to Raoult's law, $y_E > x_E$ for ethanol in water at all compositions. Then distillation to gasohol should be no problem because it is constantly enriching. But experiments show that $y_E < x_E$ when $x_E > 0.9$. If you put 10% water into your gas tank, water separates and you have a major problem on your hand.

The reason this happens is that the water does not entirely "like" the ethanol. We can characterize this disdain with modified Raoult's Law ($K_i = \gamma_i P_i^{sat}/P$). If a little ethanol mixes with the water, that is fine and $\gamma_W=1$. But when water is surrounded by 90% ethanol, it can get very uncomfortable and $\gamma_W \rightarrow 2$. At $x_E = 0.9$ and 78°C, ethanol is comfortable and $K_E = P_E^{sat}/P \approx 1$ but $K_W = \gamma_W P_W^{sat}/P \approx 1.1$. So the water becomes richer in the vapor than the ethanol and distillation fails. This causes the separation to make gasohol to be less direct and more expensive both in terms of dollars and in terms of energy efficiency. They nod when I say this, but five minutes have already elapsed.

In the remaining 20 minutes, I introduce a simplified version of the MOSCED model and apply it in an example. Then I assign two homework problems. I refer to this model as the SSCED (simplified separation of cohesive energy density) model. The MOSCED model is a modification of Scatchard-Hildebrand theory that separates the cohesive energy density into a dispersion term, a polarity term, and two hydrogen bonding terms (one for acidity and one for basicity).[1] The simplifications of SSCED are designed to convey key concepts in a manner that is consistent with presentations throughout thermodynamics. Quantitative precision is not necessary for this conceptual introduction. On the other hand, the interpretation of a term like the binary interaction parameter, k_{ij}, is fundamental and intellectually challenging to students. The concept that $k_{ij} < 0$ indicates favorable mixing can be illustrated graphically with the square-well potential, and reinforced with ConcepTesting[2] as demonstrated in the assessment section below. The SSCED model reinforces that concept while the Scatchard-Hildebrand model does not, as discussed in the rationale section along with other finer points about the advantages and limitations of the SSCED model. The presentation section immediately after this introduction closely follows the notes for the freshman lecture. I conclude with a brief review of the assessments of student learning and a perspective on how students may benefit from presentation of such a model at an early stage in the curriculum.

2. Presentation

Resuming from the first five minutes of the lecture, the technical name for the factor, γ_i, is the "activity coefficient." When $\gamma_i = 1$ the situation of the ith component is "ideal." When $\gamma_i < 1$, the ith component is extremely comfortable. Such a formulation would make a great solvent if you had a nasty stain to remove. When $\gamma_i > 1$, the component is uncomfortable, like the water in 90% ethanol. Finally, when $\gamma_i > 10$, the component "hates" its environment so much

that it separates, like the water in gasoline. A very simple computational model can describe all of these situations and help to design formulations to achieve chemical engineering goals. It is,

$$RT \ln \gamma_1 = V_1 (1 - \Phi_1)^2 [(\delta_2' - \delta_1')^2 + 2 k_{12} \delta_1' \delta_2'] \tag{1}$$

Where $R = 8.314$ J/mole-K, T is the temperature in Kelvins, $V_i = MW_i / \rho_i^L$ is the liquid molar volume at 298K and $\Phi_i = x_i V_i / \sum x_j V_j$ is the volume fraction, analogous to weight fraction. The bracketed terms require some explanation. k_{12} is a correction factor that characterizes specific interactions, principally hydrogen bonding. We discuss k_{12} later. The other term addresses the "solubility parameter." If we assume for the moment that $k_{12} = 0$, then $\Delta \delta'$ provides a concise and quantitative measure of γ_i. If $\Delta \delta' = 0$, then the solution is ideal and Raoult's Law is fine. Otherwise, the solution becomes non-ideal.

