

**NOT NEVER NOHOW**

Dear Editor:

Professor Barduhn's letter in the last issue of *CEE* noted that the prefix "a" to a word often infers the negative (*e.g.*, symmetric *vs.* asymmetric), and that this should apply to "diabatic" and "adiabatic." Consequently, non-adiabatic should have the same meaning as diabatic. This is an interesting thought.

I wonder whether Professor Barduhn is aware that the word *bat* is the root of all these words. Performing the usual series expansion on that little word:

1. We first obtain *batic* which means to act like a bat, or to be batty.
2. Then comes *abatic* which refers to non-batlike behavior.
3. Obviously *diabatic*, must mean to behave like two non bats, or to not be batty twice in a row (there is still some argument about these different interpretations).
4. Continuing this series expansion by adding another prefix "a" then gives *adiabatic*, which, without question, refers to not behaving like two non-bats.
5. And finally, we are impelled inexorably by this crescendo of steely logic to conclude that *non-adiabatic* means to never not behave like two non-bats, at least not two times in a row, nohow, nowhere and at no time—not never.

But what has this to do with hot air and heat flow?

Sincerely,  
**Octave Levenspiel**  
Oregon State University

**WOMEN IN SCIENCE VIDEOTAPES**

Dear Editor:

Those involved with chemical engineering education might be interested in our videotape series.

The Women In Science Videotape Series consists of eight videotapes designed to present women scientists and students from across the country in an upbeat and positive light. Seven of the tapes focus on women in the following fields: biomedical science, chemistry, computer science, dentistry, engineering, geoscience, and physics/astronomy. The eighth videotape features general career opportunities in science and addresses the barriers that discourage young women from pursuing science careers.

Funded by a grant from the Women's Educational Equity Act Program of the U. S. Department of Education, the videotapes are intended to encourage young women to take high school and college courses in math and science and to seriously consider careers in science or technology. The series was designed to be used by secondary school and college instructors or counselors, and is appropriate for career fairs, classroom use, individual counseling sessions, and public television.

Each color videotape cassette is approximately thirty minutes long and is available in two formats: 3/4-inch U-matic or 1/2-inch VHS. Included with the videotapes are brochures/posters containing specific career information for each of the fields. A user's guide accompanies each of the first seven videotapes and contains pre- and post-viewing activities, discussion questions, salary informa-

tion, additional resources, and the videotape script. These tapes are currently available for preview rentals or purchase.

Sincerely,  
**Joyce B. Williams**  
Women in Science  
Educational Resources  
University of Michigan  
Ann Arbor, MI 48109

**ChE CASE STUDIES AVAILABLE**

Dear Editor:

Those who teach chemical engineering thermodynamics know how difficult it is to find suitable examples which are realistic and, at the same time, give good insight into the scientific significance of thermodynamics. Those who teach plant design are concerned with finding problems that reflect industrial reality but at the same time do not excessively burden the student who has only limited time for performing complex calculations.

With ever-increasing use of computers in chemical process design, teachers of chemical engineering are properly concerned about giving students some experience in the use of computers for solving industrially-significant problems. In response to this concern, we have established some case-study problems in applied chemical thermodynamics which may be of help to chemical engineering teachers, especially in plant-design courses.

Each of the case-study problems, briefly described below, presents first, some introductory background information; second, a statement of the design problem; and third, the necessary thermodynamic framework for formulation of the problem toward a solution. To assist in reaching a solution, each case study also includes some self-explanatory examples in addition to the necessary computer programs and subroutines. For each program, we give input and output information as well as program documentation that explains how to use the programs and describes the subroutines.

1. *Vapor-Liquid Equilibria for the System Acetone-Methanol. Effect of Pressure on Azeotropic Composition* is concerned with vapor-liquid equilibria for an azeotropic mixture obtained from production of methanol by oxidation of butane [1]. At pressures close to atmospheric, the acetone/methanol mixture has an azeotrope which contains 83 mol percent acetone. The problem is to find the pressure range where no azeotrope exists, allowing complete separation by distillation. To describe the thermodynamic behavior of the vapor, we use the virial equation of state, truncated after the second virial coefficient, with virial coefficients obtained from the Hayden-O'Connell correlation [2]. Activity coefficients for the liquid phase are determined from the UNIQUAC equation. The two-dimensional Newton-Raphson iteration technique is used to solve the equations that give the conditions where no azeotrope is formed.

2. *Vapor-Liquid Equilibria for Aqueous Mixtures of Weak, Volatile Electrolytes and Other Gases*, is concerned with aqueous mixtures of weak, volatile electrolytes as found, for example, in coal-gasification processes, where aqueous streams containing  $\text{NH}_3$ ,  $\text{CO}_2$ ,  $\text{H}_2\text{S}$ , or  $\text{SO}_2$  must be purified. To design equipment for purification by stripping, it is necessary to calculate vapor-liquid equilibria for aqueous mixtures containing these volatile solutes that partially ionize in water. To describe the behavior of volatile, ionizing solutes in water, we must satisfy simultaneously phase equilibria and chemical (ionization) equilibria, along with the constraints of material balances. The program provides necessary computer details to achieve the desired simultaneous solution; in addition, the program enables the user to do dew-point, bubble-point and flash

Continued on page 51.

The chapters devoted to Pascal are probably adequate to become acquainted with the language provided one has had prior programming experience. I would not recommend this text to a novice. The author provides a number of examples in the form of sample programs which are useful; but, in my opinion, it would be much better if he also provided exercises.

