

Ministerul Educației și Cercetării  
Universitatea Tehnică din Cluj-Napoca  
Facultatea de Știința și Ingineria Materialelor  
Catedra de Chimie

Programul:	Cercetare de Excelență
Modul: II	Proiecte de Dezvoltare a Resurselor Umane pentru Cercetare
Tipul proiectului:	Proiecte de cercetare de excelenta pentru tinerii cercetători
Cod proiect:	ET108/2006
Denumirea proiectului:	Procese la Interfața fazelor: Modelare matematica, Optimizare numerica, Implementare web, cu aplicatii în separarea și caracterizarea seriilor de compuși chimici biologic activi
Etapă:	Finală/2007

## *Lucrare în extenso*

### *Cuprins*

<i>Etape, obiective și activități</i>	<i>– pag. 02</i>
<i>Activități și rezultate</i>	<i>– pag. 03</i>
<i>Etapa 1, Activitatea 1</i>	<i>– pag. 04</i>
<i>Etapa 1, Activitatea 2</i>	<i>– pag. 09</i>
<i>Etapa 1, Activitatea 3 și Etapa 2, Activitatea 1</i>	<i>– pag. 16</i>
<i>Etapa 2, Activitatea 3</i>	<i>– pag. 23</i>
<i>Etapa 2, Activitatea 4</i>	<i>– pag. 29</i>
<i>Etapa 3, Activitatea 1</i>	<i>– pag. 45</i>
<i>Etapa 3, Activitatea 2</i>	<i>– pag. 100</i>
<i>Etapa 3, Activitatea 3</i>	<i>– pag. 101</i>
<i>Et1, Activitatea 4, Et2, Activitatea 2, și Et3, Activitatea 4</i>	<i>– pag. 104</i>
<i>Publicații</i>	<i>– pag. 107</i>
<i>Concluzii</i>	<i>– pag. 136</i>

### ***Etape, obiective și activități***

Pentru etapele anului 2007 obiectivele planificate au fost:

- ÷ Colectarea datelor experimentale (electroforeza, spectrofotometrie)
- ÷ Dezvoltarea modelelor matematice
- ÷ Parametrizarea variabilelor: proprietati de suprafata ale lichidelor, repartitie si distributie intre faze
- ÷ Implementarea modelelor matematice in module de calcul numeric
- ÷ Obținerea parametrilor de model si de experiment prin optimizare numerica
- ÷ Concretizarea modelelor

Activitățile prevăzute a se desfășura au fost:

- ÷ Separarea prin electroforeza a triazinelor
- ÷ Achiziția datelor spectrofotometrice (intensitate luminoasa) in cinetica reactiei ionilor de cupru si tiosulfat
- ÷ Inglobarea in modelul matematic al ecuatiilor de caracterizare a proprietatilor de suprafata ale lichidelor
- ÷ Participari la manifestari stiintifice si dobandirea de competente complementare
- ÷ Inglobarea in modelul matematic al ecuatiilor de caracterizare a repartitiei si distributiei intre faze
- ÷ Participari la manifestari stiintifice si dobandirea de competente complementare
- ÷ Construirea functiilor obiectiv si a formulelor de iteratie
- ÷ Implementarea rutinelor si programelor de calcul
- ÷ Testarea functiilor obiectiv
- ÷ Corelarea cu experimentele, alegerea functiilor obiectiv optime
- ÷ Calcularea parametrilor de model prin optimizare, si a parametrilor de experiment prin formule de calcul
- ÷ Participari la manifestari stiintifice si dobandirea de competente complementare

**Activitățile au fost realizate și obiectivul planificat a fost atins.**

*Activități și rezultate*

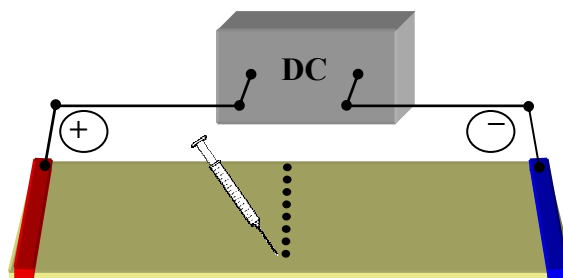
### Etapa 1, Activitatea 1. Separarea prin electroforeza a triazinelor

Electroforeza este definită ca transportul particulelor încărcate electric într-un câmp electric produs de curent electric.

Particulele pot fi ioni simpli (cum este cazul triazinelor) macromolecule complexe (ca proteinele și coloizii) sau materie specifică (cum este cazul celulelor vii - eritrocite sau bacterii).

Separarea electroforetică este bazată pe rata de migrare diferențiată în masa fazei lichide diferită de reacțiile care apar la electrozi. Rezoluția poate fi semnificativ îmbunătățită când un element de discontinuitate este introdus în faza lichidă (cum este un gradient de pH).

Schema experimentului de electroforeză este redat în figura de mai jos:



Pentru electroforeza pe hârtie de ser, pe lângă camera de electroforeză și redresor (fig. 1) mai sunt necesare și benzi de hârtie de filtru Whatman (25cmX2cm), soluție de tampon concentrată (66 g 5,5'-dietilbarbiturat de sodiu (medinal), 35.1 g acetat de sodiu hidratat cu 3 molecule de apă, 0.2 g mertiolat de sodiu, care se dizolvă într-un balon cotat de 1000 ml cu apă distilată și se corectează pH-ul la pH = 9 cu acid acetic glacial), soluție de tampon de lucru (obținută prin dizolvarea 1/10 a soluției tampon concentrate cu apă distilată), soluție de colorare (10 g amidoshwartz 10B, 900 ml alcool metilic, 100 ml acid acetic glacial) și soluție de spălare (100 ml acid acetic glacial, 400 ml metanol, 500 ml apă distilată) și soluție de eluare (4 g hidroxid de sodiu, 1000 ml apă distilată).

Algoritmul de lucru este redat mai jos:

1. Se prepară gelul de  $\beta$ -esterază în mediu de TG la pH = 8; fie acesta G1;
2. Se prepară gelul de PGM în mediu de TG la pH = 8; fie acesta G2;
3. Se prelevă 10 probe de amestecuri de triazine;
4. În 10 eprubete cu dop se pun câte 2 ml de apă distilată și se așează pe un strat de gheață;
5. Se etichetează tuburile după conținut pentru a evita confuzia;

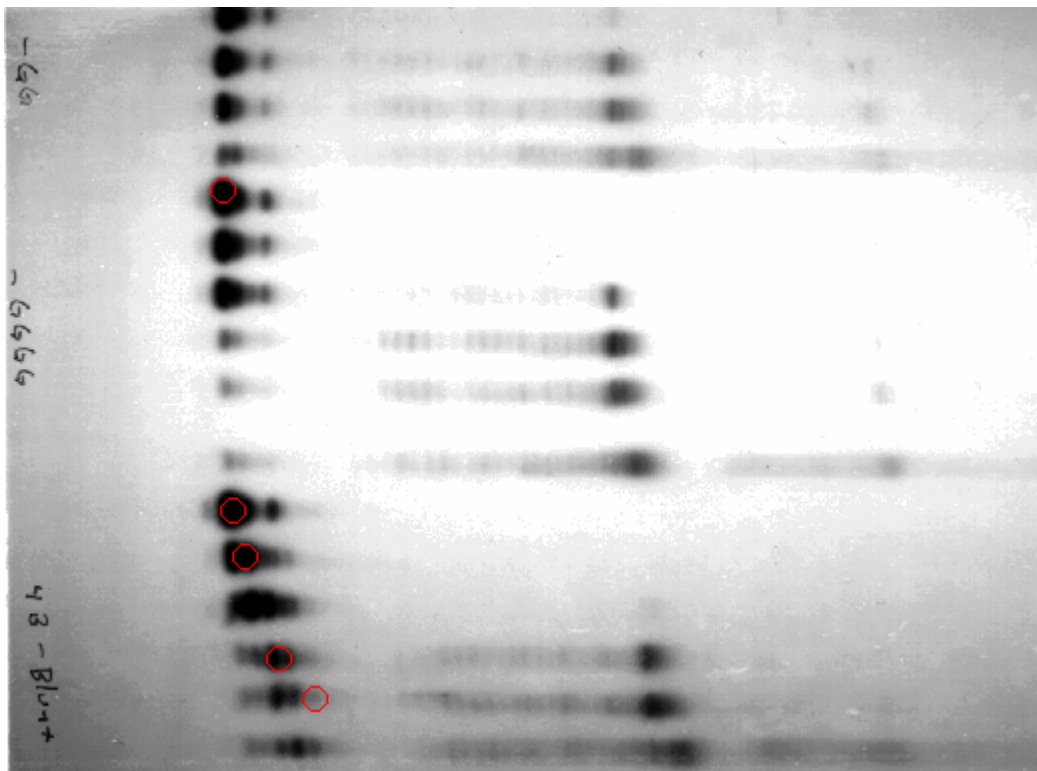


***ET108/2006 – Et. Finală/2007 – Lucrare in extenso***

2. Se impregnează fiecare bandă cu tamponul de electroforeză și se fixează orizontal (prin adeziune de rame) astfel ca cel puțin 1 cm din cele două capete să fie în soluția tampon;
3. Se efectuează preelectroforeza pentru echilibrarea sistemului:
  - 3.1. Se conectează redresorul la sursa de tensiune, se fixează amperajul la 0.2 mA/cm de lățime;
  - 3.2. Se lasă în funcțiune timp de 30 min.;
  - 3.3. Se întrerupe curentul electric;
4. Se aplică proba:
  - 4.1. Se aplică 5-10  $\mu$ l ser sub forma unei benzi;
  - 4.2. Se așteaptă 10 min.;
5. Se efectuează migrarea electroforetică:
  - 5.1. Se stabilește legătura la sursa de curent;
  - 5.2. Pentru migrare rapidă (4-5 ore) se reglează tensiunea la borne de 320-350 V și amperajul la 0.3-0.5 mA/cm de lățime de bandă;
  - 5.3. Se deconectează sursa de tensiune.
6. Se efectuează determinările:
  - 6.1. Se scot benzile de hârtie din camera cromatografică;
  - 6.2. Se pun în etuvă la 100°C timp de 10-15 min. pentru uscare;
  - 6.3. Se introduc în soluția de colorare timp de 15 min.;
  - 6.4. Se îndepărtează excesul de colorant prin trecerea proteinogramei prin 3 băi de spălare (până la decolorarea benzii);
  - 6.5. Se tamponează cu hârtie de filtru uscată;
  - 6.6. Se introduc în etuvă la 80°C timp de 10-15 min.;
  - 6.7. Se pregătesc 5 eprubete;
  - 6.8. Se decupează fiecare bandă începând cu banda corespunzătoare albuminei;
  - 6.9. Se mărunțește fiecare bandă și se introduce în eprubeta corespunzătoare;
  - 6.10. Se pipetează în fiecare eprubetă câte 5 ml soluție de eluare;
  - 6.11. Se agită energic;
  - 6.12. Pentru o bună eluare se lasă 30 min.;
  - 6.13. Se citește extincția fiecărei fracțiuni față de apă distilată la  $\lambda = 590$  nm folosind un spectrofotometru;

6.14. Se calculează ponderea fiecărei fracțiuni în amestec prin raportarea extincției sale la suma extincțiilor (5 fracțiuni):  $c_i[\%] = 100 \cdot E_i / \Sigma E_j$ .

