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Computers In Chemistry

Computer Algebra Systems as Tools for Chemical Education

A NEW DIMENSION IN PROBLEM SOLVING TECHNIQUES

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With a Computer Algebra System at hand, students can look forward to taking college science courses…

In recent years a number of exciting developments have emerged in the area of scientific computational tools for classroom use. Computer Algebra Systems (CASs), for example, Maple, are at the forefront of this arena. Such tools have been long sought by teachers of physical chemistry, inherently a mathematics intensive subject. With a CAS at hand, students can look forward to taking college science courses, like physical chemistry, without the usual mathematics anxiety. These tools can be used to do numerical and symbolic mathematics including calculus and linear algebra. In addition, they have wonderful graphics capabilities that include three-dimensional plots, contour plots, and animations. This paper describes the implementation of Maple in two junior-level physical

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chemistry courses. The materials used for beginning workshops are presented here and additional examples of Maple's graphic and algebraic capabilities are described.

Introduction

An area of the undergraduate chemistry curriculum, that requires mathematical versatility of students, is physical chemistry. Experience shows that a vast majority of students who take this course feel intimidated by the mathematics required to understand the principles. As one author recently stated [1]: "There is a suspicion among students that physical chemistry is the *Great White Whale* of the chemistry curriculum." Mathematics is the language of physical chemistry. Students need to understand this language well enough to appreciate the formulations of the principles and the techniques used to apply them for solving model problems. It is generally agreed that the frightful reputation of physical chemistry courses is, in part, due to students' lack of fluency in basic symbolic (algebra and calculus) and numeric mathematics. Today, numerical calculations and other data manipulations are routinely performed on desk-top computers and sophisticated pocket calculators [2, 3]. This has alleviated some of the difficulty that students traditionally have had in physical chemistry courses. Until recently, however, there was little affordable computational help available to students to deal with the algebra, calculus, and graphical aspects of physical chemistry. Fortunately, there now are a number of symbolic, as well as numeric, computational packages available for desk-top computers. These programs help take away the mathematical fear for students enrolled in physical chemistry courses. Comparative reviews of the earlier versions of a few of these programs have been reported previously [4].

Maple represents an exciting development in scientific computational software for desktop computers [5]. This interactive command-line driven program not only does commonly encountered numerical computations to any desired degree of accuracy, but it is also a powerful symbolic processor that can be used to solve algebra, calculus, and other advanced mathematics problems with ease. Maple contains more than 2500 routines and has a built-in programming language that "allows the flexibility to extend existing routines or create new ones" [6]. Powerful graphing capabilities are available for representing data. These include two- and three-dimensional graphing with animation. CASs have the potential for revolutionizing the way we teach science and mathematics and the way we analyze and approach problems. Practical problems that

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were formerly in the domain of graduate schools can now be meaningfully solved and discussed in undergraduate courses. Experts have compared the emergence of CASs with such milestones as FORTRAN in the 1960s and calculators in the 1970s [7].

This paper deals with the use of Maple in physical chemistry courses at the State University College at Geneseo. Maple V, release 3 (Microsoft Windows version), is installed on all personal computers at Geneseo. There are 15 486-based PCs available to students in the chemistry department. During the first week of classes physical chemistry students are given a hands-on introduction to Maple in a workshop environment during two 75-minute sessions or three 50-minute sessions. In addition to showing students how to *start* and *quit* a Maple session in the Windows environment, this workshop covers the topics discussed below. Prepared examples, also given here, are printed and distributed to students. The topics selected cover most of the commands students are likely to use at the beginning of the course. These introductory sessions are sufficient for them to use and explore Maple for routine class assignments. Additional topics and commands are introduced throughout the semester via special examples.

This paper demonstrates the use of some of the features of a CAS that help students save time in doing routine tasks correctly and in exploring new uses for desktop computers (i.e., complex numerical calculations, symbolic algebra and calculus, and creating and manipulating three-dimensional graphs and animations).

