TRAINING SOFTWARE FOR REACTION KINETICS VIA WEB

Mihaela Ligia UNGUREŞAN, Lorentz JÄNTSCHI

Technical University of Cluj-Napoca, Romania,
http://mihaela.academicdirect.ro, http://lori.academicdirect.ro

Abstract: An original client-server interface to use for interactive students work with computer was build. The program serves for training in field of reaction kinetics of simple and complex reactions. The program was build using PHP language and is available through web at the address:
http://vl.academicdirect.ro/molecular_dynamics/reaction_kinetics
The program makes the activity of teaching and learning about the kinetics of chemical reactions to be more efficient, the students being able to determine from the graphics of concentration depending on time, for slow as well as fast reactions, the reaction rate, halftime, the reaction order.

Keywords: reaction kinetics, client-server application, e-learning

1. INTRODUCTION

The chemical kinetics is about the rate and mechanism of chemical reactions [1,2]. The research of the reaction mechanisms starts from establishing the experimental rate law that involves the dependence of rate law on the concentration of the reactants, products, and catalyses, on temperature and on the interpretation of the activation parameters. The rate law is the mathematical form of the kinetic law of the action of masses [3,4].

The kinetic study of a reaction involves establishing the rate law, identifying the constants, establishing the reaction mechanisms according to the rate law, establishing the dependences of the reaction rates depending on time.

2. METHOD AND RESULTS

A client server application was build. For implementation of the software, *HTML* language was choused from reason of easy to run and use. Only a computer with windows operating system and Microsoft Internet Explorer ≥ 4.0 is enough to run all *.htm* files. A set of *PHP* programs for computing simulated values was implemented. *PHP* (post processed hypertext) language is a very easy to use and is a server dedicates software. The *PHP* page request is send to the web server, and the server using *mod_php* module process the page, compile the program, execute the instructions, and send to the client process data in html format.

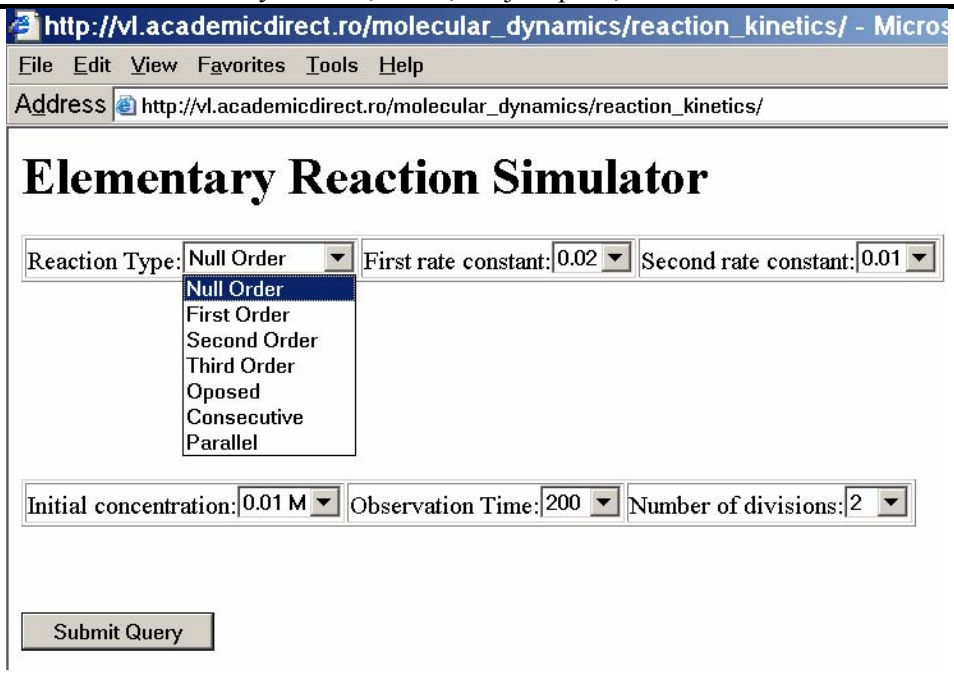

Fig. 1. http://vl.academicdirect.ro/molecular_dynamics/reaction_kinetics web interface

Depending on the option chosen by the user, the program generates columns of calculated values and displays them (fig. 2). The data are modifiable so that the user, as he wishes, can modify the calculated values in simulation, introducing his own values (resulted for instance from experimental measurements) [5, 6].

