energy for the synthesis using bromoethane as the substrate is significantly lower, thus suggesting that the reaction will be much faster if this compound is used as the reactant. Finally, costs of the two reactants are compared using data from the commodities literature.

The approach to solving this problem relies exclusively on the use of molecular modeling to obtain information that is not readily available from any of the standard data sources—hence the use of quantum chemistry to estimate parameters that are of considerable practical utility for both reactor and process-design purposes is well illustrated.

We have recently added a new senior-level course to our curriculum, "Molecular Perspectives in Chemical Engineering." This course presents students with a comprehensive overview of the use of molecular modeling and simulation techniques in several different applications, including estimation of thermophysical and reaction rate data, sorption equilibria and diffusion rates, phase equilibrium simulation, and prediction of transport properties.

An outline for this course, including descriptions of the computational exercises that are currently in use, is given in Table 2. Examples of molecular modeling exercises used in the capstone chemical engineering molecular simulation course can also be found by accessing the CSM website at <http://www.mines.edu/Academic/chemeng>.

## CONCLUSIONS

Molecular-scale modeling has reached a level of sophistication and accuracy that makes it an essential and highly useful tool for chemical engineers, yet the methods, capabilities, and limitations of this tool are not yet well known across the chemical engineering profession. The use of molecular-scale modeling is becoming increasingly important in industry as researchers and product developers look for ways to cut the costs and time associated with development of new products.

At CSM, we have addressed this problem by incorporating atomistic modeling methods throughout our curriculum at the undergraduate level in both the chemistry and chemical engineering course sequences. We believe that this approach represents a new educational paradigm in chemical engineering, and we are committed to integration of these concepts across the curriculum.

## REFERENCES


1. Wei, J., *Adv. Chem. Eng.,* **16**, 51 (1991)
2. Bird, R.B., W.E. Stewart, and E.N. Lightfoot, *Transport Phenomena,* Wiley & Sons, New York, NY (1960)
3. Landau, R., *Chem. Eng. Prog.,* **52**, Jan (1997)
4. Drexler, K.E., *Proc. Natl. Acad. Sci. US,* **78**, 5275 (1981)
5. Gibney, K., *ASEE Prism,* **8**(1), 23 (1998)
6. Hehre, W.J., L. Radom, P.v.R. Schleyer, and J.A. Pople, *Ab Inito Molecular Orbital Theory,* Wiley & Sons, New York, NY (1986)
7. Burkert, U., and N.L. Allinger, *Molecular Mechanics* ACS Monograph 177, American Chemical Society (1982)
8. Frenkel, D., and B. Smit, *Understanding Molecular Simulation,* Academic Press (1996)
9. Clark, M., R.D. Cramer III, and N. van Opdensch, *J. Comp. Chem.,* **10**, 982 (1989)
10. Halgren, T.A., *J. Comp. Chem.,* **17,** 490 (1996)
11. Quirke, N. *Chem. Eng. Prog.,* Feb (1996)
12. Rowley, R.L., and J.F. Ely, *Molecular Simulation,* **7**, 303 (1991)
13. Moore, J.D., S.T. Cui, P.T. Cummings, and H.D. Cochran, *AIChE J.,* **43**, 3260 (1997)
14. Cui, S.T., H.D. Cochran, P.T. Cummings, and S.K. Kumar, *Macromolecules,* **30**, 3375 (1997)
15. Chialvo, A.A., and P.T. Cummings, *J. Chem. Phys.,* **105**, 8274 (1996)
16. Hansen, E., and M. Neurock, *Computers in Chem. Eng.,* **22**, 1045 (1998)
17. Chen, N., and R.T. Yang, *Ind. Eng. Chem. Res.,* **35**, 4020 (1996)
18. Sungpet, A., "Reactive Polymer Membranes for Olefin Separations," PhD Thesis, Colorado School of Mines (1997) ❐


## ChE letter to the editor

Dear Sir:

The article by Rugarcia, et al., titled "The Future of Chemical Engineering Education" [*CEE,* **34**, 16, (2000)] is interesting and thought provoking. However, it begins with a caricature of a poor lecture and returns to the theme of the inferiority of the lecture format later in the paper with the assertion that "the superiority of alternative methods. . .has been demonstrated in thousands of empirical research studies." This view has become widely accepted among the proponents of "new" teaching methods. At the risk of being branded as a Luddite (probably true), I am compelled to offer a modest and purely anecdotal defense of the lecture format.

Looking back on my own experience as an undergraduate, the classes that I most enjoyed were all formal lectures in physics, chemistry, and even geology. These lectures were given to large classes (sometimes several hundred students) and I am sure that the lecturers would have been horrified at the thought of following a course textbook or of presenting worked examples during a lecture. What was presented was an in-depth review stressing the fundamental principles and the logic and coherence of our understanding of the subject. It is perhaps ironic that the notes from several of these courses were later published as successful textbooks! Well-thought-out and well-rehearsed demonstration experiments, performed by a teaching assistant, were sometimes included. Questions, assignments, and practice examples were handled in parallel tutorial sessions, given by either a faculty member or a PhD student, each with no more than

*Continued on page 177.*

► *In this work, the solid sample is considered as the single mass-transfer resistance; nevertheless, boundary-layer resistance can arise, particularly when binary mixtures are transported through a very permeable media; in that event, the influence of hydrodynamic conditions on overall transfer (concentration polarization phenomenon) is a good indication that can be best achieved by a magnetic Rushton turbine already existing on the setup.*

► *The independent temperature jackets for the two compartments also offer an opportunity to experiment with the incidence of non-isothermal conditions, already shown to strongly affect the observed transfer rate of a pure organic vapor.*[15]

## ACKNOWLEDGMENTS

The authors gratefully acknowledge the numerous valuable comments of the manuscript's reviewers.