Introduction to Maple

Part (A): Simple Activities (50 minutes)

All of the initial workshop sessions are conducted in a computer laboratory with a maximum of two students sharing a computer. A 15-minute lecture introduces students to starting and quitting Maple in the Windows environment, saving and retrieving Maple generated files and their formats, and the general features of Maple as a command driven program [8]. After this initiation, students work from a handout that gives the command lines necessary for specific tasks. Workshop Handout I contains the command lines shown in sheet1.pdf (18 Kbytes) (bold face lines starting with the > symbol). Using Handout I students become familiar with the Maple commands for simple manipulations. Any notation with which they are not familiar is explained as they use the handouts. The actual display students see after executing the command lines in the handout is also

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given in sheet1.pdf. Students are then encouraged to explore similar commands on their own.

Part (B): Dealing with Functions (50 minutes)
In this workshop session students are introduced to the way Maple deals with functions. The workshop handout for this session consists of the command lines shown in sheet2.pdf (45 Kbytes). Here students learn to define a function of a single variable, calculate its value for a given argument, display its graph, and carry out symbolic differentiation and integration followed by simplification of the results. When Maple is unable to integrate an expression analytically, it is possible to find a numerical value for the integral. This simple yet very useful exercise gives students a glimpse of the symbolic and numeric manipulation power of CASs. Functions of two or more variables are treated in a similar manner. A display of the screens resulting from the successful execution of the command lines in this handout is also shown in the sheet2.pdf.

Part (C): Plotting Experimental Data and Performing a Least-Squares Fit (35 minutes)
This is the topic for the third and final workshop session. It deals with a set of command lines illustrating plotting procedures for [*x, y*] points, and for doing a least squares fit of experimental data to linear and quadratic equations. The workshop handout for this session consists of the command lines shown in sheet3.pdf (14 Kbytes). This is a straight forward problem that might be more easily performed, except for the animation, with any of a number of lower-level software packages (e.g., spreadsheets). However, by doing familiar problems using a CAS students become better acquainted with its powerful command-line syntax and more easily apply it to more difficult problems. In this workshop students learn to enter data lists, use the STATS package to do least-squares fits, create data sequences for plotting of points, and use the PLOTS package to produce an animated display containing multiple graphs. The animation is achieved by a repeated sequential display of three plot-frames: the first frame with the experimental data, the second frame with the experimental data and the linear fit, and the third frame containing all three. A display of the screens resulting from the successful execution of the command lines in the handout is also given in sheet3.pdf.

Part (D): Exploring Maple Using the HELP key. (15 minutes)
At the end of the third workshop session some time is spent in discussing the online HELP facility and related Maple literature. Students are encouraged to explore further using two online facilities provided by the vendor: Maple HELP and Maple Tutorial.

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Maple HELP: Maple V, release 3, has an online HELP facility that can be invoked to obtain information on any topic or subtopic using the syntax:

?topic

?topic, subtopic

The information provided includes a brief description of the *topic* and a list of related topics and subtopics for further exploration. For example, the command **??** describes the HELP facility itself.

Maple Tutorial: An online tutorial is also included with Maple V, release 3. Information about the tutorial can be obtained by the HELP command: *?tutorial*. There are 13 lessons and two quizzes contained in this tutorial. It covers topics of interest to a person just starting to use Maple. Students should complete this entire tutorial during the first two weeks of classes.

Maple Literature

In addition to the on-line facilities mentioned above, there are many good reference books, textbooks, and manuals available to users of Maple [9–16]. For beginning students we recommend the books by Char et al. [11] and Heck [15]. For seekers of help and information on the Internet, there is a *Maple Users' Group*, MUG, at maple-list@daisy.waterloo.ca. Useful Maple related information is also available from its Web Site: http://www.maplesoft.com. Maple-based problem solving techniques and other topics of interest now regularly appear in the *Maple Technical Newsletter* [17], published twice a year.

Examples from Physical Chemistry

During the semester additional Maple techniques are introduced to students, as they are needed in the course, via a number of worked out and well-documented examples. The examples discussed here are intended to illustrate how a CAS can be used to enhance the understanding of chemical principles by making the associated mathematics and