The solubility parameter is related to the energy density of a compound. This energy can be quantified by the heat of boiling. When you boil water, for example, molecules are extracted from their congenial environment to a lonely vapor, where they can share no energy with others. They prefer to share energy. That is why you must add heat. More heat must be added if they share more energy. If the same boiling pot is used to characterize various compounds, then more small molecules will fit in it than large ones, and even more heat is required. Therefore, it is the energy density that characterizes how strongly a compound sticks to itself. This kind of energy density is something quite different from the explosive energy density of a compound like dynamite, so we need a distinctive name for it. That name is the cohesive energy density, defined by,

$$\delta^2 = (U^{vap} / V) = \text{J/cm}^3 \tag{2}$$

where U^{vap} is the energy of vaporization and the rationale for squaring δ is explained in the thermodynamics course. In the absence of hydrogen bonding, $\delta = \delta'$. Therefore, in terms of δ', discomfort of a component in solution is not caused by dislike for the other components, but by a strong preference for its own company. You may have heard that an extroverted engineer is one who looks at *your* feet when he is talking to you. Any introverted engineers in the room should relate to this perspective on the definition of discomfort. It is a sad perspective, but true.

In the presence of hydrogen bonding, the hydrogen bonding contribution must be separated from δ, hence the name for this model as the SSCED model (simplified separation of cohesive energy density model, pronounced "sked" like sled with a "k"). This separation is given by

$$\delta^2 = (\delta')^2 + 2 \alpha \beta \tag{3}$$

Where α characterizes the compound's acidity and β characterizes the basicity. The acidity and basicity can be measured spectroscopically by probing how strongly compounds interact with a standard reference base and a standard acid. Sample values of δ', α, and β are given in Table 1. Note that water stands out in Table 1 as a compound with remarkably high energy density, both in terms of δ' and in terms of $\alpha\beta$. The water molecule is very small, essentially the size of a single oxygen atom, but it has a large dipole moment (reflected in δ') and strong hydrogen bonding (reflected in $\alpha\beta$).

We now return to the quantity k_{12}. If $k_{12} = 0$, then $\gamma_i > 1$, always, but there are situations when $\gamma_i < 1$. When mixing acids with water for example, the compounds "like each other" so much that you need to be careful. A more moderate example is given by mixing acetone with chloroform, in which case mixture boiling experiments show that $\gamma_i < 1$. The proton of the chloroform is made mildly acidic by the electronegative chlorine atoms pulling on its electrons. The high density of electrons on the carbonyl oxygen makes it mildly basic. Organic chemistry

courses should reinforce these concepts of electron distributions. These considerations are represented by the guideline that

$$k_{12} \approx (\alpha_2 - \alpha_1)(\beta_2 - \beta_1)/(4\delta_1\delta_2) \qquad (4)$$

Table 1. Sample values of physical properties.

	T_c(K)	P_c(MPa)	ω	C_P/R	MW	ρ_{298}	δ(J/cm^3)$^{1/2}$	α(J/ cm^3)$^{1/2}$	β(J/ cm^3)$^{1/2}$
Benzene	562.2	4.90	0.211	9.82	78	0.87	18.65	0.63	2.24
Methanol	512.6	8.10	0.566	5.28	32	0.79	19.25	17.43	14.49
Ethanol	516.4	6.38	0.637	7.88	46	0.79	18.67	12.58	13.29
Acetone	508.2	4.70	0.306	8.96	58	0.79	19.64	0.00	11.14
Chloroform	536.4	5.40	0.216	7.90	119.2	1.48	18.88	5.80	0.12
Water	647.3	22.12	0.344	4.04	18	1.00	27.94	50.13	15.06
Iso-octane	544.0	2.57	0.303	22.50	114	0.70	14.11	0	0
MTBE	497.1	3.43	0.266	15.37	88	0.74	15.17	0	7.4

For the chloroform+acetone example, this formula gives

$$k_{12} = (5.8-0)(0.12-11.14)/(4*19.64*18.88) = -0.035 \qquad (5)$$

Note how the order of subtraction results in a negative value for k_{12} when one of the components is acidic and the other is basic. If you switched the subscript assignments, then $\Delta\alpha$ would be negative and $\Delta\beta$ would be positive, but k_{12} would still be negative. This negative value makes the value of γ_i smaller, and that is basically what happens when hydrogen bonding is favorable.

Something else happens when one compound forms hydrogen bonds but the other is inert. Taking iso-octane(1) as representative of gasoline and mixing it with water(2),

$$k_{12} = (0-50.13)(0 -15.06)/(4*27.94*14.11) = 0.479 \qquad (6)$$

This large positive value will add to the large $(\Delta\delta')^2$ such that $\gamma_1 >> 10$, indicating the liquid phase split that we anticipated. We can quantify the phase split by noting that $x_i \approx 1/\gamma_i$ when $\gamma_i > 100$. Knowing the saturation limit of water contaminants can be useful in environmental applications.

