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SIMULATION OF KINETICS CHEMICAL REACTIONS

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Abstract: The present paper its presents the mathematical simulation of the kinetics of simple and complex reactions, using the program PHP is available through http Internet protocol at the address:

http://academicdirect.ro/virtual_library/molecular_dynamics/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, $t_{1/2}$, the reaction order.

Keywords: Chemical kinetics, reaction order, simulation, rate law.

1. Introduction

The chemical kinetics[1] is about the rate and mechanism of chemical reactions. 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.[2] The kinetic study of a reaction involves establishing the rate law, identifying the rate constants, establishing the reaction mechanisms according to the rate law, establishing the dependences of the reaction rates depending on time.

2. Software

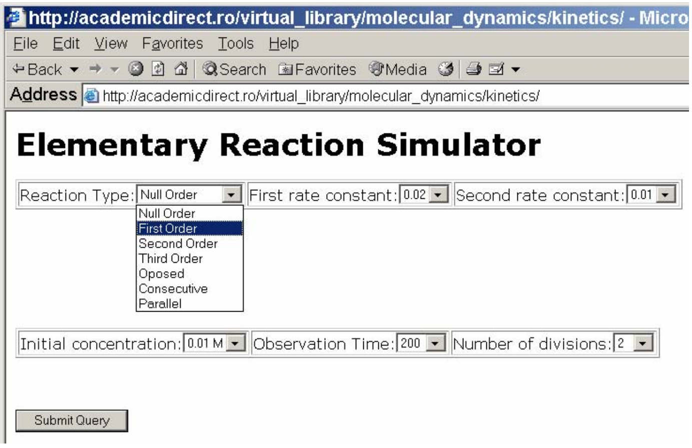
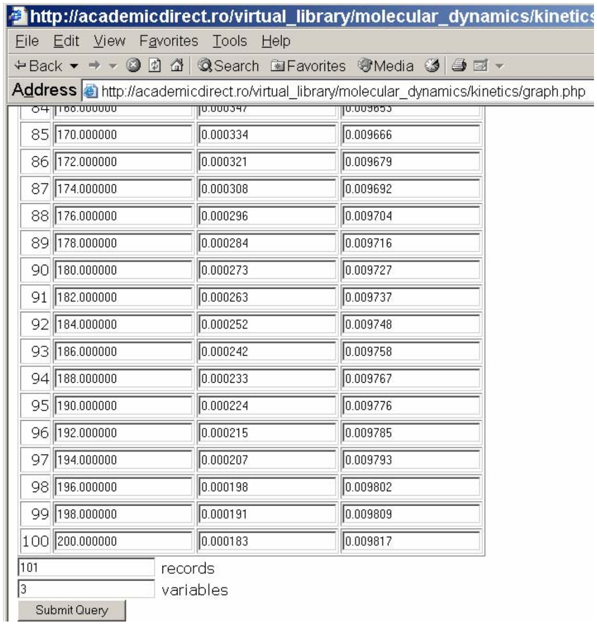


Fig. 1. http://academicdirect.ro/virtual_library/molecular_dynamics/kinetics/

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 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. 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).[3,4]



85	170.000000	0.000334	0.009666
86	172.000000	0.000321	0.009679
87	174.000000	0.000308	0.009692
88	176.000000	0.000296	0.009704
89	178.000000	0.000284	0.009716
90	180.000000	0.000273	0.009727
91	182.000000	0.000263	0.009737
92	184.000000	0.000252	0.009748
93	186.000000	0.000242	0.009758
94	188.000000	0.000233	0.009767
95	190.000000	0.000224	0.009776
96	192.000000	0.000215	0.009785
97	194.000000	0.000207	0.009793
98	196.000000	0.000198	0.009802
99	198.000000	0.000191	0.009809
100	200.000000	0.000183	0.009817

101 records
3 variables

Fig. 2. http://academicdirect.ro/virtual_library/molecular_dynamics/kinetics/graph.php

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, parallel and consecutive reactions[5] are presented as follows.

```
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;}
```