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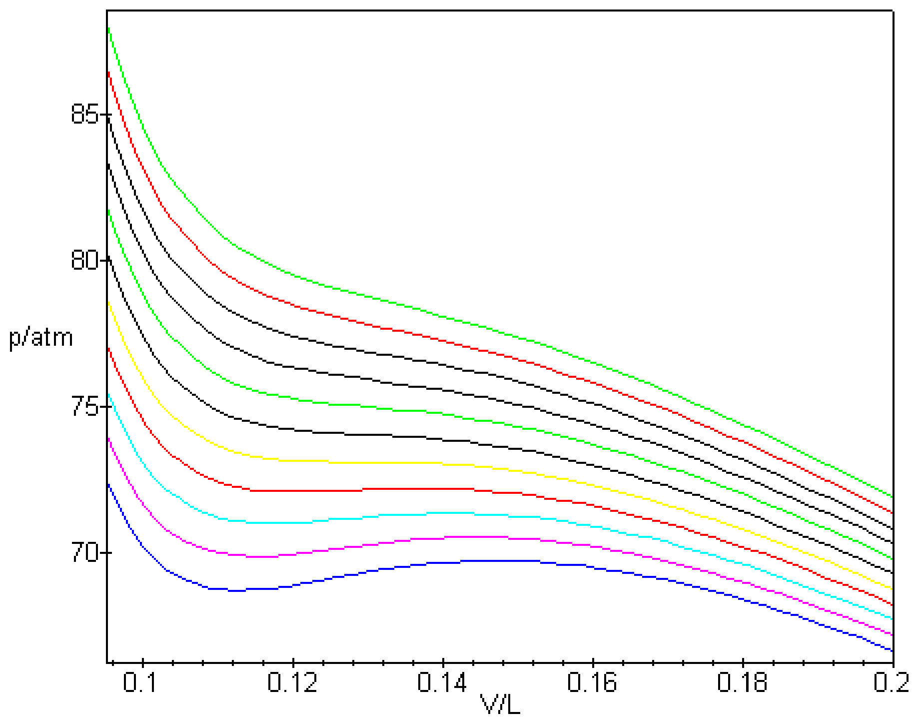

FIGURE 1. THE VAN DER WAALS ISOTHERMS FOR CO_2.

graphics-displays easier to manipulate. Below we discuss two such examples. Example 1: 2-D plots, Surface plots, Contour plots, and Animations Functions of two or more variables are routinely encountered in chemistry. The plotting of such functions without the help of a computer is a fairly time consuming and cumbersome task. The availability of CASs makes it extremely easy to create a variety of displays of these functions. Visualizations are important because they allow students to analyze and study the physical significance of these functions. In sheet4.pdf (13 Kbytes) we give the syntax for defining and displaying functions of two and three variables.

Example 1A(i) illustrates the van der Waals equation of state of a real gas in which the pressure, *p*, depends upon the temperature, *T*, and the molar volume, *V*, of the gas. The PLOT command is used to generate Figure 1, which shows the familiar *isotherms of* CO_2, the *p* versus *V* curves at various *T* values. All figures referred to here can be generated by executing the Maple file, sheet4.ms (This Maple file is available as supporting material for downloading from the Abstract page. Readers must have access to Maple in order to use it.).

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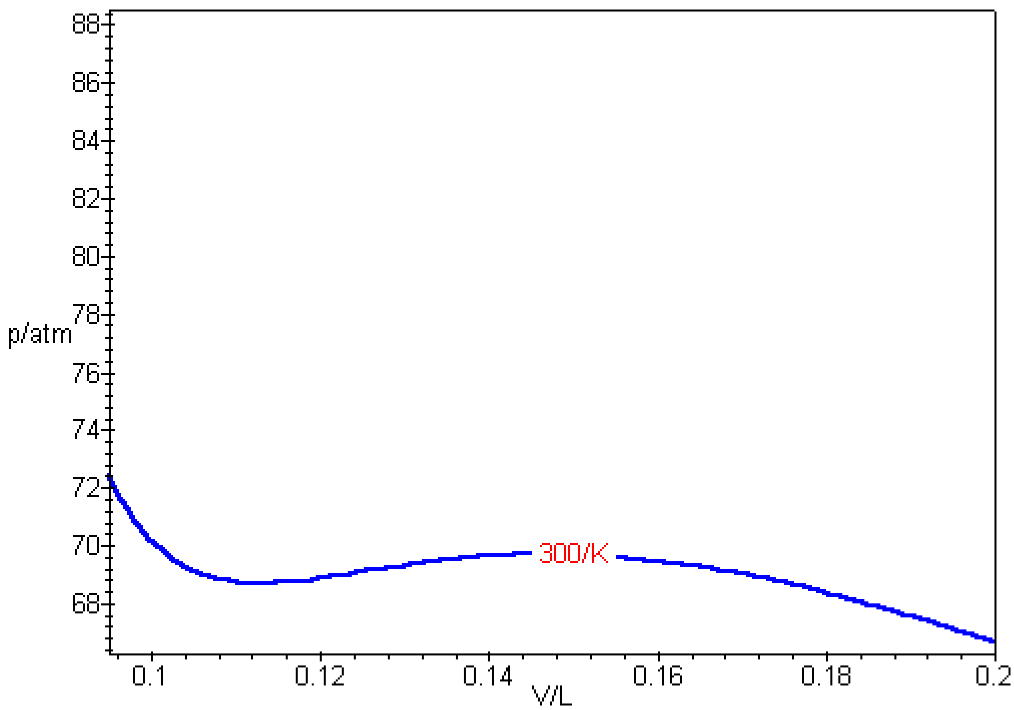