As a final example, note that we recover an ideal solution when both components hydrogen bond, as in the case of methanol+ethanol.

$$k_{12} = (17.43-12.58)(14.49-13.29)/(4*19.25*18.67) = 0.003 \qquad (7)$$

In this case, we see that hydrogen bonding itself is not the cause of solution non-ideality. A mismatch of hydrogen bonding causes non-ideality.

Applications of these insights abound in chemical engineering. For example, what third compound could you add to ethanol+water to make the solution more ideal so that pure ethanol could be obtained? The extension of the SCED model to multicomponent systems is simple, as discussed in the thermodynamics course. How soluble is vitamin-C in the blood stream relative to its solubility in body fat? What about vitamin-E? Aspirin? Tylenol? You just need to know the activity coefficients of these compounds in water and n-octanol (a reasonable approximation of body fat). What solvent should you use to safely remove an undesirable embellishment from a classical painting? The embellishment probably used a different paint, so you need to find a solvent with $\gamma_i < 1$ in the embellished paint but $\gamma_i > 1$ in the classical paint. Quantitative understanding of fields from art restoration to zoology to agribusiness would be impossible without unifying concepts like hydrogen bonding. Students should retain these concepts and reinforce them as they take complementary courses throughout their curriculum.

Example 1.

Estimate the *K*-value for 10mol%chloroform in 90% acetone at 350K and 0.1MPa. You may assume that $\log_{10}(P^{sat}/P_c)=7(1+\omega)(1-T_c/T)/3$.

Solution:
The value of k_{12} = -0.035 is given by Eq. (5). V_C = 119.2/1.48= 80.5 and V_A = 58/0.79 =73.4.
The volume fraction is: Φ_C = 0.1*80.5/(0.1*80.5+0.9*73.4) = 0.109
γ_C = exp{ 80.5*(1-0.109)²*[(19.64-18.88)² - 2*0.035*18.88*19.64]/(8.314*350) } = 0.573.
P_C^{sat} = 5.40*10^(7*1.216*(1-536.4/350)/3) = 0.166 MPa.
$K_C = \gamma_C *P_C^{sat}/P$ = 0.573*0.166/0.1 = 0.951

Homework 1.

Gasohol is made by distilling a solution known as beer (~5mol% ethanol). Compute the *K*-values of ethanol and water at 5mol% ethanol and 365K and compare them to the K-values at 95mol%ethanol and 350.6K. Assume that P = 0.1MPa. Explain the impact of activity coefficient on your results. You may assume that $\log_{10}(P^{sat}/P_c)=7(1+\omega)(1-T_c/T)/3$.
Solution: k_{12} = (12.58-50.13)(13.29-15.06)/(4*18.67*27.94) = 0.032
At 358.5K and 5% ethanol, P_E^{sat} = 0.1327 and P_W^{sat} = 0.0658 MPa according to the assumed vapor pressure equation. The water is nearly pure and computation confirms that γ_W = 1.016.
Details for ethanol: Φ_E = 0.05*58.5/(0.05*58.5+0.95*18) = 0.146.
γ_E = exp{ 58.5*(1-0.146)² [(18.67-27.94)² + 2*0.032*18.67*27.94]/(8.314*358.5) } = 5.517.
This gives K_E = 7.319 and K_W = 0.669.
At 350.6K and 95% ethanol, P_E^{sat} = 0.0997 and P_W^{sat} = 0.0491 MPa according to the assumed vapor pressure equation. The ethanol is nearly pure and computation confirms that γ_E = 1.001.
For water,
γ_W = exp{ 18*[(18.67-27.94)² + 2*0.032*18.67*27.94]/(8.314*350.6) } = 2.046
This gives K_E = 0.998 and K_W = 1.002.
Overall, non-ideality makes distillation easier at low concentrations of ethanol, but the large activity coefficient switches to the water at high ethanol concentrations and makes it slightly more volatile. This is why distillation fails to purify ethanol this system.

Homework 2.