Un exemplu de împrăștiere obținută la electroforeza triazinelor este redat în figură următoare:

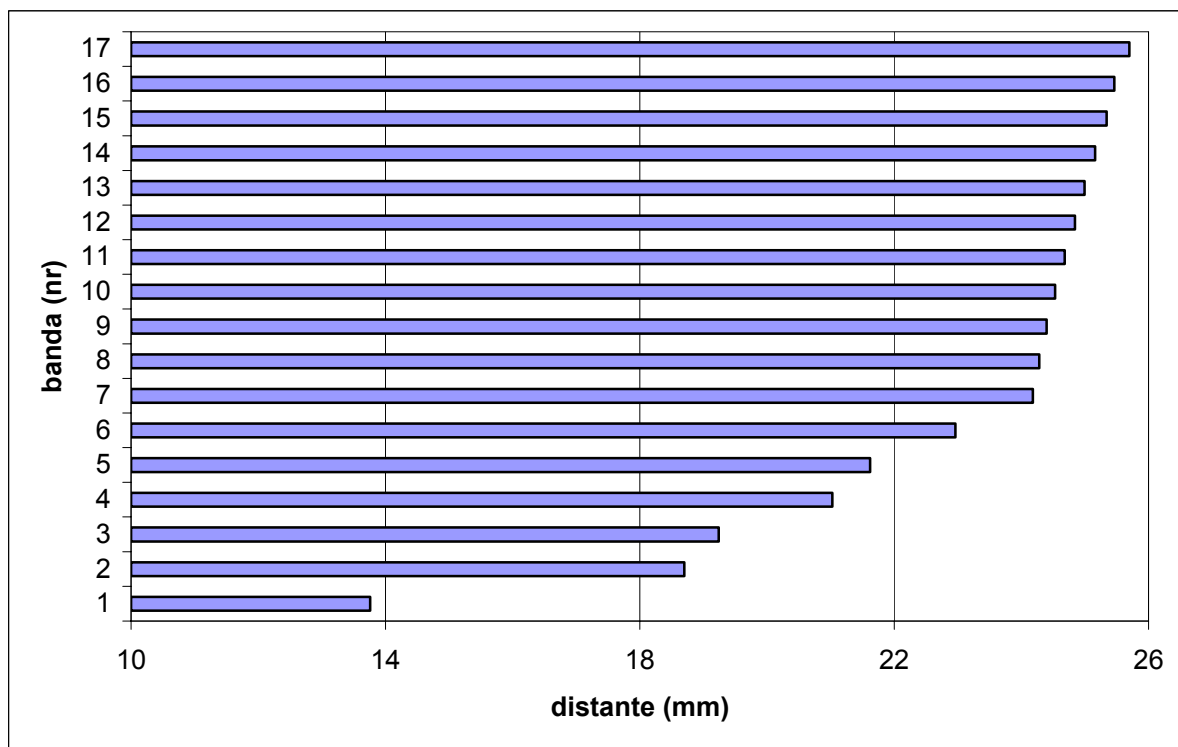


Rezultatele experimentale pentru cele două preparate de gel sunt redate în tabelul următor:

Deplasari	P1	P2	P3	P4	P5	P6	P7	P8	P9	P10	Medii
Banda1	13.7	13.7	13.7	13.8	13.7	13.9	13.9	13.6	13.8	13.8	13.76
Banda2	18.7	18.6	18.8	18.6	18.6	18.6	18.7	18.7	18.8	18.9	18.70
Banda3	19.1	19.3	19.3	19.1	19.3	19.3	19.4	19.2	19.3	19.1	19.24
Banda4	21.2	21.1	21.1	20.9	20.9	20.8	21.1	21.2	21	21	21.03
Banda5	21.5	21.7	21.7	21.6	21.5	21.5	21.6	21.6	21.7	21.8	21.62
Banda6	22.9	22.9	22.9	23	23.1	22.9	23	23	22.9	23	22.96
Banda7	24.2	24.2	24.3	24.1	24.1	24.2	24.3	24.1	24.1	24.2	24.18
Banda8	24.3	24.3	24.4	24.2	24.2	24.3	24.4	24.2	24.2	24.3	24.28
Banda9	24.4	24.4	24.5	24.3	24.3	24.4	24.7	24.3	24.3	24.4	24.40
Banda10	24.7	24.5	24.6	24.4	24.4	24.5	24.9	24.4	24.4	24.5	24.53
Banda11	24.8	24.6	24.7	24.5	24.5	24.7	25	24.5	24.7	24.8	24.68
Banda12	24.9	24.8	25	24.6	24.7	24.9	25.1	24.7	24.8	24.9	24.84
Banda13	25	25.1	25.1	24.7	24.9	25.1	25.2	24.8	24.9	25.1	24.99
Banda14	25.1	25.4	25.3	24.8	25	25.2	25.7	24.9	25	25.2	25.16
Banda15	25.6	25.5	25.6	25	25.2	25.3	-	25.1	25.1	25.7	25.34
Banda16	-	-	-	25.5	25.4	25.6	-	25.3	25.5	-	25.46

Banda17	-	-	-	-	-	-	-	25.7	-	-	25.70
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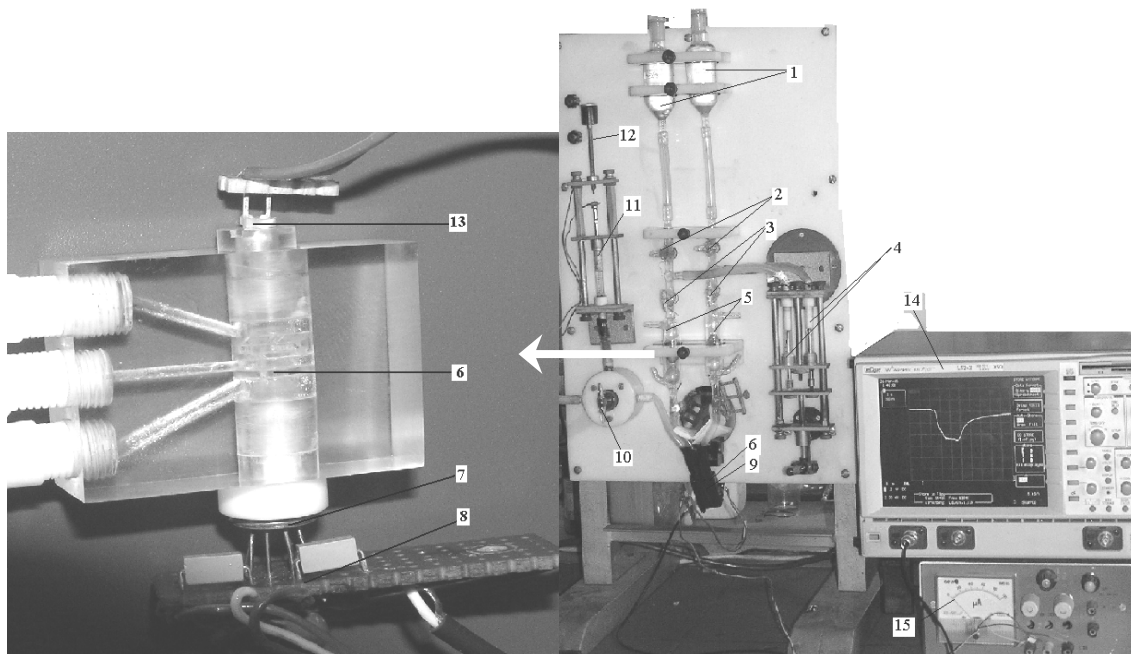
Următorul grafic prezintă benzile medii înregistrate pentru separarea electroforetică amestecului de triazine:



► Concluzii: știind că frecvent un amestec de triazine conține peste 20 de triazine (rareori mergând până la 30), metoda de separare prin electroforeză a reușit separarea a cel puțin 57% dintre acestea și a cel mult 85% dintre acestea. Metoda electroforetică de separare a triazinilor se dovedește un foarte bun instrument în separarea triazinilor atunci când amestecul de triazine conține un număr redus de triazine (până la 15 triazine, aceasta fiind de fapt valoarea modei - cel mai frecvent număr, 4 din 10 cazuri - pentru numărul de benzi distinct identificate în separarea triazinilor). Pentru probe cu număr mare de triazine se impun metode cuplate de analiză cum ar fi metode cromatografice, la care optimizarea fazei mobile să permită o mai mare sensibilitate.

**Etapa 1, Activitatea 2. Achiziția datelor spectrofotometrice (intensitate luminoasă) în cinetica reacției ionilor de cupru și tiosulfat**

Următoarea instalație (construită la Universitatea Tehnică din Cluj-Napoca - Dr. Mihaela Ligia UNGUREȘAN) a fost folosită pentru achiziția datelor spectrofotometrice:



Legendă

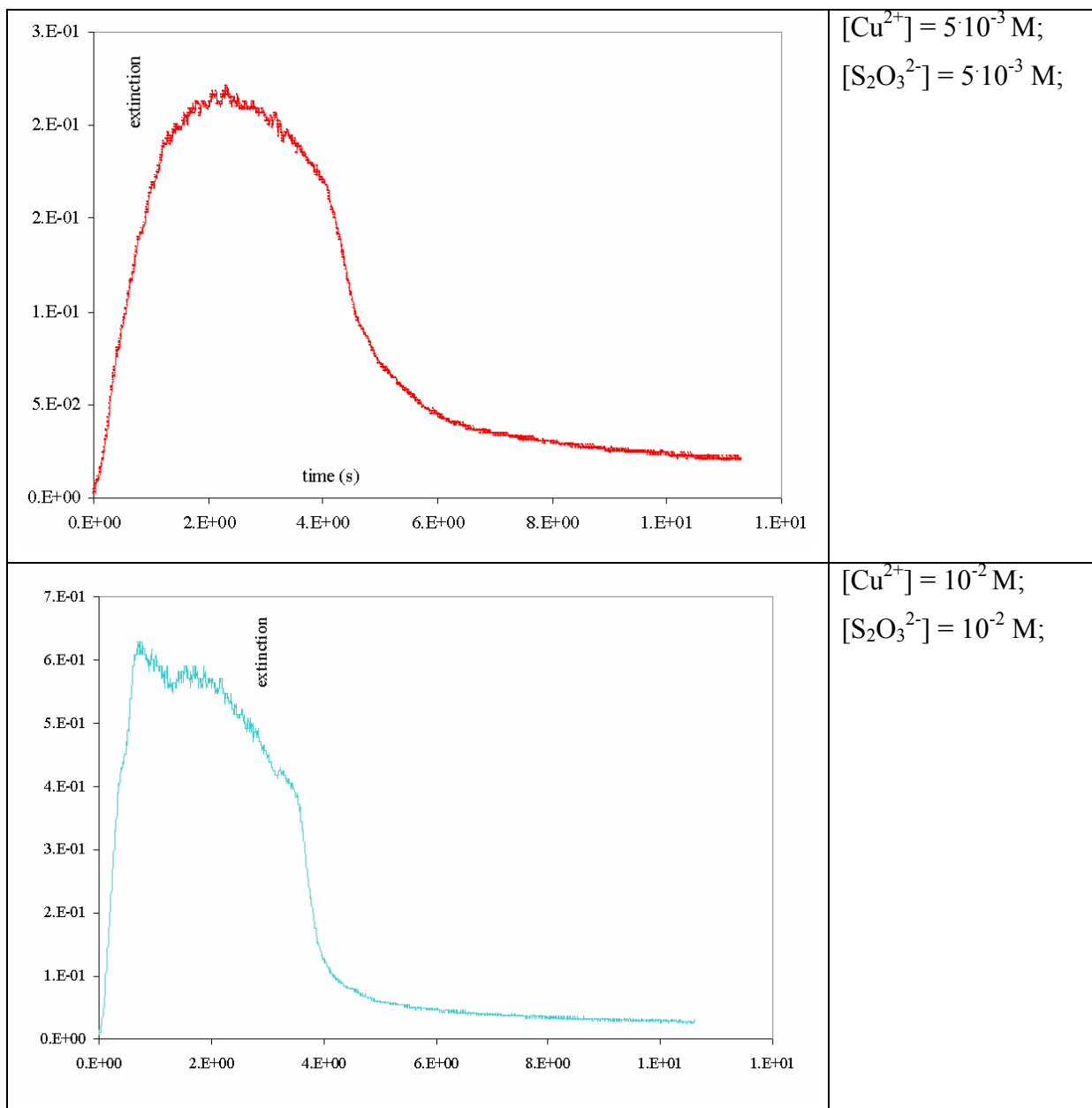
1. rezervoare cu soluțiile celor doi reactanți ( $\text{Cu}(\text{ClO}_4)_2$ ;  $\text{Na}_2\text{S}_2\text{O}_3$ ); 2. robineti superiori; 3. robineti inferiori; 4. sistem dozare reactanți; 5. refrigerenți; 6. celula de măsură; 7. traductor de măsură (detector cu fotodiodă); 8. circuit electronic pentru prelucrarea semnalului; 9. cameră obscură; 10. robinet cu trei căi pentru evacuarea produșilor de reacție; 11. electrod mobil; 12. electrod fix; 13. sursă de lumină monocromatică (LED); 14. osciloscop cu memorie; 15. microampermetru.