FIGURE 2. AN ANIMATION (ANIM1BJ.MOV, 595 KBYTES) OF THE VAN DER WAALS PRESSURE-VOLUME ISOTHERMS FOR CO_2.

Note: Figure 2 is the first screen of the animation. Clicking on it should start the animation)

An alternative and attractive way of displaying such functions for a particular gas, characterized by its a and b values, is to animate the *p* versus *V* curves using *T* as a parameter. The result is a “motion-picture” showing various isotherms of the gas at a speed the user can control. See the animation in Figure 2. Example 1A(ii), Maple sheet4.pdf gives the commands that accomplish this.

Another way to look at a function of two variables is to make a three-dimensional plot, in which the variables represent two of the dimensions and the function represents the third dimension. Example 1A(iii), Maple sheet4.pdf, demonstrates how this can be accomplished in Maple. The resulting $p(V, T)$ surface plot for CO_2 gas is shown in Figure 3. Maple allows the user to look at such surfaces from various orientations. The orientation selected for the surface shown here accentuates the valley and the peak present in a narrow range of variables, *V* and *T*.

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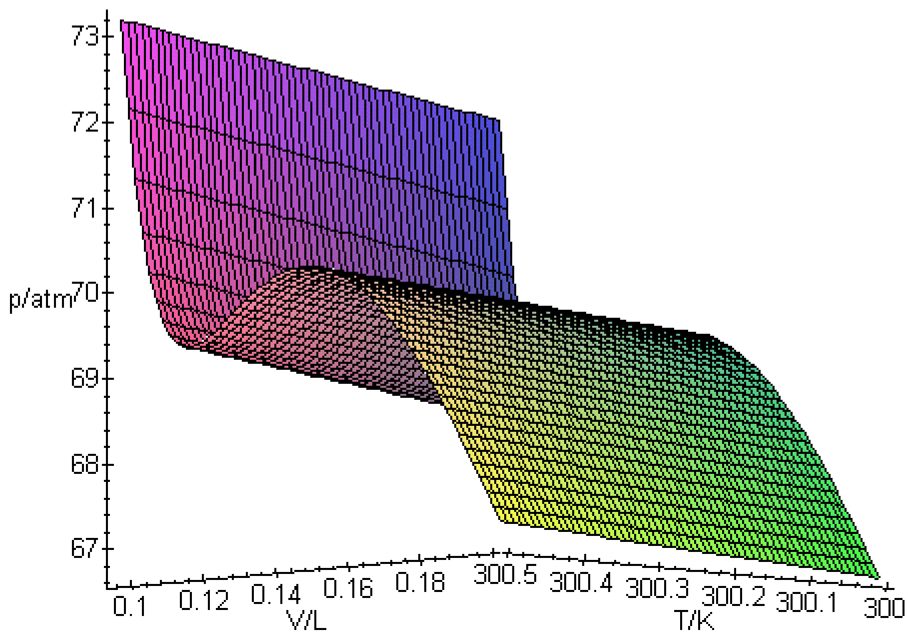

FIGURE 3. THE VAN DER WAALS SURFACES FOR CO_2.

Surfaces are often plotted in the form of *contour diagrams*. This is easily accomplished in Maple using its contour plotting commands. Example 1A(iv), Maple sheet4.pdf, gives the syntax to generate the contour diagram for CO_2 shown in Figure 4. It corresponds to the surface shown in Figure 2.