The mathematical functions that are used represents the concentrations of reactants at a certain moment, of the reactants, intermediates, as well as of the reaction products, the variable x being representing the time, c being the initial concentration, and k, k_1, k_2 being rate constants. The expressions of the integrated forms of the rate laws are expressed for reaction of zero order, first, second, third, opposed reactions, parallel and consecutive reactions are presented as follows [7, 8]:

- function ordin1($x,$k,$c){return $c*exp(-$x*$k);}
- function ordin1p($x,$k,$c){return $c*(1.0-exp(-$x*$k));}
- function ordin1c1($x,$k1,$k2,$c){return $c*exp(-$x*$k1);}
- function ordin1c2($x,$k1,$k2,$c){
- return $c*$k1*(exp(-$x*$k1)exp($x*$k2))/($k2-$k1);}
- function ordin1c3($x,$k1,$k2,$c){
- return $c*(1.0-$k2*exp(-$x*$k1)/($k2-$k1)+$k1*exp(-$x*$k2)/($k2-$k1));}
- function ordin1p1($x,$k1,$k2,$c){return $c*exp(-$x*($k1+$k2));}
- function ordin1p2($x,$k1,$k2,$c){
- return $k1*$c*(1.0-exp(-$x*($k1+$k2)))/($k1+$k2);}
- function ordin1p3($x,$k1,$k2,$c){
- return $k2*$c*(1.0-exp(-$x*($k2+$k1)))/($k2+$k1);}
- function ordin2($x,$k,$c){return $c/(1.0+$k*$x);}
- function ordin2p($x,$k,$c){return $c-$c/(1.0+$k*$x);}
- function ordin01($x,$k,$c){if ($k*$x<$c) return $k*$x; else return $c;}
- function ordin02($x,$k,$c){if ($k*$x<$c) return $c-$k*$x; else return 0.0;}
- function ordin31($x,$k,$c1,$c2,$c3){return $c1-$k*$c1*$c2*$c3*$x;}
- function ordin32($x,$k,$c1,$c2,$c3,$c4){return $c4+$k*$c1*$c2*$c3*$x;}

- function ordinr1($x,$k1,$k2,$c1,$c2){return $c1-($k1*$c1-$k2*$c2)*$x;}
- function ordinr2($x,$k1,$k2,$c1,$c2){return $c2-($k2*$c2-$k1*$c1)*$x;}

A program execution for first order reaction type (first rate constant: 0.02 s^{-1}, initial concentration 0.01 $mol \cdot l^{-1}$, observation time: 200 s) are presented in fig. 2:

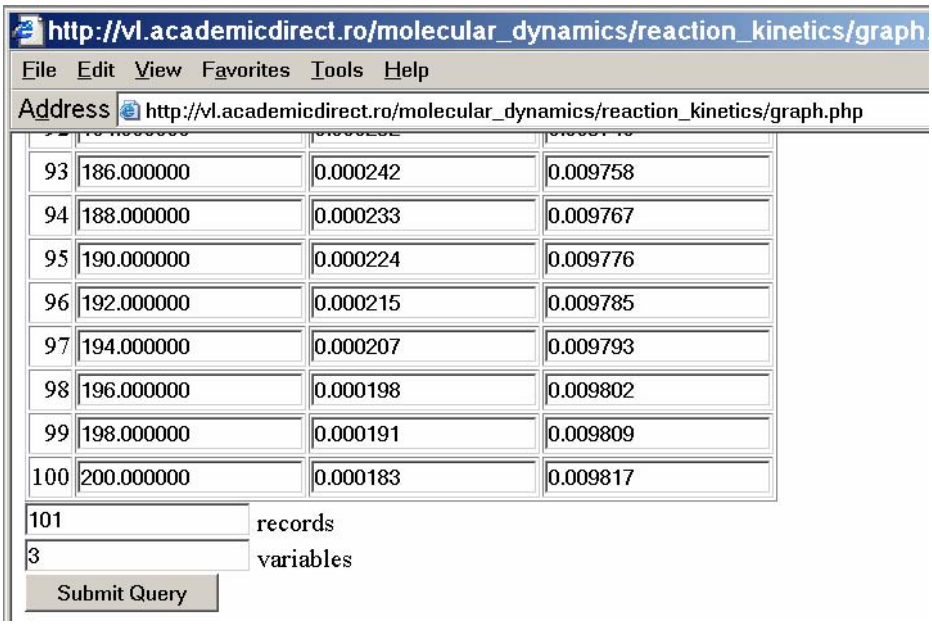

Fig. 2. http://vl.academicdirect.ro/molecular_dynamics/reaction_kinetics/graph.php

The data in fig. 2 are taken over by a program of graphic representation (fig. 3):

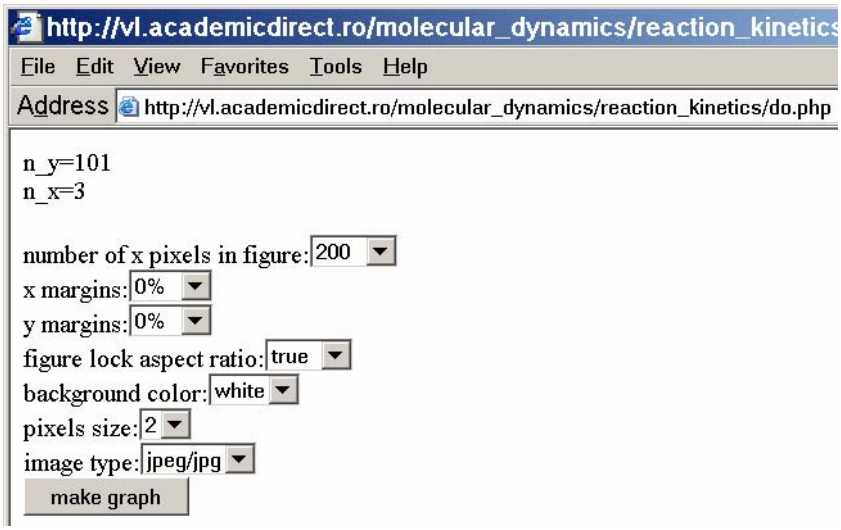

Fig. 3. http://vl.academicdirect.ro/molecular_dynamics/reaction_kinetics/do.php

The program allows choosing the options wanted (number of pixels, margins, background, pixels size, image type). Based on the options chosen by the user, the program makes the graphic (fig. 4):

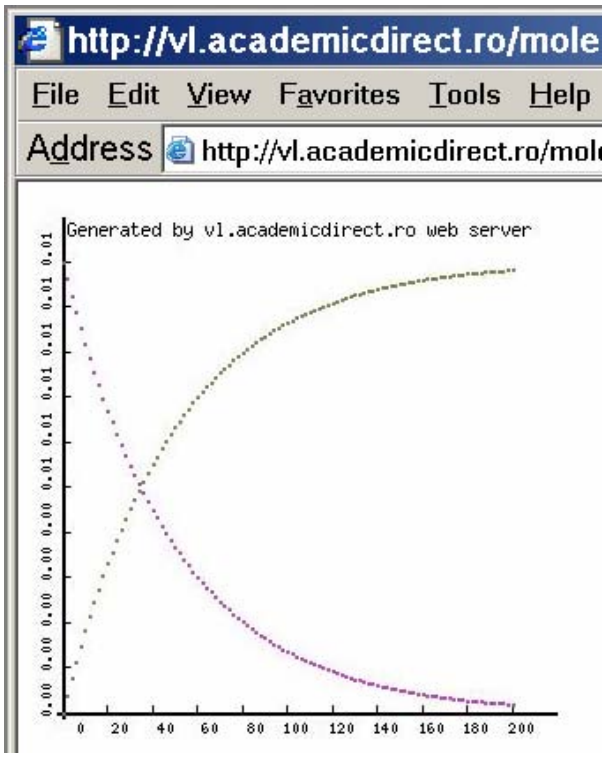

Fig. 4. http://vl.academicdirect.ro/molecular_dynamics/reaction_kinetics/plot.php