O serie de lucrări recente ale Dr. Mihaela Ligia UNGUREȘAN și coautorii tratează problematica determinării ordinului de reacție la amestecul dintre cupru și tiosulfat:

Nr	Lucrare
1	Mihaela Ligia UNGURESAN, G. NIAC, <i>Investigation of <math>\text{Cu}^{2+}</math>-<math>\text{S}_2\text{O}_3^{2-}</math> Reaction Kinetics</i> , Inorganic Reaction Mechanisms, cod: IRM04062/L, 6, Issue 3, 2007.
2	Mihaela Ligia UNGURESAN, G. NIAC, Emanoil SURDUCAN, Vasile SURDUCAN, <i>Instalatie de curgere oprita pentru studiul cineticii reactiilor rapide în solutii. Reactia dintre <math>\text{Cu}^{2+}</math> și <math>\text{S}_2\text{O}_3^{2-}</math></i> , Revista de Chimie, 58(1), 40 - 43, 2007.
3	Mihaela Ligia UNGURESAN, G. NIAC, <i>Composition of the Intermediate of the Fast</i>

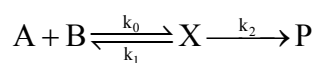
	<i>Interaction Between Copper(II) and Thiosulfate ions in Aqueous Solution</i> , Revue Roumaine de Chimie, 52(5), 483-487, 2007.
4	Mihaela Ligia UNGURESAN, G. Niac, <i>PART I.Visible Spectrum of the Copper(II)-Thiosuphate Complex</i> , Physical Chemistry: An Indian Journal, Vol.II, Issue 1, 2007.
5	Mihaela Ligia UNGURESAN, G. Niac, <i>PART II.Formation Constant of CuS<sub>2</sub>O<sub>3</sub> in Aqueous Solution</i> , Physical Chemistry: An Indian Journal, Vol.II, Issue 1, 2007.

► Următoarele grafice reprezintă datele experimentale de extincție la diferite concentrații ale reactanților:



**ET108/2006 – Et. Finală/2007 – Lucrare in extenso**

► Folosind datele obținute din 3 experimente ( $10^{-2}$ ,  $5 \cdot 10^{-3}$ ,  $10^{-3}$  M pentru concentrațiile reactanților) și presupunând un model de cinetică de forma:



care presupune următoarele ecuații matematice între concentrațiile reactanților:

$$\frac{dX}{dt} = k_0 A^{y_0} B^{y_1} - k_1 X^{y_2} - k_2 X^{y_3} \quad \frac{dA}{dt} = -k_0 A^{y_0} B^{y_1} + k_1 X^{y_2} \quad \frac{dB}{dt} = -k_0 A^{y_0} B^{y_1} + k_2 X^{y_3} \quad \frac{dP}{dt} = k_2 X^{y_3}$$

► Variabilele măsurate sunt  $[X]$  (în termeni de extincție  $E = \varepsilon[X]$ , unde  $\varepsilon$  înglobează și constanta de experiment, lungimea camerei de amestecare și detecție) și timpul  $t$ .

► Constantele necunoscute sunt  $\varepsilon$ ,  $y_0$ ,  $y_1$ ,  $y_2$ ,  $y_3$ ,  $k_0$ ,  $k_1$ ,  $k_2$ .

► Scopul optimizării numerice a fost obținerea constantelor necunoscute pornind de la valorile cunoscute ale variabilelor. Expresiile diferențiale ce rezultă din ecuațiile matematice de mai sus sunt:

$$d[A] = -k_0 [A]^{y_0} [B]^{y_1} dt + k_1 X^{y_2} dt; \quad d[B] = -k_0 [A]^{y_0} [B]^{y_1} dt + k_1 [X]^{y_2} dt \\ d[X] = (k_0 [A]^{y_0} [B]^{y_1} - k_1 [X]^{y_2} - k_2 [X]^{y_3}) dt$$

Ecuațiile de iterație numerică sunt:

$$D_{i-1} = k_0 A_{i-1}^{y_0} B_{i-1}^{y_1} dt - k_1 X_{i-1}^{y_2} dt \\ A_i = A_{i-1} - D_i; \quad B_i = B_{i-1} - D_i; \quad X_i = X_{i-1} + D_{i-1} - k_2 X_{i-1}^{y_3}$$

Expresia ce a fost supusă algoritmului de optimizare numerică este:

$$\hat{E} = a[X], \text{ unde } \hat{E} \text{ este estimatorul extincției experimentale}$$

Valorile de start folosite în optimizare au fost:

$$\div [A]_0 = 10^{-3}; 5 \cdot 10^{-3}; 10 \cdot 10^{-3} \text{ (în funcție de experiment);}$$

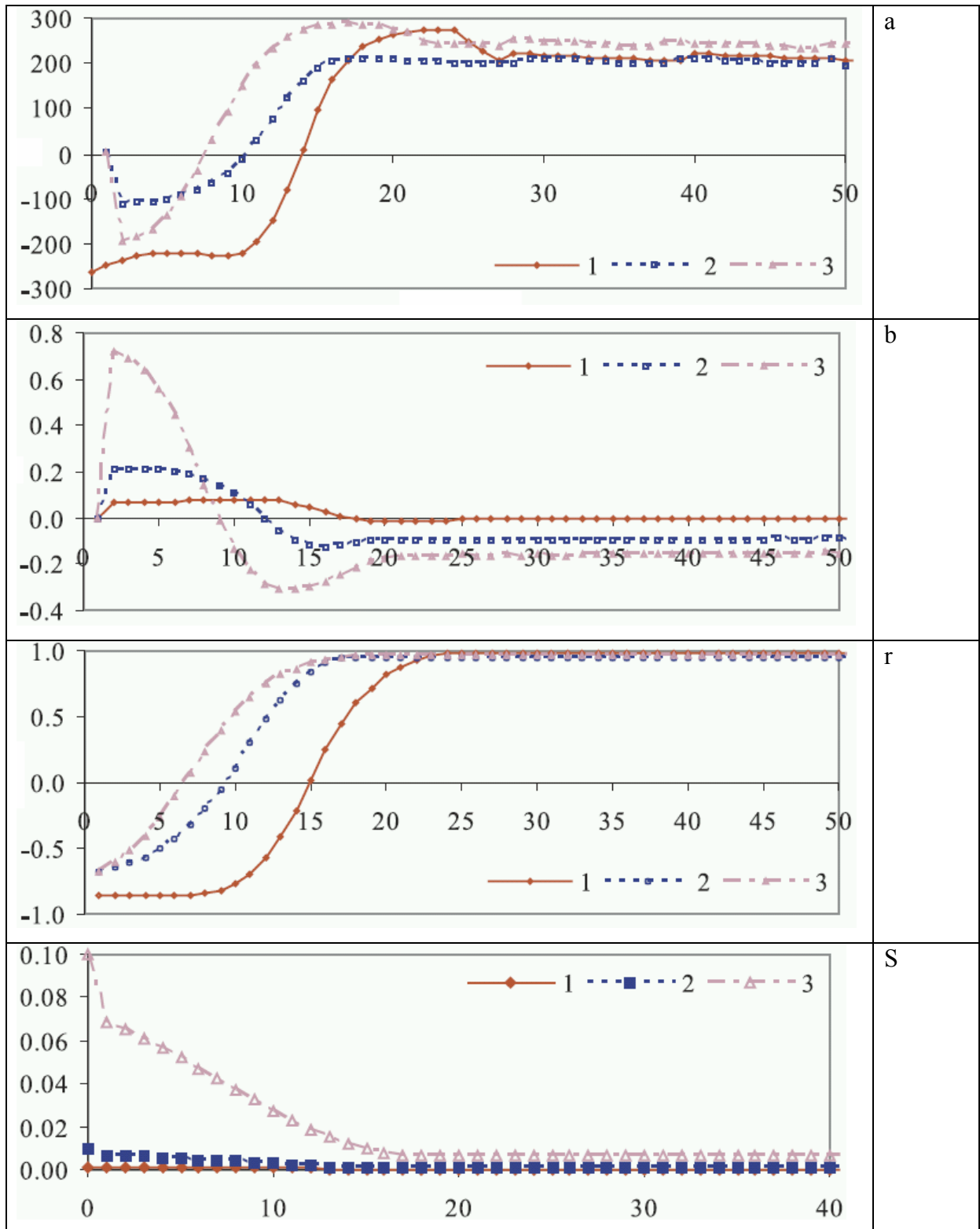
$$\div [B]_0 = 10^{-3}; 5 \cdot 10^{-3}; 10 \cdot 10^{-3} \text{ (în funcție de experiment);}$$

$$\div [X]_0 = 0;$$

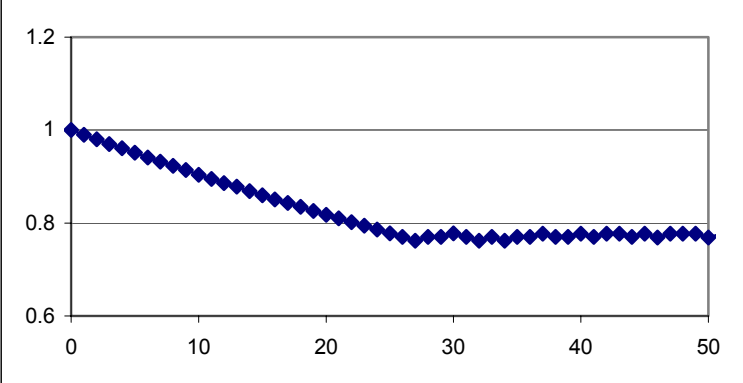
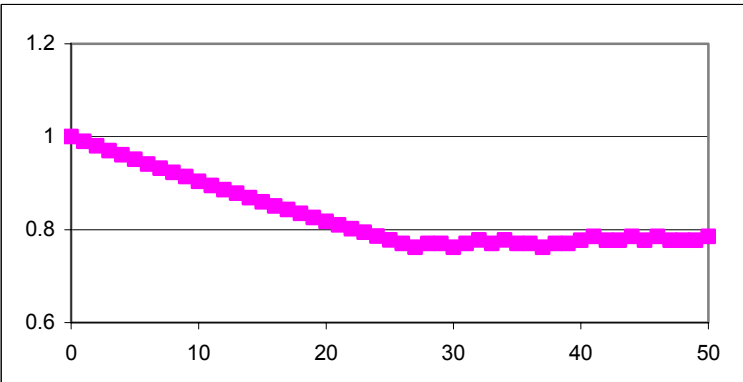
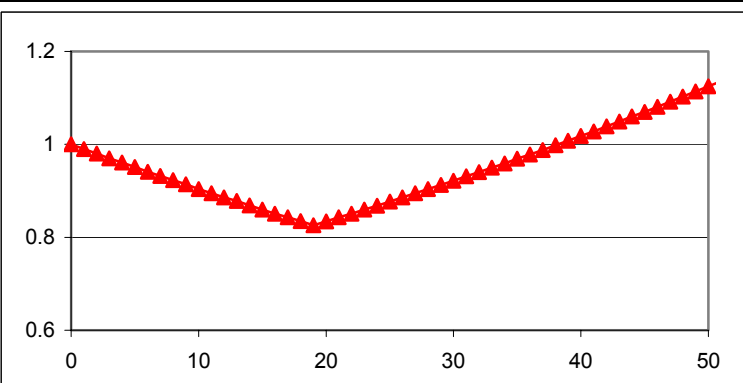
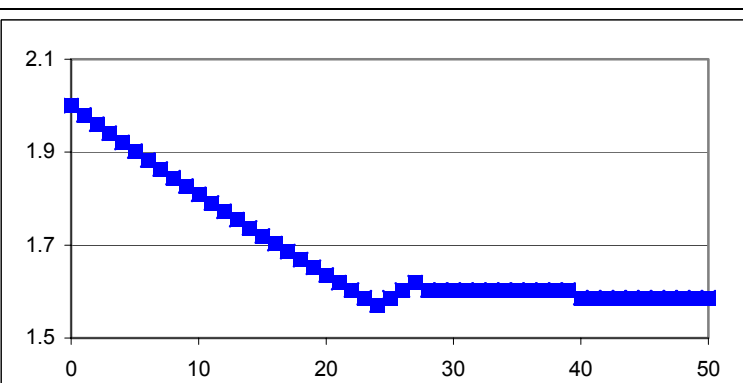
$$\div k_0 = 1; k_1 = 1; k_2 = 1; y_0 = 1; y_1 = 1; y_2 = 1; y_3 = 1;$$