Another commonly encountered function in chemistry is the Maxwell distribution of speeds among ideal gas molecules. As shown in Example 1B, this function depends upon three variables: molar mass, M, temperature, T, and speed, c. A pedagogically useful way of displaying such functions is to plot the surfaces $f(c, T)$ for a given M or $f(c, M)$ for a given T. This can be done by using the commands shown in examples 1B(i) or 1B(ii), respectively from Maple sheet4.pdf. The "He-tent," shown in Figure 5, is an example of the $f(c, T)$ surface for helium and the "300-K tent," shown in Figure 6, is an example of the $f(c, M)$ surface at 300 K.

The most captivating way of displaying such surfaces, however, can not be reproduced in printed medium. It uses animation. In Maple this is accomplished by calculating a set of surfaces, $f(c, T)$ for different values of M or $f(c, M)$ for different values of T, and

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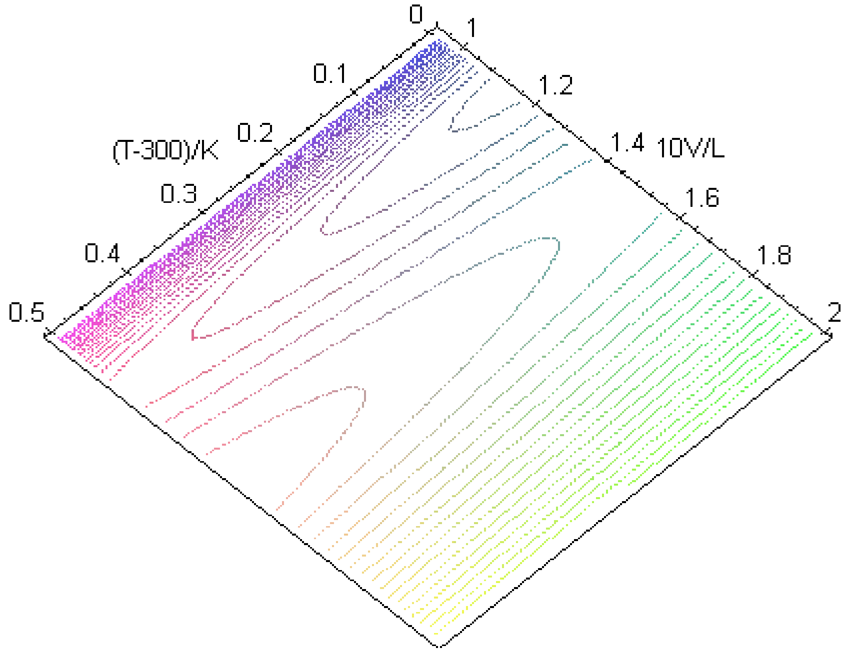

FIGURE 4. A CONTOUR PLOT OF THE VAN DER WAALS SURFACE FOR CO_2.

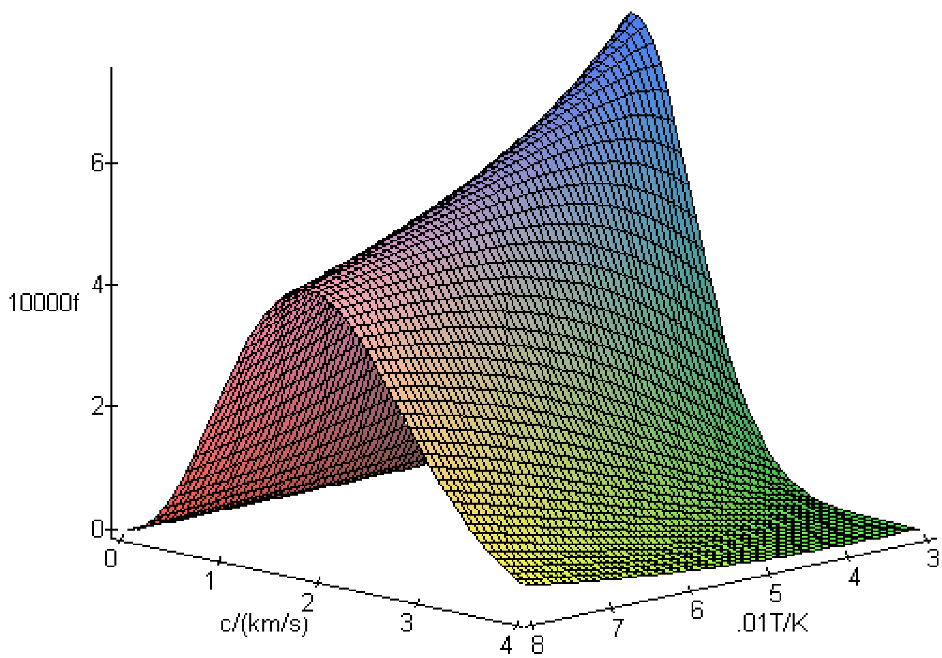

FIGURE 5. AN *F*(*C*, *T*) SURFACE FOR HELIUM – THE “HELIUM TENT”.