The MC68000 is a powerful microprocessor, but it is relatively complicated (compared to, say, the 6502) to program and use effectively as a laboratory instrument. In my opinion the brief introduction to MC68000 assembly language programming in chapters 14 to 21 is inadequate, even for someone who has had experience. The addressing modes are one of the most important and powerful features provided with the MC68000 instruction set. Yet to spend only one short chapter discussing the addressing modes and to provide virtually no practice exercises is extraordinary. Assembly language programming for 16 (and larger) bit processors gets to be cumbersome without the use of an assembler. ASM, the assembler provided with the System 9000, is a crucial part of the system and also deserves more than one chapter if it is to be learned effectively. Again, practice exercises would be very helpful.

Although the author does not suggest it specifically, it seems that this book might better be described as an adjunct to the documentation provided with the System 9000. The eclectic approach used in the book should help to keep the many details in the system documentation in perspective and, at the same time, provide an easier path toward getting the System 9000 doing something useful. □

## LETTER TO THE EDITOR

Continued from page 7.

calculations for multicomponent aqueous systems containing volatile, weak electrolytes and other gases. To solve the equations of phase equilibrium, we use the method of Nakamura *et al* [3] to calculate fugacity coefficients in the vapor phase; for the liquid phase, we use Henry's constants and an extension of the theory for electrolyte solutions developed by Pitzer [4] to describe the temperature and concentration dependence of activity coefficients. A sophisticated numerical technique is used to solve the many simultaneous equations of equilibrium.

3. *Gas-Hydrate Phase Equilibria* presents a program for calculating the conditions of pressure, temperature and gas composition required for formation of hydrates. Gas hydrates are formed when water and light gases (*e.g.*, natural gases, refrigerants, oxygen, nitrogen) are at equilibrium at low temperatures and high pressures. Gas molecules become trapped in cavities (or cages) contained in the crystalline lattice structure formed by water molecules; the trapped gas molecule stabilizes the lattice. A quantitative understanding of conditions for hydrate formation is necessary, for example, to design gas production from underground fields of natural-gas hydrates, or to control sea-water desalination plants

where hydrates are used to separate water from salt. Hydrate-formation is particularly important in the transportation of natural gas, where hydrates can clog pipelines. In this case study, we use a modified van der Waals-Platteeuw [5] framework to estimate hydrate-formation conditions. Fugacities in the vapor phase are computed from the Chueh-Prausnitz [6] modification of the Redlich-Kwong equation of state.

4. *Isothermal Flash Calculations for Multicomponent Mixtures of Organic Liquids Using UNIFAC* combines the UNIFAC method [7] for establishing activity coefficients with a step-limited Newton-Raphson routine to assist the user in performing isothermal flash calculations for a wide variety of mixtures of organic liquids, containing up to 10 components. We use an isothermal flash calculation to obtain the pressure (or temperature) that produces the optimum separation of two hydrocarbons from a multicomponent stream. The program includes a data bank with group surface areas, group volumes and group-group interaction parameters as required to calculate activity coefficients with UNIFAC.

5. *Estimation of Activities of Solvents in Polymer Solutions Using UNIFAP*, uses an extension of the UNIFAC method for calculation of liquid-phase activities of solvents in polymer solutions. In polymer production, these activities are required to design devolatilization equipment, necessary to recover the solvent from the polymer solution by evaporation. UNIFAP [8] is a group-contribution method that can be used to estimate vapor-liquid equilibria for a variety of polymer mixtures where no experimental mixture data are available. The computer program includes a data bank which contains the pertinent group parameters.

Copies of these case studies are available from J. M. Prausnitz (Department of Chemical Engineering, University of California, Berkeley, California 94720). Magnetic tapes for computer programs (written in FORTRAN IV) are available for purchase. These tapes are 9 track at 1600 bpi, in EBCD with 80-character (card-image) record.

The undersigned are grateful to the Camille and Henry Dreyfus Foundation, New York, for financial support and to V. Brandani, E. M. Pawlikowski and F. E. Anderson for extensive assistance in preparing the case studies. They welcome comments on the use of these case studies for education of future chemical engineers.

J. M. Prausnitz

E. G. Azevedo

University of California, Berkeley

## REFERENCES

- (1) Lowenheim, F. A., and M. K. Moran, *Faith, Keyes, and Clark's Industrial Chemicals*, 4th Ed., John Wiley, New York (1975).
- (2) Hayden, J. G., and J. P. O'Connell, *Ind. Eng. Chem. Proc. Des. Dev.*, **14**, 209 (1975). See Reference (9).
- (3) Nakamura, R., G. J. F. Breedveld, and J. M. Prausnitz, *Ind. Eng. Chem. Proc. Des. Dev.*, **15**, 557 (1976).
- (4) Pitzer, K. S., *J. Phys. Chem.* **77**, 268 (1973).
- (5) Van der Waals, J. H., and J. C. Platteeuw, *Adv. Chem. Phys.*, **2**, 1 (1959).
- (6) Chueh, P. L., and J. M. Prausnitz, *Ind. Eng. Chem. Fund.*, **6**, 492 (1967).
- (7) Gmehling, J., P. Rasmussen, and A. Fredenslund, *Ind. Eng. Chem. Proc. Des. Dev.*, **21**, 118 (1982).
- (8) Oishi, T., and J. M. Prausnitz, *Ind. Eng. Chem. Proc. Des. Dev.*, **17**, 333 (1978).
- (9) Prausnitz, J. M., E. A. Grens, T. F. Anderson, C. A. Eckert, R. Hsieh, and J. P. O'Connell, *Computer Calculations for Multicomponent Vapor-Liquid and Liquid-Liquid Equilibria*, Prentice-Hall (1980).