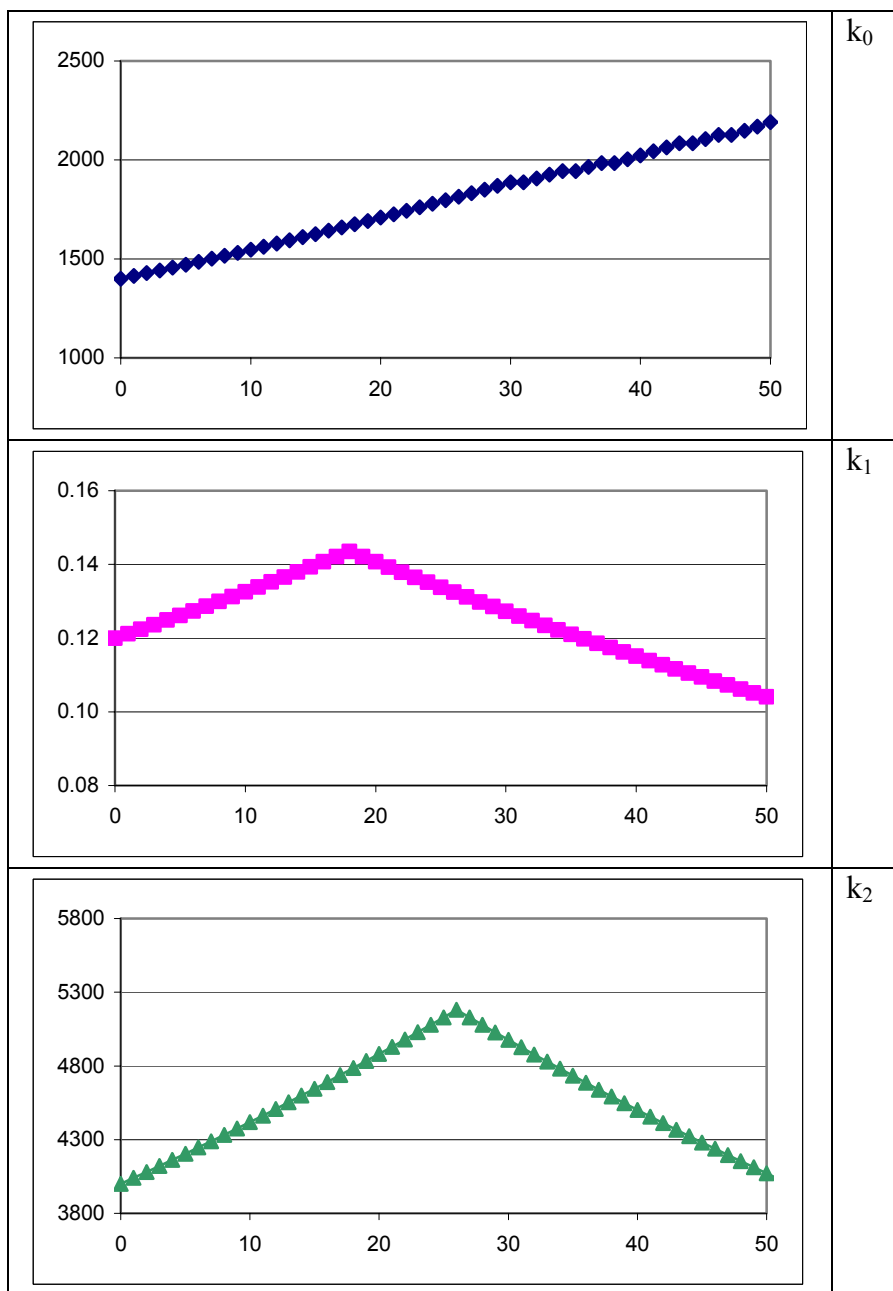
$$\div \varepsilon_0 = 200.$$

► A fost aplicată procedura de optimizare pentru fiecare set de date experimentale (1100 de perechi extincție-timp pentru  $10^{-3}$ , 1300 pentru  $5 \cdot 10^{-3}$ , 6500 pentru  $10 \cdot 10^{-3}$ ) și rezultatele optimizării (în termeni de coeficienți ai ecuației de regresie  $a$  și  $b$ , corelație  $r$  și sumă de reziduuri  $S$ ) sunt redată în figurile următoare în funcție de pasul de iterație:



► Figurile de mai sus arată că convergența se obține pentru toate cele 3 cazuri începând cu iterația 25. Valorile constantelor necunoscute în funcție de iterație sunt redată în graficele următoare (pentru unul dintre experimente):

 <p>A line graph with a blue line and diamond markers. The y-axis ranges from 0.6 to 1.2 with major ticks at 0.6, 0.8, 1.0, and 1.2. The x-axis ranges from 0 to 50 with major ticks at 0, 10, 20, 30, 40, and 50. The data points start at (0, 1.0) and decrease to approximately 0.77 at x=50.</p>	<p><math>y_0</math></p>
 <p>A line graph with a magenta line and square markers. The y-axis ranges from 0.6 to 1.2 with major ticks at 0.6, 0.8, 1.0, and 1.2. The x-axis ranges from 0 to 50 with major ticks at 0, 10, 20, 30, 40, and 50. The data points start at (0, 1.0) and decrease to approximately 0.78 at x=50.</p>	<p><math>y_1</math></p>
 <p>A line graph with a red line and triangle markers. The y-axis ranges from 0.6 to 1.2 with major ticks at 0.6, 0.8, 1.0, and 1.2. The x-axis ranges from 0 to 50 with major ticks at 0, 10, 20, 30, 40, and 50. The data points start at (0, 1.0), reach a minimum of approximately 0.82 at x=20, and rise to approximately 1.12 at x=50.</p>	<p><math>y_2</math></p>
 <p>A line graph with a blue line and square markers. The y-axis ranges from 1.5 to 2.1 with major ticks at 1.5, 1.7, 1.9, and 2.1. The x-axis ranges from 0 to 50 with major ticks at 0, 10, 20, 30, 40, and 50. The data points start at (0, 2.0) and decrease to approximately 1.6 at x=50.</p>	<p><math>y_3</math></p>



► Rezultatele statisticii variaționale pe cele 3 seturi de date sunt redate în tabelul de mai jos:

E	$y_0$	$y_1$	$y_3$	$k_0$	$k_2$	$S$	$C_0$	$a$	$b$	$r$	$IS$
1	0.82	0.81	1.51	3.46	2.30	1.81	1	219	-0.0005	0.980	107
2	0.80	0.79	1.57	1.02	2.04	66.6	5	189	-0.0821	0.955	99
3	0.75	0.75	1.57	0.82	2.10	582	10	227	-0.1300	0.962	99

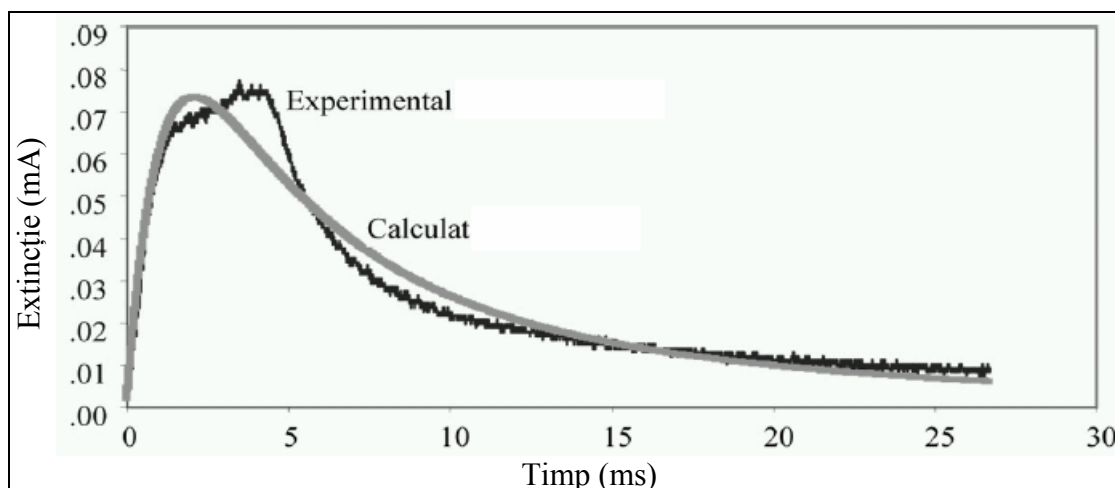
$k_0$  și  $k_2$ : valori  $\cdot 10^{-3}$

► Așa cum arată graficele de mai sus, valorile pentru  $\varepsilon$ ,  $y_0$ ,  $y_1$ ,  $y_3$ ,  $k_0$  și  $k_2$  obținute reprezintă certitudini (toate acestea stabilizându-și valoarea peste iterația 107) în timp ce valorile pentru  $y_2$  și  $k_1$  reprezintă incertitudini (neputând fi obținute prin procedura de optimizare).

Următorul tabel redă valorile pentru certitudini împreună cu intervalele de încredere obținute:

Mărime	Simbol	Valoare
Ordin parțial de reacție reactant	$y_0$	$0.787 \pm 0.08$
Ordin parțial de reacție reactant	$y_1$	$0.787 \pm 0.08$
Ordin parțial de reacție intermediar	$y_3$	$1.53 \pm 0.1$
Constantă de viteză a reacției de echilibru directe	$k_0$	$(1.8 \pm 0.2)(1 + [A]_0[B]_0 \cdot 10^4) \cdot 10^3$
Constantă de viteză a reacției ireversibile	$k_2$	$(2.15 \pm 0.2) \cdot 10^3$
Coeficient de extincție	$\varepsilon$	$211 \pm 22$

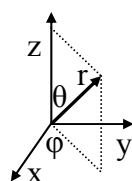
► Următorul grafic redă suprapunerile ce rezultă din aplicarea constantelor necunoscute obținute pentru fiecare experiment peste valorile experimentale obținute din experimentul în care concentrațiile inițiale ale reactanților au fost de  $10^{-2}$  (toate cele 3 curbe teoretice fiind în fapt suprapuse una peste cealaltă și peste valoarea lor medie din tabelul de mai sus):



**Etapa 1, Activitatea 3 și Etapa 2, Activitatea 1. Înglobarea în modelul matematic al ecuațiilor de caracterizare a proprietăților de suprafață ale lichidelor și înglobarea în modelul matematic al ecuațiilor de caracterizare a repartiției și distribuției între faze**

Problema cea mai importantă aferentă acestor activități a fost elaborarea modelului matematic al fenomenului de difuzie, prezent atât în cazul fenomenelor de repartiție și distribuție între faze cât și în cadrul diferitelor proprietăți de suprafață pe care lichidele le manifestă.