The follows code sequences serve for displaying the graphic on browser client [9]:

```
$n = $_POST['n']; // number of records
$m = $_POST['m']; // number of variables
for($k=0;$k<$m;$k++){
$temp=sprintf("x_%d",$k);
$x[$k] = split('[;/]',$_POST[$temp]); } // x values
$x_size = $_POST['p']; // number of x pixels in figure
$k = $_POST['k']; // figure lock aspect ratio
$b = $_POST['b']; // background color
$z = $_POST['z']; // pixels size
$t = $_POST['z']; // line size
$r = $_POST['r']; // x margins
$s = $_POST['s']; // y margins
switch ($_POST['g']) {
case 'png':header ("Content-type: image/png");imagepng($image);break;
case 'gif':header ("Content-type: image/gif");imagegif($image);break;
case 'jpg':
header ("Content-type: image/jpeg");imageinterlace($image,1);imagejpeg($image);
} // Content-type
```

Another interesting example of program running is for consecutive reactions (fig. 5, first rate constant: 0.02 s^{-1}, second rate constant: 0.01 s^{-1}, initial concentration: 0.01 $mol \cdot l^{-1}$, observation time: 200 s):

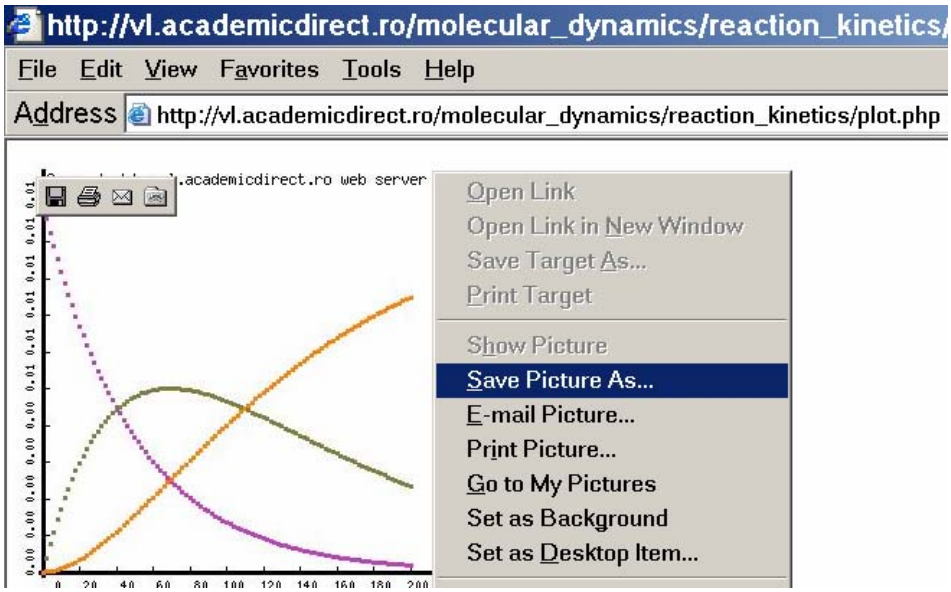

Fig. 5. The graphic representation of the consecutive reactions of the first order

The obtained graphic can be saved on to the disk, as we can observe in fig. 5.

3. CONCLUSIONS

Considering the advantages of implemented software technology (machine and operating system portability, graphical interface and database connectivity features, easiest of programs developing, free type license agreement, http capability) the programming language and the program itself is the one of the best choice now available.

The program is successfully used for student practice in field of chemical kinetics. The program permits to observe more efficient the evolution of reaction in real time.

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