The American experience with methyl tert-butyl ether (MTBE) in the 90's broaches qualification as a fiasco. Rumor has it that congressmen from corn states thought that a mandate for 10% "oxygenated fuel" would boost demand for ethanol. Within four years MTBE was the number one synthetic chemical produced in the world. What nobody anticipated was how MTBE might affect groundwater. It imparts a bitter taste and nasty smell even at parts per billion. Gasoline is stored in underground tanks, and the tanks leak. Estimate the solubility of MTBE in water at 298K and compare it to that of iso-octane and benzene.
Solution: For iso-octane, Eq. (6) gives k_{12} = 0.479.
$x_O=1/\gamma_O$ = 1/exp{ 114/0.70*[(14.11-27.94)² + 2*0.479*14.11*27.94]/(8.314*298) } = 5.7E-17
For benzene, k_{12} = (0.63-50.13)(2.24 -15.06)/(4*27.94*18.65) = 0.304
x_B=1/exp{ 78/0.87*[(18.65-27.94)² + 2*0.304*18.65*27.94]/(8.314*298) } = 4.0E-8
For MTBE, k_{12} = (0-50.13)(7.4 -15.06)/(4*27.94*15.17) = 0.226
x_M=1/exp{ 88/0.74*[(15.17-27.94)² + 2*0.226*15.17*27.94]/(8.314*298) } = 1.7E-9

So the solubility of MTBE is roughly 8 orders of magnitude higher than that of iso-octane. This estimate would need to be checked with experimental data, but the essential observation is that the basicity of the ether suggests checking it out. Benzene is interesting because its estimated solubility is even higher than that of MTBE. Benzene does not taste or smell like MTBE, but it is carcinogenic. Nevertheless, nobody seems to be talking about the solubility of benzene in groundwater… at the moment.

3. Rationale

The SSCED model provides a simplified and generalized introduction to the MOSCED model, but the MOSCED model is designed for other purposes. Specifically, it is designed for infinite dilution activity coefficients instead of being a solution model at all concentrations. The MOSCED model is given by,

$$\ln \gamma_2^\infty = \frac{V_2}{RT}\left[(\lambda_2 - \lambda_1)^2 + \frac{q_1^2 q_2^2 (\tau_2 - \tau_1)^2}{\psi_1} + \frac{(\alpha_2 - \alpha_1)(\beta_2 - \beta_1)}{\xi_1} \right] + aa \ln\left(\frac{V_2}{V_1} \right) + 1 - \left(\frac{V_2}{V_1} \right)^{aa} \tag{8}$$

Where λ_i is the dispersion factor, τ_i is the polarity factor, q_i is a factor ranging from 0.9 to 1. aa, ψ_i and ξ_i are adjustable parameters characterizing solvent properties. At infinite dilution, they are specific values, but they must depend on composition to change from one solvent to the next. That composition dependence is not addressed by the MOSCED model, but it poses no problem for experts in thermodynamics. Parameters of an activity model like UNIQUAC could be determined from the infinite dilution activity coefficients and activity coefficients at all compositions computed from UNIQUAC. But activity models like UNIQUAC tend to be covered after models like MOSCED. The MOSCED model is based primarily on van der Waals mixing. The terms involving $(\Delta\lambda)^2$ and (V_2/V_1) comprise the Scatchard-Hildebrand and Flory-Huggins contributions derived from the van der Waals equation when constant packing fraction is assumed.[3] The other contributions are based on phenomenological arguments. The UNIQUAC model is based on the concept of local compositions. Developing the nuances of fitting parameters to one activity model then interpolating the free energy based on an entirely different activity model could undermine the attention span of sophomores as well as freshmen. Another alternative would be to articulate composition dependencies for all the parameters. This would take the model away from a simple explanation. On the other hand, eliminating the polarity factor (ie. $\psi = \infty$), setting $aa = 0$, and $\xi = 2$ for all compositions makes the model much simpler and more broadly applicable while retaining the separation that enables consideration of hydrogen bonding influences.

The SSCED model was derived from the MOSCED model by minimizing deviations in a somewhat crude manner. The factor of 2 multiplying $\alpha\beta$ in Eq. (1) was determined by minimizing the differences between the physical contributions of the two models. Analyzing the physical contributions showed that $\delta^2 \approx (\lambda^2 + \tau^2/2)$ for non-associating compounds. Note that $\delta = \delta'$ in the absence of association. For associating compounds, Eq. (1) was rewritten as