Fie un sistem de coordonate carteziene, pe care se exprimă simultan și coordonatele sferice:



Pornind de la ecuația difuziei:

$$\frac{\partial \varphi(x, y, z, t)}{\partial t} = K \cdot \Delta \varphi(x, y, z, t), \quad \Delta = \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$$

pentru a o aplica la sisteme cu simetrie sferică (funcția de proprietate este în coordonate polare  $\varphi = \varphi(r, \varphi, \theta)$  și variază doar în funcție de r) este necesar să facem transformarea la coordonate polare a operatorului de derivare. Fie deci:

$$\varphi = \varphi(r, \varphi, \theta), \text{ cu } \frac{\partial \varphi}{\partial \varphi} = 0 \text{ și } \frac{\partial \varphi}{\partial \theta} = 0$$

unde ecuațiile exprimă faptul că  $\varphi$  variază doar în funcție de r. Ecuațiile de transformare între coordonatele carteziene (x,y,x) și coordonatele polare (r,θ,φ) sunt:

$$\begin{cases} x = r \cdot \cos(\varphi) \cdot \sin(\theta) \\ y = r \cdot \sin(\varphi) \cdot \sin(\theta) \\ z = r \cdot \cos(\theta) \end{cases}, \quad \begin{cases} r = \sqrt{x^2 + y^2 + z^2} \\ \varphi = \arctan(y/x) \\ \theta = \arctan(\sqrt{x^2 + y^2}/z) \end{cases}$$

Exprimăm derivata de ordinul 1 a lui  $\varphi$  în raport cu x și ținem seama de schimbarea de variabile:

$$\frac{\partial \varphi}{\partial x} = \frac{\partial \varphi}{\partial r} \cdot \frac{\partial r}{\partial x} + \frac{\partial \varphi}{\partial \varphi} \cdot \frac{\partial \varphi}{\partial x} + \frac{\partial \varphi}{\partial \theta} \cdot \frac{\partial \theta}{\partial x}$$

Folosim acum relațiile de mai sus, când rezultă:

$$\frac{\partial \varphi}{\partial x} = \frac{\partial \varphi}{\partial r} \cdot \frac{\partial r}{\partial x}, \quad \frac{\partial \varphi}{\partial y} = \frac{\partial \varphi}{\partial r} \cdot \frac{\partial r}{\partial y}, \quad \frac{\partial \varphi}{\partial z} = \frac{\partial \varphi}{\partial r} \cdot \frac{\partial r}{\partial z}$$

unde ecuațiile rezultă în mod analog. Calculăm derivatele de ordinul 1 ale lui r în raport cu x, y și z:

$$\frac{\partial r}{\partial x} = \frac{x}{\sqrt{x^2 + y^2 + z^2}}, \quad \frac{\partial r}{\partial y} = \frac{y}{\sqrt{x^2 + y^2 + z^2}}, \quad \frac{\partial r}{\partial z} = \frac{z}{\sqrt{x^2 + y^2 + z^2}}$$

și le exprimăm în funcție de r, θ și φ:

$$\frac{\partial r}{\partial x} = \cos(\varphi) \cdot \sin(\theta) = \frac{x}{r}, \quad \frac{\partial r}{\partial y} = \sin(\varphi) \cdot \sin(\theta) = \frac{y}{r}, \quad \frac{\partial r}{\partial z} = \cos(\theta) = \frac{z}{r}$$

și le introducem în relația de mai sus, unde, pentru simetrie s-au lăsat rapoartele x/r, y/r și z/r:

$$\frac{\partial \varphi}{\partial x} = \frac{x}{r} \cdot \frac{\partial \varphi}{\partial r}, \quad \frac{\partial \varphi}{\partial y} = \frac{y}{r} \cdot \frac{\partial \varphi}{\partial r}, \quad \frac{\partial \varphi}{\partial z} = \frac{z}{r} \cdot \frac{\partial \varphi}{\partial r}$$

Calculăm și derivatele de ordinul 2 după formulele:

$$\frac{\partial}{\partial x} \frac{\partial \varphi}{\partial x} = \frac{\partial r}{\partial x} \cdot \frac{\partial}{\partial r} \frac{\partial \varphi}{\partial x} + \frac{\partial \varphi}{\partial x} \cdot \frac{\partial}{\partial \varphi} \frac{\partial \varphi}{\partial x} + \frac{\partial \theta}{\partial x} \cdot \frac{\partial}{\partial \theta} \frac{\partial \varphi}{\partial x}$$

Ținem seama de relația de mai sus și de independența de r a rapoartelor x/r, y/r și z/r:

$$\frac{\partial}{\partial x} \frac{\partial \varphi}{\partial x} = \frac{\partial r}{\partial x} \cdot \frac{x}{r} \cdot \frac{\partial}{\partial r} \frac{\partial \varphi}{\partial r} + \frac{\partial \varphi}{\partial x} \cdot \frac{\partial}{\partial \varphi} \frac{x}{r} \cdot \frac{\partial \varphi}{\partial r} + \frac{\partial \theta}{\partial x} \cdot \frac{\partial}{\partial \theta} \frac{x}{r} \cdot \frac{\partial \varphi}{\partial r}$$

Înlocuind:

$$\frac{\partial}{\partial x} \frac{\partial \varphi}{\partial x} = \left(\frac{x}{r}\right)^2 \cdot \frac{\partial^2 \varphi}{\partial r^2} + \left(\frac{\partial \varphi}{\partial x} \cdot \frac{\partial}{\partial \varphi} \frac{x}{r} + \frac{\partial \theta}{\partial x} \cdot \frac{\partial}{\partial \theta} \frac{x}{r}\right) \cdot \frac{\partial \varphi}{\partial r}$$

Însumând acum cele 3 ecuații de tipul de mai sus obținem:

$$\Delta \varphi = \frac{\partial^2 \varphi}{\partial r^2} + \left(\frac{\partial \varphi}{\partial x} \cdot \frac{\partial}{\partial \varphi} \frac{x}{r} + \frac{\partial \theta}{\partial x} \cdot \frac{\partial}{\partial \theta} \frac{x}{r} + \frac{\partial \varphi}{\partial y} \cdot \frac{\partial}{\partial \varphi} \frac{y}{r} + \frac{\partial \theta}{\partial y} \cdot \frac{\partial}{\partial \theta} \frac{y}{r} + \frac{\partial \varphi}{\partial z} \cdot \frac{\partial}{\partial \varphi} \frac{z}{r} + \frac{\partial \theta}{\partial z} \cdot \frac{\partial}{\partial \theta} \frac{z}{r}\right) \cdot \frac{\partial \varphi}{\partial r}$$

și dacă se ține seama că φ nu depinde de z:

$$\Delta \varphi = \frac{\partial^2 \varphi}{\partial r^2} + \left(\frac{\partial \varphi}{\partial x} \cdot \frac{\partial}{\partial \varphi} \frac{x}{r} + \frac{\partial \theta}{\partial x} \cdot \frac{\partial}{\partial \theta} \frac{x}{r} + \frac{\partial \varphi}{\partial y} \cdot \frac{\partial}{\partial \varphi} \frac{y}{r} + \frac{\partial \theta}{\partial y} \cdot \frac{\partial}{\partial \theta} \frac{y}{r} + \frac{\partial \theta}{\partial z} \cdot \frac{\partial}{\partial \theta} \frac{z}{r}\right) \cdot \frac{\partial \varphi}{\partial r}$$

Să calculăm termenii ce apar în relația de mai sus. Derivatele de ordinul 1 ale lui φ sunt:

$$\frac{\partial \varphi}{\partial x} = \frac{-y}{x^2 + y^2} = \frac{1}{r} \cdot \frac{-\sin(\varphi)}{\sin(\theta)}, \quad \frac{\partial \varphi}{\partial y} = \frac{x}{x^2 + y^2} = \frac{1}{r} \cdot \frac{\cos(\varphi)}{\sin(\theta)}, \quad \frac{\partial \varphi}{\partial z} = 0$$

iar ale lui θ:

$$\frac{\partial \theta}{\partial z} = \frac{-\sqrt{x^2 + y^2}}{x^2 + y^2 + z^2} = -\frac{\sin(\theta)}{r}, \quad \frac{\partial \theta}{\partial x} = \frac{x}{\sqrt{x^2 + y^2}} \cdot \frac{z}{x^2 + y^2 + z^2} = \frac{\cos(\varphi) \cdot \cos(\theta)}{r},$$

$$\frac{\partial \theta}{\partial y} = \frac{y}{\sqrt{x^2 + y^2}} \cdot \frac{z}{x^2 + y^2 + z^2} = \frac{\sin(\varphi) \cdot \cos(\theta)}{r}$$

Cealalți termeni sunt:

$$\frac{\partial x}{\partial \varphi} = -\sin(\varphi) \cdot \sin(\theta), \quad \frac{\partial y}{\partial \varphi} = \cos(\varphi) \cdot \sin(\theta), \quad \frac{\partial x}{\partial \theta} = \cos(\varphi) \cdot \cos(\theta), \quad \frac{\partial y}{\partial \theta} = \sin(\varphi) \cdot \cos(\theta),$$

$$\frac{\partial z}{\partial \theta} = -\sin(\theta)$$

Putem acum înlocui în expresia ce apare în fața derivatei de ordinul 1 a proprietății:

$$\left( \frac{\partial \varphi}{\partial x} \cdot \frac{\partial x}{\partial \varphi} + \frac{\partial \theta}{\partial x} \cdot \frac{\partial x}{\partial \theta} + \frac{\partial \varphi}{\partial y} \cdot \frac{\partial y}{\partial \varphi} + \frac{\partial \theta}{\partial y} \cdot \frac{\partial y}{\partial \theta} + \frac{\partial \theta}{\partial z} \cdot \frac{\partial z}{\partial \theta} \right) = \frac{1}{r} \cdot \frac{\sin(\varphi)}{\sin(\theta)} \cdot \sin(\varphi) \cdot \sin(\theta) +$$

$$\frac{\cos(\varphi) \cdot \cos(\theta)}{r} \cdot \cos(\varphi) \cdot \cos(\theta) + \frac{1}{r} \cdot \frac{\cos(\varphi)}{\sin(\theta)} \cdot \cos(\varphi) \cdot \sin(\theta) + \frac{\sin(\varphi) \cdot \cos(\theta)}{r} \cdot \sin(\varphi) \cdot \cos(\theta) +$$

$$\frac{\sin(\theta)}{r} \cdot \sin(\theta) = \frac{1}{r} \cdot (\sin^2(\varphi) + \cos^2(\varphi) \cdot \cos^2(\theta) + \cos^2(\varphi) + \sin^2(\varphi) \cdot \cos^2(\theta) + \sin^2(\theta)) = \frac{2}{r}$$

Înlocuind rezultă expresia finală a Laplacianului în coordonate polare pentru sistemele ce difuzează în simetrie sferică:

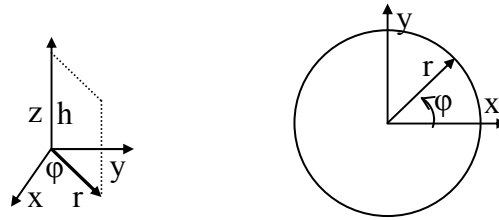
$$\Delta \varphi = \frac{\partial^2 \varphi}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial \varphi}{\partial r}$$

și deci ecuația difuziei (1) devine:

$$\frac{\partial \varphi(r, t)}{\partial t} = K \cdot \left( \frac{\partial^2 \varphi(r, t)}{\partial r^2} + \frac{2}{r} \cdot \frac{\partial \varphi(r, t)}{\partial r} \right)$$

Ecuția de mai sus este deosebit de utilă în cazul proceselor catalizate, în care catalizatorul introdus în sistem difuzează în toate direcțiile în mod uniform, introducând o simetrie sferică.

