APPLICATIONS OF TECHNOLOGY IN TEACHING CHEMISTRY
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PERSONAL COMPUTERS IN TEACHING PHYSICAL CHEMISTRY

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ABSTRACT:
The advanced course in Physical Chemistry for students of
Chemical Faculty of Moscow State University deals with classical
and statistical thermodynamics, kinetics and catalysis.
The main aims of using PC are:
- complex calculations in particularly solving equations and
  systems of equations having no analytical solution
   (e.g. nonisothermal kinetics),
- analysis of functions behaviour at the parameter variations
   (e.g. heat capacity at polytropic processes),
- illustrative graphics in two and three dimensions (e.g. S-T
  state diagram of water and potential energy surfaces),
- dynamical models of processes - "moving pictures"
   (e.g. chemical reaction proceeding),
- combination of previous items with text in a hypertext system,
  producing an "electronic handbook".
We use for this purpose some standard and original
programs (chemical equilibria calculations, formal kinetics
of chemical reactions, oscillating reactions et al).

I. TEACHING PHYSICAL CHEMISTRY

Special group of students with profound studying of mathematics
and physical chemistry exists at Moscow State university for
many years. Fundamental course of physical chemistry for these
students contains classical and statistical thermodynamics,
kinetics and catalysis.

We use PC at teaching physical chemistry to students of this
group with main proposes:

A. During practical work:

1. To treat experimental data obtained during   laboratory
sessions with the help of various   programs: statistical
calculations (mainly linear least squares) by our original
program REPRO; spreadsheets provided calculations and chart
drawing, etc;

2. To carry out problems modelling the behavior of complex systems, for example: investigation of oscillating chemical reactions using our original program Lotka-Volterra. This model is defined with the following kinetic scheme:

```
        k1
  A + X ---> 2X
        k2
  X + Y ---> 2Y
        k3
  Y + B ---> E
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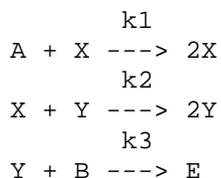
With the help of computer program student may investigate this chemical process in time. One can change parameters of this system (k1, k2, k3 and the initial concentration of A, B, X, Y substances) and see the conforming graph with the kinetic curves for X and Y substances. Teacher may also set the values for rate constants and put a test graph to student, who in this case must estimate these values from graph using the following relationships:

time of oscillations period is equal to:

$t = 2*pi/SQRT(k1*k3*[A]*[B])$ and

$k2*(X1-X2)-k3*[B]*ln(X1/X2) = k1*[A]*ln(Y1/Y2)-k2*(Y1-Y2),$

where X_i, Y_i are the current values of intermediates X, Y and letters in brackets denote concentration for corresponding substances (which are constant for this model).
Fig. 1 is the snapshot of the PC screen with such test graph.

3. To calculate chemical equilibrium for studied reaction from thermodynamic data of its components using our original program CHET.

B. During class work:

1. Solving complicated equations, for example:
determination of rate constant values for two step consequent reaction

```
    k1     k2
  A --> B --> C.
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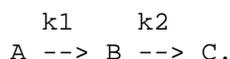
In this case the location of maximum for intermediate (B) concentration is determined by two equations:

$t([B]max) = ln(m)/(k2-k1)$ and

$[B]max = [A]o*m^{(m/(1-m))},$

where m=k2/k1. Usually this equations are solved graphically or by repeated trials. The numerical calculation is very simple if we use solving program like Borland's EUREKA (fig. 2).