## NOMENCLATURE

- A sample surface area
- a asymptote slope
- c concentration
- $c_0$ upstream concentration
- $c_L$ downstream concentration
- D diffusion coefficient
- $E_{D,P}$ energy of activation for diffusion (D) and permeability (P)
- L sample thickness
- P pressure
- $\wp$ permeability
- R perfect gas constant
- S sorption coefficient
- t time
- T temperature
- V downstream volume

***Greek Symbols***

- $\theta$ time lag
- $\Delta H_s$ heat of sorption

## REFERENCES

1. Cussler, E.L., *Diffusion: Mass Transfer in Fluid Media,* Cambridge University Press (1984)
2. Crank, J., *The Mathematics of Diffusion,* Oxford Science Publications (1975)
3. Barrer, R.M., and G. Skirrow, "Transport and Equilibrium Phenomena in Gas-Elastomer Systems. I. Kinetic Phenomena," *J. of Poly. Sci.,* **3**, 549 (1984)
4. Vieth, W.R., *Diffusion In and Through Polymers. Principles and Applications,* Hanser, Oxford University Press (1991)
5. Rutherford, S.W., "Review of Time-Lag Permeation Technique as a Method for Characterization of Porous Media and Membranes," *Adsorption,* **3**, 283 (1997)
6. Frisch, H.L., "The Time-Lag in Diffusion I.," *J. of Phys. Chem.,* **62**, 93 (1957)
7. Brandrup, J., and E.H. Immergut, *Polymer Handbook,* 3rd ed., Wiley Interscience (1980)
8. Van Krevelen, D.W., *Properties of Polymers: Their Correlation with Chemical Structure, Their Numerical Estimation and Prediction from Additive Group Contributions,* 3rd ed., Elsevier Science Edition (1990)
9. Robb, W.L., "Thin Silicone Membranes: Their Permeation Properties and Some Applications," *Annals. of New York Acad. Sci.,* **146**, 119 (1968)
10. Paul, D., and A.T. DiBenedetto, "Diffusion in Amorphous Polymers," *J. of Poly. Sci.,* **C10,** 17 (1965)
11. Siegel, R.D., and R.W. Coughlin, "Errors in Diffusivity as Deduced from Permeation Experiments with the Time-Lag Technique," *AIChE J. Symp. Series,* **120**, 68 (1986)
12. Barrer, R.M., and H.T. Chio, "Solution and Diffusion of Gases and Vapors in Silicone Rubber Membranes," *J. of Poly. Sci.,* **C10,** 111 (1965)
13. Yasuda, H., and K. Rosengren, "Isobaric Measurement of Gas Permeability of Polymers," *J. of Appl. Poly. Sci.,* **14**, 2839 (1970)
14. Jordan, S.M., and W.J. Koros, "Permeability of Pure and Mixed Gases in Silicone Rubber at Elevated Pressures," *J. of Poly. Sci.,* **B28**, 795 (1990)
15. Hillaire, A., and E. Favre, "Isothermal and Non-Isothermal Permeation of an Organic Vapor Through a Dense Polymer Membrane," *Ind. & Engg. Chem. Res.,* **38**(1), 211 (1999) ❒

---

# Letter to the Editor

*Continued from page 167.*

three undergraduates.

Used in this way, a lecture course provides a highly effective way not only for the dissemination of information but also for capturing the interest of students. The formal lectures does *not* provide a good format for developing problem-solving skills, for dealing with engineering design, or even for presenting and discussing solutions to pre-assigned problems.

Unfortunately, in many (if not most) universities the lecture format has been widely misused since it has become the universal workhorse. This may be a more serious issue in engineering education where "design" and "problem solving" constitute a major portion of the curriculum. Nevertheless, within the chemical engineering curriculum, there are many subject areas that are well-suited to the lecture approach and, in the hands of a skilled practitioner and especially if supported by appropriate tutorial sessions, this approach can be very effective. Essentially this same point is made by Wankat and Oreovicz in *Teaching Engineering.* This is one of the references cited in the present article as showing the superiority of alternative approaches! Such a conclusion is hardly surprising since, in any attempt at a quantitative assessment, it would be very difficult, if not impossible, to establish whether the apparent disadvantages of a lecture course are really intrinsic to the format or stem from an inappropriate application of this format. There seems to be a clear danger that, in the current enthusiasm for "new" instructional methods, the very real advantages (and equally real limitations) of the lecture format will be overlooked.

**Douglas M. Ruthven**
*University of Maine*