$$\delta^2 = (\delta')^2 + m\alpha\beta \tag{9}$$

where m was an adjustable parameter. Minimizing the objective function $\sum\{(\delta')^2 - (\lambda^2 + \tau^2/2)\}^2$ for 30 compounds in the database of Lazzaroni et al. where δ' was computed from Eq. (9) yielded an optimal value of $m \approx 2.2$. The factor of 4 in the denominator of Eq. (4) was determined by minimizing deviations in vapor-liquid equilibrium (VLE) data for the 10 binary systems of the first five compounds in Table 1, and three VLE systems involving water with special emphasis on ethanol+water. These particular mixtures were chosen to illustrate the range

of possibilities from strong solvation to hydrophobicity. Coincidentally, this manner of separation retains the consistent interpretation of cohesive energy density as a primary consideration (e.g. $\delta_W' > \delta_B' > \delta_O'$, where W means water, B means benzene, and O means iso-octane). This consistency is not immediately apparent in MOSCED's λ parameters.

Other simple alternatives include the Hansen solubility parameters[4,5] and the original Scatchard-Hildebrand model.[5,6] The problem with the Scatchard-Hildebrand model is that it overestimates the non-ideality of the solution. For example, matching the experimental data for methanol+benzene requires a negative value of $k_{12}= -0.035$ when the Scatchard-Hildebrand model is applied. Students then conclude that methanol and benzene must "like" each other, because that is what k_{12} should mean. But in this case, the negative k_{12} is cancelling the overestimation of the non-ideality from the "unseparated" cohesive energy density. A similar problem occurs with water and nearly any other compound. Even ethanol+water is predicted to be immiscible with the Scatchard-Hildebrand model. This kind of "two steps forward and one step backward" makes the presentation unnecessarily confusing. The Hansen solubility parameters, on the other hand, have the advantage of being simpler than SSCED in some sense, because there is a single hydrogen bonding parameter instead of two. Nevertheless, Hansen's method cannot account for activity coefficients less than one. This undermines the scope of conceptual reasoning that should form the long term basis for students' thermodynamic insight. In deference to Hansen's method, however, the separate contributions to the solubility parameter are constrained to sum to the original Scatchard-Hildebrand value. This adaptation from Hansen's method is helpful in clarifying that SSCED provides separation, but no elimination.

An advantage of the MOSCED model is its direct accounting of the specific molecular interactions involved in hydrogen bonding. This accounting is based on spectroscopic measurements that are independent of the desired activity coefficients.[7] Kamlet-Taft parameters are dimensionless measures of acidity and basicity, but the MOSCED model recasts their values to provide dimensional consistency with solubility parameters. This may open the door to more creative ways for students to mesh analytical techniques with engineering applications, as in catalysis for example. Interactions of zeolite acid sites with molecular base sites may seem less mysterious when the existence of molecular base sites has been acknowledged at the outset. This improved chemical insight can be pervasive throughout the curriculum.

Eq. (1) was deliberately expressed in terms of k_{12} instead of simply substituting Eq. (4) directly, as in MOSCED. Note that Eq. (4) is described as a "guideline." This means that it is a starting point, but it leaves open the possibility of refining the value. The value of experimental data is hinted at in the presentation and several assignments at the sophomore level lead students through the process of finding relevant data and inferring refined values of k_{12}. A model like UNIFAC can predict activity coefficients but sheds no light on the underlying chemical interactions that lead to the behavior. Furthermore, the UNIFAC model makes it difficult to refine predictions in light of experimental data for specific systems of interest.

Another alternative would be Wertheim's theory.[8] Wertheim's theory forms the basis of hydrogen bonding equations of state like the PCSAFT[9] and ESD[10] models. It is also based on rigorous statistical mechanics instead of phenomenological arguments. Therefore a simplified integration of Wertheim's theory with Scatchard-Hildebrand theory would have an advantage as a natural segue to the more sophisticated theories. In fact, this was considered to be the preferred alternative initially. Unfortunately, hydrogen bonding compounds tend to operate at higher packing fractions, and this undermines a simple extension of the constant packing fraction

assertion. Some compromise may be feasible long term, but the current form of the SSCED model is satisfactory for present purposes.

Finally, it may be possible to relate the dispersion, acidity, and basicity parameters to ab initio characterizations, as in the COSMO-RS model.[11] This would reinforce the value of quantum mechanical computations throughout the curriculum, but freshmen (and sophomores) would be unlikely to appreciate this level of sophistication. It would make more sense to recast the ab initio results as reinforcing the SSCED concepts after the fact, in the Junior or Senior year.