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

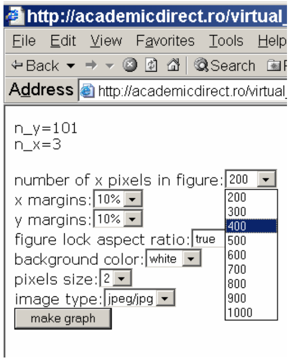


Fig. 3. http://academicdirect.ro/virtual_library/molecular_dynamics/kinetics/do.php

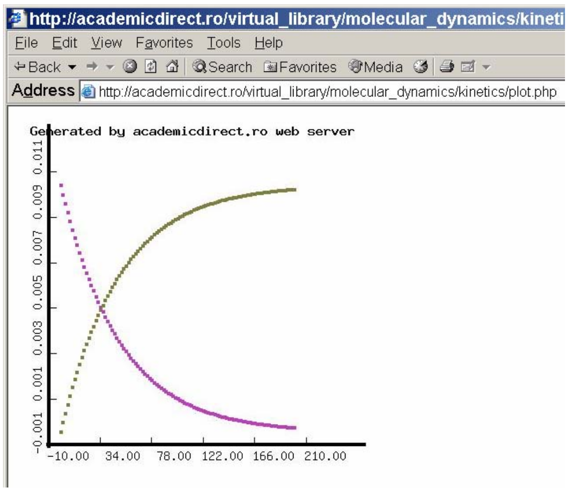


Fig. 4. http://academicdirect.ro/virtual_library/molecular_dynamics/kinetics/plot.php

We present as follows a few code sequences for displaying the graphic on browser client:

```
$n=$HTTP_POST_VARS['n'];//number of records; $m=$HTTP_POST_VARS['m'];//number of variables
```

```
for($k=0;$k<$m;$k++){$temp=sprintf("x_%d",$k);; $x[$k]=split('[;/]',$HTTP_POST_VARS[$temp]);//x values}
$x_size = $HTTP_POST_VARS['p'];//number of x pixels in figure; $k = $HTTP_POST_VARS['k'];//figure lock
aspect ratio; $b = $HTTP_POST_VARS['b'];//background color; $z = $HTTP_POST_VARS['z'];//pixels size; $t =
$HTTP_POST_VARS['z'];//line size; $r = $HTTP_POST_VARS['r'];//x margins; $s = $HTTP_POST_VARS['s'];//y
margins;switch($HTTP_POST_VARS['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
```

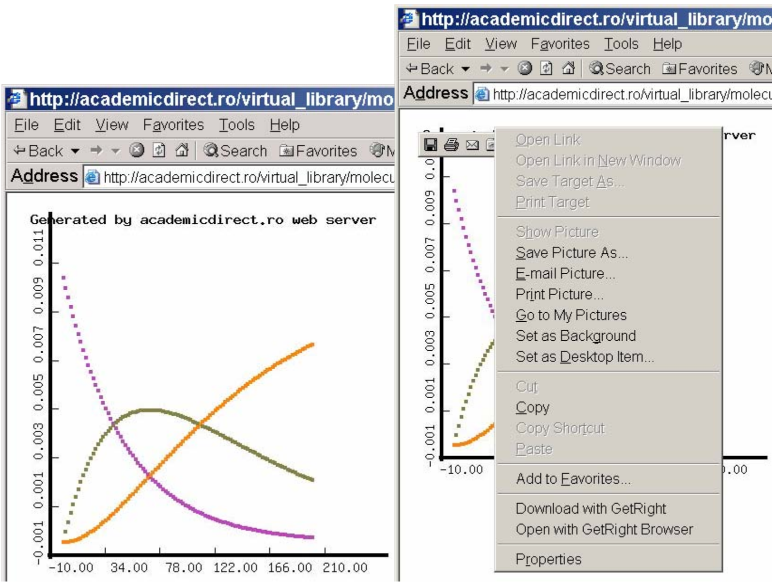


Fig. 5: The graphic representation of the consecutive reactions of the first order

The graphic obtained can be saved on the disk, as we can observe in fig.5.[6]

3. Conclusions

Considering the advantages of implemented software technology 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.

References

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