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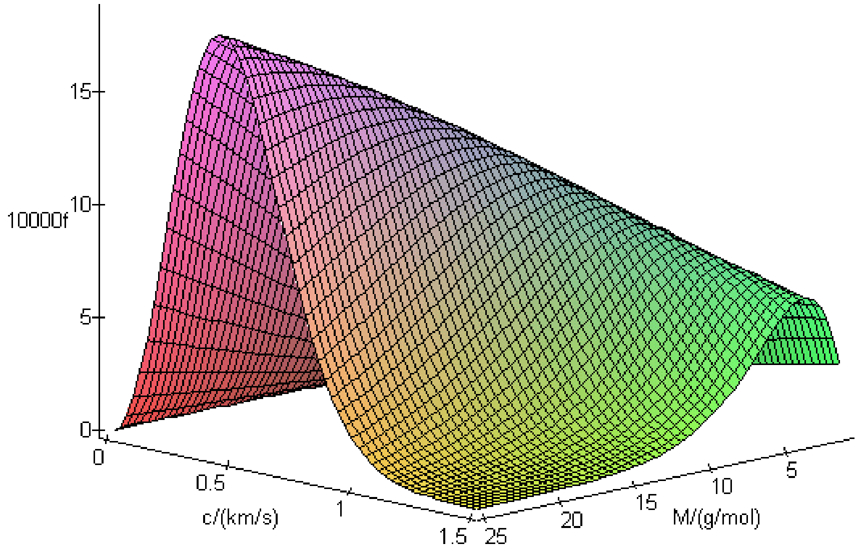

FIGURE 6. AN *F*(*C*, *M*) SURFACE FOR IDEAL GASES – THE “300-K TENT”.

repeatedly displaying them in a sequence. The Maple commands to accomplish this are given in B(iii). Upon execution of the command lines the calculated $f(c, T)$ surfaces are repeatedly displayed for various values of the molar mass. The animation characteristics, such as the size of the picture, animation rate, etc., are controlled by the viewer. See Figure 7

Example 2. Symbolic Algebra

There are numerous algebraic problems in physical chemistry that are either very time consuming or very difficult for students. CASs can make it easier for them to perform the needed algebraic manipulations. For illustration, a celebrated problem from the area of chemical kinetics is used [1, p. 1014]. The problem is this:

Given the following mechanism for the formation of HBr(g) from H_2(g) and Br_2(g),

$Br_2 \rightarrow 2Br$	rate constant k_1
$Br + H_2 \rightarrow H + HBr$	rate constant k_2
$H + Br_2 \rightarrow Br + HBr$	rate constant k_3
$HBr + H \rightarrow Br + H_2$	rate constant k_4

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$Br + Br \rightarrow Br_2$ rate constant k_5

show that the *steady state approximation* gives this expression for the rate of formation of HBr(*g*).

$$\frac{d[\mathrm{HBr}]}{dT} = \frac{k[\mathrm{H_2}]\,[\mathrm{Br_2}]^{1/2}}{[\mathrm{Br_2}] + k_p[\mathrm{HBr}]}$$

where k and k_p are constants. The Maple solution to this problem is presented in sheet5.pdf (19 Kbytes). The chemical and mathematical steps followed are explained by the comments given in this sheet. It involves the symbolic solution of two simultaneous equations, referred to as equations 1 and 2 in the sheet, followed by algebraic manipulations involving substitution, factoring, expansion, and simplification. Students can benefit (in time and difficulty) by using Maple to carry out these procedures using these model solutions as guides.