There is one substantial disadvantage of the SSCED model that motivates the coverage of more advanced models like UNIQUAC and SAFT. Since it has only one binary interaction parameter, the magnitude of deviations from non-ideality can be adjusted, but not the skewness. The skewness of the Gibbs energy is controlled by the volume ratio in the SSCED model. However, this limitation pertains to quantitative modeling, not to the conceptual and educational device intended here.

4. Assessment

Assessments of student learning have not been performed for the freshmen yet, but a very similar presentation pertains to the sophomores and this has been assessed in class through the ConcepTest methodology and through traditional examination questions. These are less personal than looking students in the eye to gage their understanding, but they do provide objectivity.

ConcepTests pose simple questions to the class and allow them to post their answers anonymously for quick compilation.[2] Electronic devices typically facilitate this approach, but it can be conducted with colored flash cards. In the strictest sense, ConcepTests should focus entirely on conceptual questions, but a small adaptation permits engagement in active learning for computational exercises as well. I refer to these as CompuTests. A few examples are given below. The (%) quantities refer to the % of students who answered correctly.

ConcepTest 1.

Referring to the figure below, cases A, B, and C correspond to characterizations of the attractive energy between two molecules as described by the square well potential. This attractive energy is given by $\varepsilon_{12}= (\varepsilon_1 * \varepsilon_2)^{\frac{1}{2}} (1- k_{12})$ where ε_{12} gives the depth of the square well. Note that the bottom of the well is $-\varepsilon_{12}$. Provide the response (A or B) corresponding to each situation.
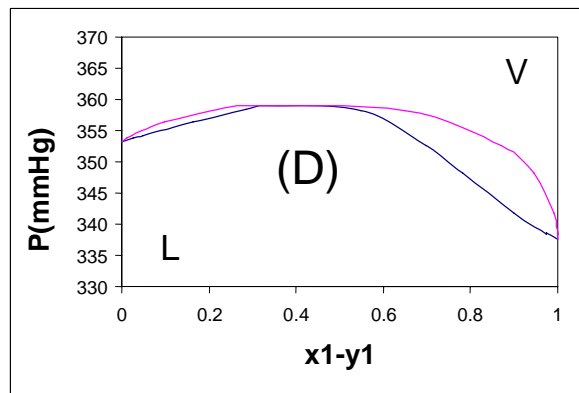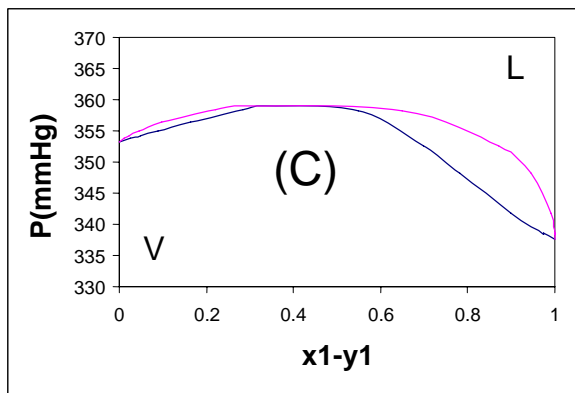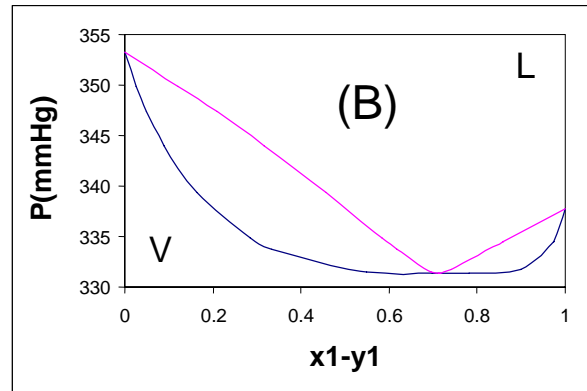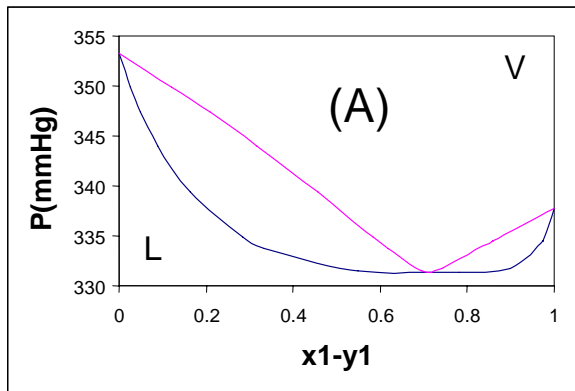
a. Which (A or B) corresponds to $k_{ij} > 0$? (72%)
b. Which corresponds to components "liking" each other? (100%)
c. Which corresponds to a higher "escaping tendency" for component 1? (94%)
d. Which will give the highest bubble point pressure? (50%)
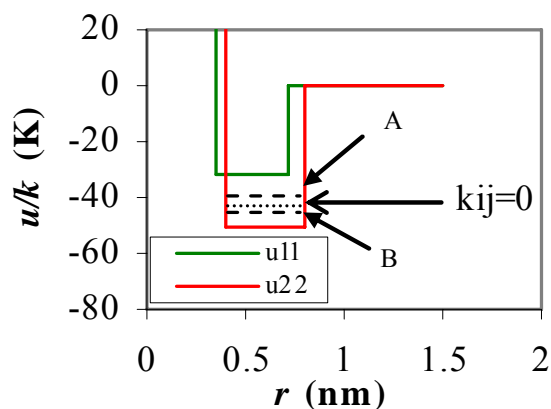
ConcepTest 2. (94%)