Ecuția de mai sus este mai practică decât cea în coordonate carteziane, și numai pentru simplul fapt că simetria (și cea sferică) este o tendință a sistemelor vii către ordine (micșoarea entropiei) în raport cu evoluția naturală a sistemelor (mărirea entropiei). O altă formulă importantă este pentru simetria cilindrică, care este detaliată mai jos:



Pentru sisteme cu simetrie cilindrică (fie  $x$  și  $y$  în planul bazei cilindrului, ca în figurile de mai sus), derivata după  $z$  este nulă, și ecuațiile (A.1) și (A.2) devin:

$$\frac{\partial \varphi(x, y, t)}{\partial t} = K \cdot \Delta \varphi(x, y, t), \quad \Delta = \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right)$$

Dacă exprimăm funcția de proprietate  $\varphi$  în coordonate cilindrice, variabilelor  $x$  și  $y$  le iau locul variabilele  $r$  și  $\varphi$ . Pentru funcția de proprietate  $\varphi(r, \varphi)$  este necesar să facem transformarea la coordonate polare a operatorului de derivare. Fie deci:

$$\varphi = \varphi(r, \varphi) \text{ și } \frac{\partial \varphi}{\partial \varphi} = 0$$

unde ecuația exprimă faptul că  $\varphi$  variază doar în funcție de  $r$  și  $h$  fiind ortogonal pe  $\varphi$  și  $r$ . Ecuațiile de transformare între coordonatele carteziene  $(x, y)$  și coordonatele polare  $(r, \varphi)$  sunt:

$$\begin{cases} x = r \cdot \cos(\varphi) \\ y = r \cdot \sin(\varphi) \end{cases}, \quad \begin{cases} r = \sqrt{x^2 + y^2} \\ \varphi = \arctan(y/x) \end{cases}$$

Exprimăm derivata de ordinul 1 a lui  $\varphi$  în raport cu  $x$  și ținem seama de schimbarea de variabile:

$$\frac{\partial \varphi}{\partial x} = \frac{\partial \varphi}{\partial r} \cdot \frac{\partial r}{\partial x} + \frac{\partial \varphi}{\partial \varphi} \cdot \frac{\partial \varphi}{\partial x}, \quad \frac{\partial \varphi}{\partial x} = \frac{\partial \varphi}{\partial r} \cdot \frac{\partial r}{\partial x}, \quad \frac{\partial \varphi}{\partial y} = \frac{\partial \varphi}{\partial r} \cdot \frac{\partial r}{\partial y}$$

unde ecuația în raport cu  $y$  rezultă în mod analog. Calculăm derivatele de ordinul 1 ale lui  $r$  în raport cu  $x$ ,  $y$  și  $z$ :

$$\frac{\partial r}{\partial x} = \frac{x}{\sqrt{x^2 + y^2}}, \quad \frac{\partial r}{\partial y} = \frac{y}{\sqrt{x^2 + y^2}}$$

și le exprimăm în funcție de  $r$  și  $\varphi$  folosind relațiile de mai sus:

$$\frac{\partial r}{\partial x} = \cos(\varphi) = \frac{x}{r}, \quad \frac{\partial r}{\partial y} = \sin(\varphi) = \frac{y}{r}$$

și le introducem în relația de mai sus, unde, pentru simetrie s-au lăsat rapoartele  $x/r$  și  $y/r$ :

$$\frac{\partial \varphi}{\partial x} = \frac{x}{r} \cdot \frac{\partial \varphi}{\partial r}, \quad \frac{\partial \varphi}{\partial y} = \frac{y}{r} \cdot \frac{\partial \varphi}{\partial r}$$

Calculăm și derivatele de ordinul 2 după formulele:

$$\frac{\partial}{\partial x} \frac{\partial \varphi}{\partial x} = \frac{\partial r}{\partial x} \cdot \frac{\partial}{\partial r} \frac{\partial \varphi}{\partial x} + \frac{\partial \varphi}{\partial x} \cdot \frac{\partial}{\partial \varphi} \frac{\partial \varphi}{\partial x}, \quad \frac{\partial}{\partial y} \frac{\partial \varphi}{\partial y} = \frac{\partial r}{\partial y} \cdot \frac{\partial}{\partial r} \frac{\partial \varphi}{\partial y} + \frac{\partial \varphi}{\partial y} \cdot \frac{\partial}{\partial \varphi} \frac{\partial \varphi}{\partial y}$$

Ținem seama și de independența de r a rapoartelor x/r și y/r:

$$\frac{\partial}{\partial x} \frac{\partial \varphi}{\partial x} = \frac{\partial r}{\partial x} \cdot \frac{x}{r} \cdot \frac{\partial}{\partial r} \frac{\partial \varphi}{\partial r} + \frac{\partial \varphi}{\partial x} \cdot \frac{\partial}{\partial \varphi} \frac{x}{r} \cdot \frac{\partial \varphi}{\partial r}, \quad \frac{\partial}{\partial y} \frac{\partial \varphi}{\partial y} = \frac{\partial r}{\partial y} \cdot \frac{y}{r} \cdot \frac{\partial}{\partial r} \frac{\partial \varphi}{\partial r} + \frac{\partial \varphi}{\partial y} \cdot \frac{\partial}{\partial \varphi} \frac{y}{r} \cdot \frac{\partial \varphi}{\partial r}$$

Rezultă:

$$\frac{\partial}{\partial x} \frac{\partial \varphi}{\partial x} = \left(\frac{x}{r}\right)^2 \cdot \frac{\partial^2 \varphi}{\partial r^2} + \frac{\partial \varphi}{\partial x} \cdot \frac{\partial}{\partial \varphi} \frac{x}{r} \cdot \frac{\partial \varphi}{\partial r}, \quad \frac{\partial}{\partial y} \frac{\partial \varphi}{\partial y} = \left(\frac{y}{r}\right)^2 \cdot \frac{\partial^2 \varphi}{\partial r^2} + \frac{\partial \varphi}{\partial y} \cdot \frac{\partial}{\partial \varphi} \frac{y}{r} \cdot \frac{\partial \varphi}{\partial r}$$

Însumând acum cele 2 ecuații de tipul de mai sus obținem:

$$\Delta \varphi = \frac{\partial^2 \varphi}{\partial r^2} + \left( \frac{\partial \varphi}{\partial x} \cdot \frac{\partial}{\partial \varphi} \frac{x}{r} + \frac{\partial \varphi}{\partial y} \cdot \frac{\partial}{\partial \varphi} \frac{y}{r} \right) \cdot \frac{\partial \varphi}{\partial r}$$

Recalcularea termenilor ce apar în relația de mai sus esterdată mai jos:

$$\frac{\partial \varphi}{\partial x} = \frac{-y}{x^2 + y^2} = -\frac{1}{r} \cdot \sin(\varphi), \quad \frac{\partial \varphi}{\partial y} = \frac{x}{x^2 + y^2} = \frac{1}{r} \cdot \cos(\varphi), \quad \frac{\partial}{\partial \varphi} \frac{x}{r} = -\sin(\varphi), \quad \frac{\partial}{\partial \varphi} \frac{y}{r} = \cos(\varphi)$$

Putem acum înlocui în expresia ce apare în fața derivatei de ordinul 1 a proprietății:

$$\left( \frac{\partial \varphi}{\partial x} \cdot \frac{\partial}{\partial \varphi} \frac{x}{r} + \frac{\partial \varphi}{\partial y} \cdot \frac{\partial}{\partial \varphi} \frac{y}{r} \right) = \frac{1}{r} \cdot \sin(\varphi) \cdot \sin(\varphi) + \frac{1}{r} \cdot \cos(\varphi) \cdot \cos(\varphi) = \frac{1}{r}$$

Înlocuind rezultă expresia finală a Laplacianului în coordonate polare pentru sistemele ce difuzează în simetrie cilindrică:

$$\Delta \varphi = \frac{\partial^2 \varphi}{\partial r^2} + \frac{1}{r} \cdot \frac{\partial \varphi}{\partial r}$$

și deci ecuația difuziei devine:

$$\frac{\partial \varphi(r, t)}{\partial t} = K \cdot \left( \frac{\partial^2 \varphi(r, t)}{\partial r^2} + \frac{1}{r} \cdot \frac{\partial \varphi(r, t)}{\partial r} \right)$$

Ecuția de mai sus se aplică cu succes îndeosebi în electrochimie, atunci când electrozii folosiți induc o simetrie cilindrică difuziei.

O problemă deosebit de importantă este bilanțul de material în reacțiile controlate difuziv. Această analiză este redată în continuare. Ecuția generală a difuziei stabilită pe baza fenomenelor de difuzie și convecție într-o regiune din spațiu ((x,y,z),(x+dx,y+dy,z+dz)) a fost

exprimată fără a se ține seama de o posibilă reacție care ar putea diminua sau mări proprietatea  $\phi$  în regiunea considerată. Această posibilă reacție în general este independentă de coordonatele spațiale și, după cum s-a văzut în exprimarea legilor de viteză pentru variația concentrației molare, variația sa se exprimă printr-o formulă generală de tipul:

$$\frac{\partial \phi(x, y, z, t)}{\partial t} = \pm \kappa \cdot \phi^{\gamma_\phi}, \gamma_\phi \text{ ordinul de reacție}$$

și completând cu termenul de mai sus se obține:

$$\frac{\partial \phi(x, y, z, t)}{\partial t} = K \cdot \Delta \phi(x, y, z, t) - \vec{\nabla} \cdot (\vec{i} + \vec{j} + \vec{k}) \phi(x, y, z, t) v(x, y, z, t) \pm \kappa \cdot \phi^{\gamma_\phi}$$

Ecuția de mai sus se numește *ecuația de bilanț de material pentru proprietatea  $\phi$*  și se aplică în numeroase procese chimice. Două exemple în acest sens sunt difuzia oxigenului în sânge și difuzia unui gaz către suprafața unui catalizator.

Soluțiile ecuației de mai sus nu sunt ușor de obținut; aceasta este o ecuație diferențială neomogenă. Rezolvarea ei analitică este posibilă numai în câteva cazuri speciale. În proiectarea reactoarelor chimice și cinetica biologică care folosesc această ecuație se utilizează metode numerice pentru rezolvarea sa pentru modelele reale de reacție.

Să exprimăm ecuația în cazul unidimensional fără convecție și un consum de proprietate de ordinul 1 ( $\gamma_\phi = 1$ ):

$$\frac{\partial \phi(x, t)}{\partial t} = K \cdot \frac{\partial^2 \phi(x, t)}{\partial x^2} \pm \kappa \cdot \phi(x, t)$$

Se poate verifica prin înlocuire că dacă  $Q(x, t)$  este soluție a ecuației fără reacție,

$$\frac{\partial Q(x, t)}{\partial t} = K \cdot \frac{\partial^2 Q(x, t)}{\partial x^2}$$

atunci  $\phi(x, t)$  dat de:

$$\phi(x, t) = Q(x, t) \cdot e^{\mp \kappa \cdot t}$$

este soluție a ecuației cu reacție. Cât despre ecuația inițială și soluția acesteia, ea este rezolvată complet în cadrul teoriei distribuțiilor, și soluția generală în  $\mathcal{R}^n$ , ( $x = (x_1, \dots, x_n)$ ) este:

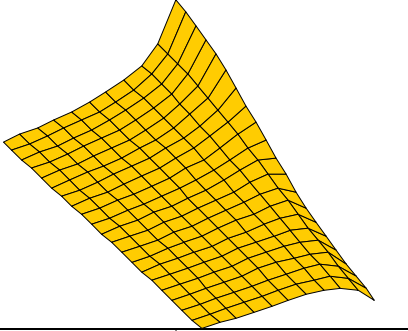
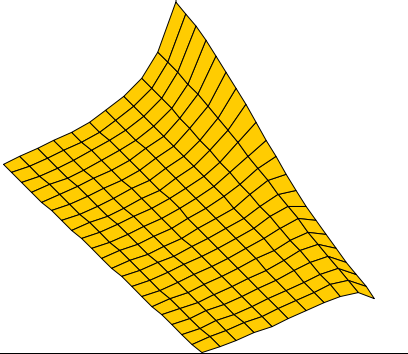
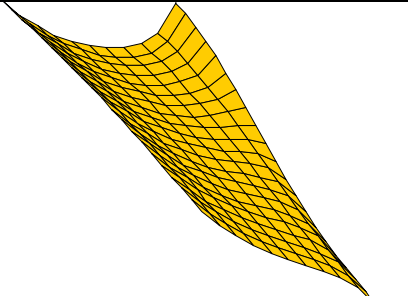
$$Q(x_1, \dots, x_n, t) = \frac{1}{(\sqrt{4K\pi t})^n} \cdot e^{-\frac{(x_1^2 + \dots + x_n^2)}{4Kt}}$$

Fie soluția din  $\mathcal{R}^1$  a ecuației; înlocuind-o pe aceasta în (12.63) obținem:

$$\phi(x, t) = \frac{1}{\sqrt{4K\pi t}} \cdot e^{-\frac{x^2}{4Kt}} \cdot e^{\mp \kappa \cdot t}$$

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

În figurile de mai jos s-au reprezentat variațiile concentrațiilor proprietății în spațiu (x) și timp (t) pentru difuzie și difuzie concurentă cu reacție chimică.