Discussion

Maple-based problem solving strategies were used in two different junior level physical chemistry courses, one for majors and the other for non-majors. In both courses, the homework was assigned with the aim of using Maple as the primary tool for dealing with all of the needed mathematics and graphing. To provide students with examples of Maple used for solving physical chemistry problems, all of the model solutions were done in Maple. The use of Maple for the course work was not mandatory. At the beginning of the course all students participated in the initial Maple workshops and did their assignments. For reasons not yet completely understood, the number of students using Maple for doing homework dropped as the semester progressed. On quizzing students about this trend it was discovered that they were somewhat frustrated by Maple's responses and its behavior when they made mistakes in entering commands. Further investigations suggested that not all of them had mastered the workshop materials and the on-line tutorial at the beginning of the semester. Some students did not try to find solutions in the on-line HELP when they ran into problems.

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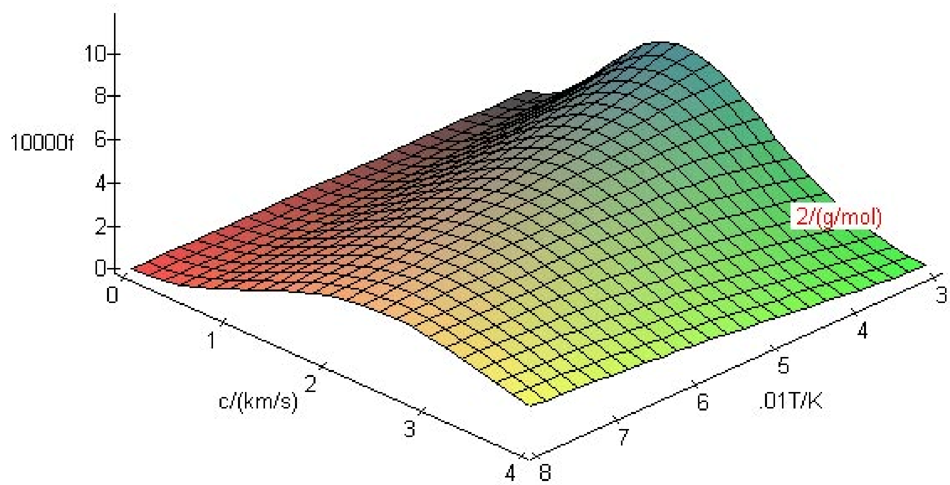

FIGURE 7. ANIMATION (ANIM2BJ.MOV, 629 KBYTES) OF THE *F*(*C*, *T*) SURFACES FOR VARIOUS IDEAL GASES.

To enhance the students' use of Maple for their course work, the following ideas are being considered.

- Should some degree of proficiency in Maple be required of all students registered for the course?

- Should attendance at the beginning of the semester Maple workshops be required of all students taking the course?

- Should students be tested on the material covered in these workshops?

- Should students submit evidence of having completed the on-line tutorials, and get credit for it? Should they be tested on the material covered in these tutorials?

- Do students have easy enough access to computers at times convenient to them?

- Should weekly assignments have some tasks that can be easily done using Maple, but would take a lot of time and effort to do without it?

- Should computers be available to students during the examination and any Maple-based materials they have developed be allowed for use during the examination?

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- Should Maple-based take-home projects be substituted for an in-class examination?
- Should an end-of-the-semester contest be run, with an appropriate reward, for students who come up with the best Maple-based solution to a challenging problem discussed in the course?

These ideas will be tried in future offerings of physical chemistry courses.

Conclusions

Computer Algebra Systems represent powerful tools for use in courses where mathematics, graphing, and visualization of the results play a significant role in the understanding of the material. Fairly sophisticated problems can be solved in a straight forward manner using these systems. They also provide an easy way to visualize the three-dimensional nature of many of the functions of chemistry. The amplification of their mathematical abilities allows students to spend more time exploring the principles of chemistry and their consequences; however, at the beginning time is needed to learn and practice the rigid command-line syntax. The beginning-of-the-semester workshops and tutorials play a key role in developing student enthusiasm for using CASs. The symbolic, numeric, graphic, and animation features must be demonstrated with carefully chosen examples that serve as models for students to follow during the course. The animation feature is key in building enthusiasm.

Obviously, students need to explore the vast majority of the commands on their own as the need arises, therefore; it is important that a significant amount of the initial workshop time be spent on the use of the on-line HELP. Some students would rather use a book instead of the on-line HELP and for these people the books by Char et al. [11] or Heck [15] are recommended.

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