Which of the following properly depicts a maximum boiling azeotrope?

"CompuTest" 1. (43%)

Arrange the following mixtures from most compatible to least compatible according the SCED solubility parameter criterion (k_{12}=0). (1) Pentane+hexane, (2) decane+decalin, (3) 1-hexene+ dodecanol, (4) pyridine+methanol, (5) diethyl ether+n-heptane

     A. 12345   B. 12534   C. 54123   D. 21543

"CompuTest" 2. (76%)

An azeotrope exists for n-butane(1)+ethyleneOxide(2) at 1.013 bars at -6.5°C and 78wt% butane. Estimate the activity coefficient of EtO (γ_2) at the azeotropic composition and temperature from the Scatchard-Hildebrand model assuming $k_{ij} = 0$.

Compound	Tc(K)	Pc(MPa)	w	CpIg/R	MW	δ(cal/cc)$^{1/2}$	ρ298
n-BUTANE	425.2	3.80	0.193	11.89	58	6.60	0.60
EtOxide	469.0	7.10	0.200	5.80	44	10.62	0.89

           (a) 0.04   (b) 1.06   (c) 1.98   (d) 2.89

Examination Question 1. (89%)

Based on the Scatchard-Hildebrand solubility parameters (k_{12}=0), arrange the following mixtures from most ideal to most non-ideal: (a) 2-pentanone+1-pentene, (b) 2-pentanone+ naphthalene, (c) ethanol +naphthalene, (d) n-hexane+ ethanol.

Examination Question 2. (61%)

A common problem with recycling polyester is the impurities from bottle caps and labels. The bottle caps typically weigh 0.05 g and the bottles are 2g. The caps are polypropylene (PP) with molecular weight of 60,000 g/mol. The bottles are polyethyleneterephthalate (PET), with molecular weight of 10,000g/mol. The solubility parameter and density of PP can be estimated from those of 224TriMethylPentane. The solubility parameter and density of PET can be approximated with those of p-xylene. Estimate the infinite dilution activity coefficient for PP in PET at 100°C assuming k_{ij}=0.

5. Conclusions

Two issues pervade teaching in the chemical engineering curriculum: time constraints and knowledge retention. If you teach too much in too little time, little is retained. If you teach too little, students cannot "connect the dots" from one isolated fact to another. The key is to articulate broadly applicable concepts, like the SCED model presented here. This mindset leverages familiar chemical concepts like acidity and basicity while dovetailing nicely with the physical interactions of the van der Waals model covered in physics coursework. Leveraging the concepts presented in other coursework has the two-fold advantage of saving time and rewarding students for retaining what they learn from course to course.

The assessments show that this perspective is accessible to sophomores at least. Assessments were not conducted for freshmen at this early stage of adapting the presentation for them, but we expect similar results to those for sophomores if sufficient effort is devoted. Students are able to quickly recognize solution non-ideality and the impact this may have on solubility and volatility. Students whose careers take them away from process design may not remember how to compute an activity coefficient five years after graduating, but they can remember that acids and bases interact strongly and that even organic chemicals can be formulated to take advantage of those interactions.

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