2. Using PC teacher can ascertain some correlations which are

not so evident for students if they see only mathematical
formulas. For example. When we analyze kinetics of chemical
reaction

```
        k
    nA --> Products
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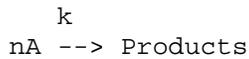
at heating with constant rise of temperature
(dT/dt=Theta=const), the rate of reaction is:

$$w = k \cdot C^n = -\frac{dC}{dT} \cdot Theta = ko \cdot \exp(-E/(R \cdot T)) \cdot C^n, \quad (*)$$

where C is concentration of substance A and n is the reaction
order. Location of function dC/dT vs T maximum is determined by
the equation:

$$-\frac{ko}{Theta} \cdot \frac{E}{R \cdot Tmax \cdot Tmax} = n \cdot C^{n-1} \cdot \exp(-E/(R \cdot Tmax)).$$

The analytical integration of differential equation for the
reaction rate (*) is impossible. So in this case we solved this
problems by means of numerical integration and drew dependence
of C and dC/dT vs T (figs. 3 and 4). And what is interesting.
Difference between concentration of substance A in reactions of
various order is negligible below the temperature of maximum
value of dC/dT (fig. 3). Therefore you want to determine
reliably order of this reaction, values of ko and E, it is
necessary to use experimental data above this temperature. It
also turns out that locations of maximum of dC/dT as function T
for different n (1-3) at constant ko and Theta lies in 5 degrees
interval (fig. 4).

3. Analysis of functions' behavior.
a. For example, very often students are thinking that there are
only two types of heat capacity: Cp and Cv. But these values
correspond only to processes at constant pressure (p) or volume
(v). Heat capacity in general case are defined by equation:

$$C = (n \cdot Cv - Cp)/(n-1),$$

where n is exponent in polytrope equation: $p \cdot v^n = const$. Analysis
of this equation shows that C=0 for adiabatic process and
indefinite for isothermal process (fig. 5).

b. Next example is analysis of dividing of chemical reactor with
ideal mixing into sections. The efficiency of such reactor may
be enhanced by dividing into sections. The question is how many
sections is significant to rise degree of conversion (y) and to
decrease the total volume of reactor as much as possible. The
ratio of total volume of m sections (m*Vi) to volume of
unsectioned reactor (V1) is equal to:

$$m \cdot Vi/V1 = m[1-(1-y)^{(1/m)}](1-y)^{((m-1)/m)}/y,$$

where m is the quantity of sections. We solved this problem with the help of spreadsheet (MicroSoft Excel) and drew the diagram (fig. 6) from which it is seen, that at small values of y dividing the reactor has little influence to its efficiency. But at high y it is significant and 3-4 sections is enough.

c. To find the answer to various problems of physical chemistry we must solve systems of differential equations. Obvious example is the analysis of chemical kinetics of complex chemical reaction. For this purpose we use KINET program written by associate professor of our faculty A.V.Abramenkov. Along using this program student write chemical equation for each simple reaction and value of rate constant of this reaction. After solving the system of differential equations it is possible to receive graph for time dependence of the concentrations for up to 15 substances involved in maximum 10 reactions and table of current concentrations. This program also allows us to determine the values of rate constants using experimental data of current concentrations.

d. One more example is to draw phase diagram of binary system after Schreder equation for ideal systems:

ln(Ni) = -(DeltaHi/R)*(Tm-T)/(Tm*T),
     T
where Ni - molar part of i-th component of binary system, Tm
       T
and DeltaHi - its melting point and heat of melting respectively, T - melting point for system with definite Ni. Students do laboratory work with diphenylamine-naphthalene system and later in computer room may calculate dependence of melting point as function of composition for it (see fig. 7). They may see that for this system cited equation satisfactory describes system behavior.

4. Viewing graphs.
a. Every student draws phase diagram of water very easily. But is is difficult to draw this chart in S, T coordinates. After seeing it on display students understand that two phase equilibria may be depicted not only as a line in p, T coordinates but as fields in S, T diagram (fig. 8).

b. Computer also allows us to draw full scale detailed chart. For instance the phase diagram of water in most of textbooks is drawn schematically. It is very useful to see real picture (fig.9,10).

c. For many students it is difficult to imagine the shape of potential energy surface when studying theory of transitional state in chemical kinetics. Using the program like SURFER it is possible to draw such picture and our experience showed that after analysis of this picture all students can draw general view of this surface and any of its section without embarrassment (fig. 11).

5. Obtaining reference information.
During classes and laboratory work we often need to obtain

equilibrium constants of chemical reactions or composition of mixture in the equilibrium state. In this case we use our own program CHET. This program uses built in data bank of thermodynamic properties of individual substances, which contains 2000 records. It can represent temperature dependencies of thermodynamic functions in tabular form, calculate equilibrium constant of a given chemical reaction or equilibrium composition of complex mixture of chemical compounds for the specified pressure and temperature.

II. SOFTWARE PROBLEMS.

A. Two reasons for using computers.
There exist at least two reasons why computers are readily used by students and teachers. The first is that computer is a universal teaching tool. It provides fast access to information (data bases, hypertext); enables modelling of experiments; adapts education speed to individual student. This stimulates the development of specific educational software. Most often this results in a large number of relatively small programs which don't resemble each other in there interface.