	Reprezentarea spațio-temporală (x,t) a fenomenului de difuzie (axa Z reprezintă concentrația proprietății) pentru $K = 2$ și $\kappa = 3$
	Reprezentarea spațio-temporală (x,t) a fenomenului de difuzie (axa Z reprezintă concentrația proprietății) concurent cu fenomenul de reacție chimică cu consum de proprietate difuzată ( $\kappa > 0$ ) pentru $K = 2$ și $\kappa = 3$
	Reprezentarea spațio-temporală (x,t) a fenomenului de difuzie (axa Z reprezintă concentrația proprietății) concurent cu fenomenul de reacție chimică cu formare de proprietate ( $\kappa < 0$ ) pentru $K = 2$ și $\kappa = -3$

**Etapa 2, Activitatea 3. Construirea funcțiilor obiectiv și a formulelor de iterație**

Pentru cinetica reacțiilor chimice scopul optimizării a fost minimizarea erorii de estimare între model și experiment folosind regresia liniară. Mai multe formule au fost elaborate și folosite, în funcție de natura erorii de estimare (și/sau legea de distribuție a acesteia). Următoarele tabele redau modelele de construcție a funcției de penalitate realizate:

	<p>Cazul clasic, cu cele două moduri de exprimare a erorii (vertical - Y variabila supusă erorii experimentale, orizontal - X variabila supusă erorii experimentale, și perpendicular (ambele X și Y supuse erorii).</p>
	<p>Valorile funcțiilor de penalitate exprimate ca funcții limită.</p>
	<p>Întreg domeniul de posibilități cuprins între ofsetul orizontal și cel vertical în funcție de gradul de afectare cu erori pe fiecare variabilă în parte și punctia PM - funcția putere</p>

Funcția putere (sau Hölder) este capabilă să măture întreaga arie determinată de cele două ofseturi:

$$\forall S \exists p \in \widehat{\mathbb{R}}^* \text{ a.i. } |a_S| = \text{PM} \left( \left| a_{(Y-aX-c)^2} \right|, \left| a_{(X-(Y-c)/a)^2} \right|, p \right)$$

ceea ce aduce ca și consecință că:

$$\left| a_{(Y-ax-c)^2} \right| \leq |a_s| \leq \left| a_{(X-(Y-c)/a)^2} \right|$$

Formule specifice sunt redată în tabelul de mai jos:

Funcția penalitate (S)	Formule de calcul
$\sum (\hat{y}_i - y_i)^2$	$Y=aX+b$ $a = \frac{M(XY) - M(X)M(Y)}{M(X^2) - M^2(X)}$ $b = \frac{M(X^2)M(Y) - M(X)M(XY)}{M(X^2) - M^2(X)}$
$\sum (\hat{x}_i - x_i)^2$	$X=aY+b$ $a = \left( \frac{M(XY) - M(X)M(Y)}{M(Y^2) - M^2(Y)} \right)^{-1}$ $b = -\frac{M(Y^2)M(X) - M(Y)M(XY)}{M(XY) - M(X)M(Y)}$
$\Sigma \frac{(\hat{y}_i - y_i)^2 (\hat{x}_i - x_i)^2}{(\hat{y}_i - y_i)^2 + (\hat{x}_i - x_i)^2}$	$Y=aX+b$ $a = -\frac{(M(X^2) - M^2(X)) - (M(Y^2) - M^2(Y))}{2(M(XY) - M(X)M(Y))}$ $\pm \sqrt{\frac{(M(X^2) - M^2(X)) - (M(Y^2) - M^2(Y))}{2(M(XY) - M(X)M(Y))} + 1}$ $b = M(Y) - aM(X)$
$\frac{m^2 + 1}{(a - m)^2} \Sigma (ax_i - y_i + b)^2$	$Y=aX+b$ $a = \frac{m^2 (M(X^2) + M^2(X)) - 2m(M(XY) - M(X)M(Y)) + (M(Y^2) - M^2(Y)) \pm \sqrt{\Delta}}{2(m(3M^2(X) - M(X^2)) + (M(XY) - M(X)M(Y)))}$ $\Delta = 2m^2 (4(M(XY) - M(X)M(Y))^2 - (M(Y^2) - M^2(Y))(3M(X^2) - 5M^2(X))) - 8m(M(XY) - M(X)M(Y))(m^2 (M(X^2) - M^2(X)) + (M(Y^2) - M^2(Y))) + m^4 (M(X^2) + M^2(X))^2 + (M(Y^2) - M^2(Y))^2$ $b = M(Y) - aM(X)$
$(Y-aX)^2, M(X)=0$	$Y=aX$

	$a = \frac{M(XY)}{M(X^2)}$
$(Y-aX)^2, M(X) \neq 0$	$Y=aX$ $a = \frac{M(Y)}{M(X)}$
$(Y-(aX+b))^2$	$Y=aX+b$ $a = \frac{M(XY) - M(X)M(Y)}{M(X^2) - M^2(X)}$ $b = \frac{M(X^2)M(Y) - M(X)M(XY)}{M(X^2) - M^2(X)}$
$(X-Ya)^2, M(Y)=0$	$X=aY$ $a = \frac{M(Y^2)}{M(XY)}$
$(X-Ya)^2, M(Y) \neq 0$	$X=aY$ $a = \frac{M(X)}{M(Y)}$
$(X-(Y-b)/a)^2$	$Y=aX+b$ $a = \frac{M(Y^2) - M^2(Y)}{M(XY) - M(X)M(Y)}$ $b = \frac{M(Y)M(XY) - M(X)M(Y^2)}{M(XY) - M(X)M(Y)}$
$GM \begin{pmatrix} a_{(Y-ax-b)^2} \\ a_{(X-(Y-b)/a)^2} \end{pmatrix}$	$Y=aX+b$ $a = \pm \sqrt{\frac{M(Y^2) - M^2(Y)}{M(X^2) - M^2(X)}}$ $b = M(Y) \mp M(X) \sqrt{\frac{M(Y^2) - M^2(Y)}{M(X^2) - M^2(X)}}$

Al doilea caz este cel al obținerii funcțiilor obiectiv pentru amestecurile de solvenți (fiecare venind cu contribuția sa în procesele de difuzie și/sau reacție care au loc în faza mobilă). Optimizarea fazei mobile la separarea cromatografică cu amestecuri de trei solvenți este posibilă atunci când numărul determinărilor experimentale ale parametrilor de separare pentru fiecare compus separat în parte se efectuează pentru un număr de compoziții distincte ale fazei mobile cel puțin egal cu numărul de variabile ale modelului matematic.

Se presupune într-un amestec de trei solvenți mărimea cantitativă a parametrului cromatografic ales depinde de compoziția fazei mobile printr-o ecuație de dependență de una din cele 2 forme:

$$M6(x_1, x_2, x_3) = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 \quad (1)$$

$$M7(x_1, x_2, x_3) = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3 \quad (2)$$

unde  $x_1, x_2, x_3$  sunt fracțiile molare ale celor 3 solvenți ( $x_1 + x_2 + x_3 = 1$ ), M6 și M7 sunt estimatori și apoi predictorii ai parametrului cromatografic ales iar  $a_1, a_2, a_3, a_4, a_5, a_6$  și  $a_7$  sunt coeficienți care sunt întâi determinați pe baza celei mai bune estimări a parametrului cromatografic ales iar apoi sunt folosiți pentru a prezice valorile acestui parametru pentru orice compoziție a fazei mobile.

Parametrii cromatografici care au fost modelați utilizând ecuațiile (1) și (2) sunt:

- $RF(i, e) = l(i)/l(e) \quad (3)$

unde  $i$  este unul din compușii de separat,  $e$  este eluentul folosit ca fază mobilă,  $l(i)$  este coordonata la care a migrat în eluentul  $e$ ,  $l(e)$  este coordonata la care a migrat eluentul, iar RF este șirul factorilor de retenție ai compușilor de separat pentru eluentul  $e$ ;

- $RS(i, j, e) = 2 * (l(i) - l(j)) / (w(i) + w(j)) \quad (4)$

unde  $i, j$  sunt doi compuși de separat,  $w(i)$  și  $w(j)$  sunt lățimile petelor compușilor, iar RS este matricea rezoluțiilor calculate pentru separarea compusului  $i$  de compusul  $j$ ;

- $RSO(i, e) = 2 * (l_o(i) - l_o(i+1)) / (w(i) + w(i+1)) \quad (5)$

unde  $l_o(i)$  este a  $i$ -a coordonată de migrare în lista ordonată a lungimilor de migrare iar RSO este matricea rezoluțiilor ordonate pentru separarea compușilor consecutivi;

- $Sm(e) = \sqrt{(\sum_j (\Delta RFT - \Delta RF(j, e))) / (n+1)} \quad (6)$

unde  $n$  este numărul de compuși de separat,  $\Delta RFT$  este factorul de retenție ideal în separare ( $1/n$ ),  $\Delta RF(j, e)$  este diferența a  $i$ -a între 2 factori de retenție consecutivi în lista ordonată a factorilor de retenție, iar  $Sm$  este separarea medie înregistrată pentru eluentul  $e$ ;

- $RSA(e) = \sum_j RSO(j, e) / n \quad (7)$

unde RSA este rezoluția medie a separării folosind eluentul  $e$ ;

- $RRP(e) = \prod_j RSO(j, e) / RSA(e) \quad (8)$

unde RRP este produsul ponderat cu media rezoluțiilor în separarea folosind eluentul e;

$$\bullet \text{ Inf}(e,m) = \sum_k (n_k/n) \log_2(n_k/n) \quad (9)$$

unde  $n_k$  este numărul de compuși care migrează în al k-lea interval echidistant din cele m în care a fost împărțită întreaga lungime de migrare  $l(e)$  iar Inf este un factor de calitate al separării calculat după metoda Logit și care se anulează pentru o separare ideală;

$$\bullet \text{ FOB}(e,m) = \sum_j a_j F_j(\text{Sm}(e), \text{Inf}(e,m), \text{RSA}(e), \text{RRP}(e)) \quad (10)$$

unde  $1 \leq j \leq 4$ ,  $F_j$  sunt funcții care exprimă fiecare câte o expresie de cei 4 parametrii,  $a_j$  sunt coeficienți aleși arbitrar sau printr-o relație de ponderare definită matematic, iar FOB este o funcție obiectiv ce caracterizează separarea cu eluentul e în raport cu alegerea coeficienților  $a_j$ , a funcțiilor  $F_j$  și respectiv a numărului de intervale m.

Prin aplicarea uneia dintre ecuațiile (3-10) pentru un șir de p experimente, rezultă o matrice MOB cu una (ecuațiile 6-10) sau mai multe linii (ecuațiile 3-5) și totdeauna p coloane, câte una pentru fiecare experiment, ale cărei elemente reprezintă valorile parametrului cromatografic care se modelează folosind una din ecuațiile (1) sau (2). Pentru ca algoritmul de optimizare să aibă o soluție unic determinată este necesar ca  $p \geq 6$  pentru ecuația (1) și respectiv  $p \geq 7$  pentru ecuația (2).

Pentru fiecare linie a matricei MOB se construiește un sistem de p ecuații liniare cu 6 sau 7 termeni (ecuația 1 și respectiv ecuația 2) în coeficienții  $a_i$  în forma:

$$\text{MOB}(j) = a_1 x_1 + a_2 x_2 + a_3 x_3 + a_4 x_1 x_2 + \dots \quad (11)$$

unde  $x_i$  sunt fracțiile molare ale fiecărui solvent ( $i = 1, 2, 3$ ) ce intră în compoziția eluentului  $e_j$  ( $j = 1, 2, \dots, p$ ).

La sistemul de ecuații liniare de forma (11) se aplică metoda celor mai mici pătrate pentru construirea sistemului de ecuații cu soluție unic determinată MMCP, care se obține după formula:

$$\text{MMCP}(k,0) = \text{M2}(\text{MOB}, A(k)), \text{MMCP}(k,1) = \text{M2}(A(k), A(l)) \quad (12)$$

unde  $k, l = 1, 2, \dots, 6$  (ecuația (1) sau 7 pentru ecuația (2)),  $A(k)$  este șirul termenilor cunoscuți din ecuația (11),  $\text{M2}$  calculează media pentru produsul șirurilor MOB și  $A(k)$ , iar MMCP este matricea extinsă a sistemului de ecuații liniare ce servește la determinarea coeficienților  $a_k$ .

Se aplică metoda Gauss pentru determinarea soluției sistemului (12).

Fie  $A0 = (a_{01}, a_{02}, \dots, a_{06})$  soluția acestui sistem (sau  $A0 = (a_{01}, a_{02}, \dots, a_{07})$ ) pentru cazul ecuației (2). (13)

Odată determinați coeficienții  $A0$  se folosesc valorile acestora pentru a efectua predicția parametrului cromatografic folosind din nou una din ecuațiile (1) și (2) și anume cea pentru care s-au determinat coeficienții.