The second reason is less discussed, but is always taken into account. All students are aware that computers will be very helpful in there post graduate life. In other words computerized education teaches not only the subject of education (chemistry), but also how chemists use computers. That's why we use much of standard software (text processors, electronic spreadsheets, solvers and so on) in education.

B. Expenses.
Besides well known advantages education with computers has some expenses. And our aim is to make them as small as possible. Our experience evidences that main difficulty in using PC is mastering various programs by students. It takes much time and diverts them from problems in physical chemistry.

C. Using interface standards.
The first step towards the minimum in computer interface expenses is to use Graphics User Interface (GUI) which has in fact become an industrial standard. If a student learns how to work with several basic packages under Windows then he or she often feels comfortable when mastering another Windows program or even when using Mac or X-Windows software.

In order to transfer education to the Windows media we should do the following:
* Provide appropriate hardware. You can hardly run Windows if you have only 1MB of memory in your computer.
* Reform freshman computer course.
* Create Windows user interface for the educational software we use.

D. Windows are not a panacea.
Though Windows has powerful facilities which allows placing textual material, complex formula, and graphics together, it

doesn't solve all interface problems. Imagine the situation when during the lesson a student must start 3-4 different programs and load several data files in them. How much time will he (or she) spend in selecting appropriate names from relatively large lists? It would be much better if all these files had direct association with some definite sense context.

Another problem with Windows comes from its multitasking capabilities. It's great that we can start several programs simultaneously, exchange their data, compare their results just on one screen. But it takes time to place multiple windows in a most convenient manner.

E. HyperBook.
Thus we had come to an idea of creating a special educational hypertext system under GUI, which we will call here "Hyperbook". Let us see its functions on one example (figure 12). The warp of the hyperbook fabric is a set of pages with educational text. We use here a broad meaning of "text" which includes formula, schemes, graphics and other illustrations. You can include some small program in this text as well. In this case we call it moving or interactive illustration. Such a program starts automatically when the page is opened (thus having definite sense context) and its window is always in a definite place on the page (compare with the previous paragraph).

As you may have noted, there are portions of highlighted text on the page on figure 12. This is another feature of hypertext – active contexts. When you activate them with, say, mouse click, the hyperbook performs some job appropriate to the sense of context. This can be showing the definition of a term, moving to another page of hyperbook or launching some application.

Our nearest intent is to create with the help of this tool computer aided physical chemistry course.

QUESTIONS FOR READERS.

We tried to use several solvers available in DOS: Eureka, Mercury, MathCAD, but all of them have significant disadvantages. Which solvers do you use if any and which is the best?

When you want to use a lot of small computer programs during the lesson do you think it is worth including them into an integrated environment like hyperbook? Or is it better to encourage their use through the commands of operating system?

Are there any other ways to lessen expenses of using computers in teaching chemistry?

FIGURES.

All figures are 640x480 16-color .GIF files.

1. Test picture for Lotka-Volterra reaction. Students ought to

estimate the values of k1, k2, k3.

2. The calculation of values of k1 and k2 for reaction A->B->C from values of t max and C max of B substance.

3. The dependence of degree of conversion (alpha) of A substance on temperature for reaction nA -> Products during constant rise of temperature (theta). n - order of reaction.

4. The dependence of d(alpha)/dT vs T for reaction nA->Products.

5. The change of heat capacity value upon increasing of n, exponent in polytrope equation (p*V^n=const). Ideal gas.

6. The influence of dividing the ideal mixing reactor into sections on degree of conversion (y). m - quantity of sections, Vi - volume of single section, V1 - volume of unsectioned reactor.

7. The phase diagram of naphthalene-diphenylamine system drawn after Schreder equation calculation. T - melting point of system, N - molar ratio of naphthalene.

8. Phase diagram of water at S, T coordinates. I - solid, II - liquid, III - vapor IV - solid-liquid, V - solid-vapor, VI - liquid-vapor transitions

9. Phase diagram of water drawn accordingly experimental data.

10. The same as at fig.9. but for the narrow interval of temperature.

11. View of potential energy (a.u.) surface for F+H2 interaction. J.S.Wright,J.Williams Chem.Phys.Lett. 184, 159 (1991).

12. Figure 12 presents contents of the window with one of the first pages of the hyperbook on chemical kinetics. Text in russian gives definitions of basic concepts of kinetics. A picture with two buttons and a graph is an interactive illustration. When the user pushes 'Start' button it begins to change in time acoording to kinetic equations, thus giving students the sense of kinetic curves and the comparison of first and second order reactions. Just above the main window there is a popup window with additional information. This windows appeared when the user clicked blue active context.