Fie  $Y$  parametrul cromatografic ales. Dacă matricea  $MOB$  (predictorul lui  $Y$ ) are mai mult de o linie, și atunci și estimatorul lui  $Y$  are mai mult de o linie. Dacă  $z$  este numărul de linii al matricei  $MOB$  (și implicit numărul de predictor) atunci putem exprima estimatorul parametrului cromatografic ales  $\hat{Y}$  sub forma unui șir:

$$\hat{Y} = (\hat{y}_1, \dots, \hat{y}_z) \quad (14)$$

Optimul se obține prin aplicarea unei funcții de maxim sau de minim (cum este caracterizarea unei separări de mai mulți compuși prin cea mai proastă separare a doi compuși ai acesteia):

$$\hat{y}_o = \text{opt}(\hat{Y}), \text{ unde } \text{opt} = \text{"max"} \text{ sau } \text{opt} = \text{"min"} \quad (15)$$

Parcurgând întreg domeniul de valori posibile pentru compoziția fazei mobile se identifică punctul de optim și anume compoziția optimă a fazei mobile  $(x_1, x_2, x_3)$ :

$$(\cdot; \cdot; \cdot) \mid \hat{Y}(\cdot; \cdot; \cdot) = \text{opt} \{ \hat{Y}(i/100, j/100, k/100) \mid i=0..100, j=0..100-i, k=100-i-j \} \quad (16)$$

**Etapa 2, Activitatea 4. Implementarea rutinelor si programelor de calcul**

Obținerea constantelor necunoscute pentru modele cinetice de reacție este o rutină extensivă în timp. Implementarea acestora s-a făcut din acest motiv în FreePascal, aplicația având astfel viteza necesară pentru a efectua calculele și a produce soluțiile în timp real.

Aplicația a beneficiat de două implementări, una pentru identificarea funcției obiectiv optime, și a doua pentru aplicarea funcției obiectiv obținute și identificarea constantelor necunoscute.

**Implementarea 0. Identificarea funcției obiectiv optime pentru modele cinetice**

```

unit functii;
interface
uses math;
const
  dt=4e-5;
  //e0=125.0; -c0
  e0=210.1;
  X0=0.00882328636334255/e0;
  A0=0.010-X0;
  B0=0.010-X0;
  N=7000;
  N_opt=1100;
  N_const=3;
  N_coefs=4;
  N_vars=N_const+N_coefs;
  dv=0.01;
  r_stop=0.999;
type
  file_name=string[10];
  x_array=array[0..N]of extended;
  v_array=array[0..N_vars]of extended;
  i_array=array[0..N_vars]of shortint;
  procedure v_af(var v:v_array; msg:file_name);
  procedure i_af(var i:i_array);
  procedure s_A0(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
  procedure s_A1(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
  procedure s_A2(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
  procedure s_A3(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
  procedure s_A4(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
  procedure s_A5(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
  procedure s_B0(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
  procedure s_B1(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
  procedure s_B2(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
  procedure s_B3(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
  procedure s_B4(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
  procedure s_B5(var x,y:x_array; md1,md2,md3,md4:extended; var s_sum: extended);
  procedure s_C0(var x,y:x_array; var s_sum: extended);
  procedure s_C1(var x,y:x_array; var s_sum: extended);
  procedure s_C2(var x,y:x_array; var s_sum: extended);
  procedure s_C3(var x,y:x_array; var s_sum: extended);
  procedure s_C4(var x,y:x_array; var s_sum: extended);
  procedure s_C5(var x,y:x_array; var s_sum: extended);
  procedure s_C6(var x,y:x_array; var s_sum: extended);
  procedure s_C7(var x,y:x_array; var s_sum: extended);
  procedure s_C8(var x,y:x_array; var s_sum: extended);
  procedure s_C9(var x,y:x_array; var s_sum: extended);
  procedure s_CA(var x,y:x_array; var s_sum: extended);
  procedure ini_mod(var v:v_array);
  procedure get_mod(var v,c:v_array; var x:x_array);
  procedure v_next(var i:i_array; var v0,vi,v1:v_array);
  procedure i_start(var i:i_array);
  function i_next(var i:i_array):boolean;
  procedure get_exp(var x:x_array;fn:file_name);
  procedure get_ini(var x,v:v_array;fn:file_name);
  procedure put_ini(var x:v_array;fn:file_name; step:longint);
  function ml(var x:x_array):extended;

```

```

function m2(var x,y:x_array):extended;
function mye(var x,y:x_array; ex,ey:extended):extended;
function mxe(var x:x_array; ex:extended):extended;
procedure one_step(var v,c:v_array);
procedure v_copy(var v1,v2:v_array);
implementation
procedure s_A0(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
//S = (E-aX)^2 //md1 = m_y2; //Ok
var
  m_xy, m_x2 : extended;
begin
  m_xy := m2(x,y);
  m_x2 := m2(x,x);
  s_sum := md1-m_xy*m_xy/m_x2;
end;
procedure s_B0(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
//S = (E-aX-b)^2 //md1 = m_y2; md2 = m_y1 //Ok
var
  a, b : extended;
  m_x, m_x2, m_xy : extended;
begin
  m_x := m1(x);
  m_x2 := m2(x,x);
  m_xy := m2(x,y);
  a := (m_xy-m_x*md2)/(m_x2-m_x*m_x);
  b := md2-a*m_x;
  s_sum := md1 - 2.0*a*m_xy - 2.0*b*md2+a*a*m_x2 + 2.0*a*b*m_x + b*b;
end;
procedure s_A1(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
//S = E^1(E-aX)^2 //md1 = m_y3; //Ok
var
  m_xy2, m_x2y : extended;
begin
  m_xy2 := mye(x,y,1.0,2.0);
  m_x2y := mye(x,y,2.0,1.0);
  s_sum := md1-m_xy2*m_xy2/m_x2y;
end;
procedure s_B1(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
//S = (E)(E-aX-b)^2 //md1 = m_y; md2 =m_y2; md3=m_y3; //Ok
var
  m_xy, m_xy2, m_x2y : extended;
  a,b : extended;
begin
  m_xy := m2(x,y);
  m_xy2 := mye(x,y,1.0,2.0);
  m_x2y := mye(x,y,2.0,1.0);
  a := (md1*m_xy2-md2*m_xy)/(m_x2y*md1-m_xy*m_xy);
  b := (md2-a*m_xy)/md1;
  s_sum := md3 - 2.0*a*m_xy2-2.0*b*md2+a*a*m_x2y+2.0*a*b*m_xy+b*b*md1;
end;
procedure s_A2(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
//S = E^0.5(E-aX)^2 //md1 = my25; //Ok
var
  m_xy15, m_x2y05 : extended;
begin
  m_xy15 := mye(x,y,1.0,1.5);
  m_x2y05 := mye(x,y,2.0,0.5);
  s_sum := md1-m_xy15*m_xy15/m_x2y05;
end;
procedure s_B2(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);
//S = (E^0.5)(E-aX-b)^2 //md1 = my05; md2 =my15; md3=my25; //Ok
var
  m_xy05, m_x2y05, m_xy15 : extended;
  a,b : extended;
begin
  m_xy05 := mye(x,y,1.0,0.5);
  m_xy15 := mye(x,y,1.0,1.5);
  m_x2y05 := mye(x,y,2.0,0.5);
  a := (m_xy15-md2)/(m_x2y05-m_xy05);
  b := (md2-a*m_xy05)/md1;
  s_sum := md3 - 2.0*a*m_xy15 - 2.0*b*md2+a*a*m_x2y05 + 2.0*a*b*m_xy05 + b*b*md1;
end;
procedure s_A3(var x,y:x_array; md1,md2,md3:extended; var s_sum: extended);

```

```

//S = (1/E) (E-aX)^2 //md1 = m y; //Ok
var
  m_x, m_x2_y : extended;
begin
  m_x := m1(x);
  m_x2_y := mye(x,y,2.0,-1.0);
  s_sum := md1 - m_x*m_x/m_x2_y;
end;
procedure s B3(var x,y:x array; md1,md2,md3:extended; var s_sum: extended);
//S = (1/E) (E-aX-b)^2 //md1 = my1; md2 =my_1; //Ok
var
  m_x, m_x2_y, m_x_y : extended;
  a,b : extended;
begin
  m_x := m1(x);
  m_x2_y := mye(x,y,2.0,-1.0);
  m_x_y := mye(x,y,1.0,-1.0);
  a := (m_x-(m_x_y/md2))/(m_x2_y-m_x_y*m_x_y/md2);
  b := (1.0-a*m_x_y)/md2;
  s_sum := md1+a*a*m_x2_y+b*b*md2+2.0*a*b*m_x_y-2.0*a*m_x-2.0*b;
end;
procedure s A4(var x,y:x array; md1,md2,md3:extended; var s_sum: extended);
//S = (1/E^0.5) (E-aX)^2 //md1 = my15; //Ok
var
  m_xy05, m_x2y_05 : extended;
begin
  m_xy05 := mye(x,y,1.0,0.5);
  m_x2y_05 := mye(x,y,2.0,-0.5);
  s_sum := md1-m_xy05*m_xy05/m_x2y_05;
end;
procedure s B4(var x,y:x array; md1,md2,md3:extended; var s_sum: extended);
//S = (1/E^0.5) (E-aX-b)^2 //md1 = my05; md2=my15; md3 = my_05; //!!!!!!!
var
  m_xy_05, m_xy05, m_x2y_05 : extended;
  a,b : extended;
begin
  m_xy05 := mye(x,y,1.0,0.5);
  m_xy_05 := mye(x,y,1.0,-0.5);
  m_x2y_05 := mye(x,y,2.0,-0.5);
  a := (m_xy05-md1)/(m_x2y_05-m_xy_05);
  b := (md1-a*m_xy_05)/md3;
  s_sum := md2-2*a*m_xy05-2*b*md1+a*a*m_x2y_05+2*a*b*m_xy_05+b*b*md3;
end;
procedure s A5(var x,y:x array; md1,md2,md3:extended; var s_sum: extended);
//S = (E+1/E) (E-aX)^2 //md1 = m y3; md2 = m y1; //Ok
var
  a : extended;
  m_x, m_xy2, m_x2y, m_x2_y : extended;
begin
  m_x := m1(x);
  m_xy2 := mye(x,y,1.0,2.0);
  m_x2y := mye(x,y,2.0,1.0);
  m_x2_y := mye(x,y,2.0,-1.0);
  a := (m_x+m_xy2)/(m_x2y+m_x2_y);
  s_sum := md1 + md2 -2.0*a*m_xy2-2.0*a*m_x+a*a*m_x2y+a*a*m_x2_y;
end;
procedure s B5(var x,y:x array; md1,md2,md3,md4:extended; var s sum: extended);
//S = (E+1/E) (E-aX-b)^2 //md1 = my2; md2 =my1; md3=my0;md4=my3; //Ok
var
  m_xy2, m_x2y, m_x, m_xy, m_x2_y, m_x_y : extended;
  a,b,d : extended;
begin
  m_xy2 := mye(x,y,1.0,2.0);
  m_x2y := mye(x,y,2.0,1.0);
  m_x := m1(x);
  m_xy := m2(x,y);
  m_x2_y := mye(x,y,2.0,-1.0);
  m_x_y := mye(x,y,1.0,-1.0);
  a := (m_xy2+m_x)*(md2+md3) - (m_xy+m_x_y)*(md1+1);
  b := (m_xy2+m_x)*(m_xy+m_x_y) - (m_x2y+m_x2_y)*(md1+1);
  d := (m_x2y+m_x2_y)*(md2+md3) - (m_xy+m_x_y)*(m_xy+m_x_y);
  a := a/d;
  b := b/d;
end;

```

```

s_sum := md4 + md2 + a*a*(m_x2y+m_x2_y)
        + 2.0*a*b*(m_xy+m_x_y)+b*b*(md2+md3)-2.0*a*(m_xy2+m_x)-2.0*b*(md1+1);
end;
procedure s_C0(var x,y:x_array; var s_sum: extended);
var
  i : longint;
  s,p : extended;
begin
  s := 0.0;
  for i:= 0 to N_opt do
    s := s + y[i]/x[i];
  s := s/(N_opt+1);
  p := 0.0;
  for i:= 0 to N_opt do
    p := p + abs(y[i]/x[i]-s);
  p := p/(N_opt+1);
  s_sum := p;
end;
procedure s_C1(var x,y:x_array; var s_sum: extended);
var
  i : longint;
  s,p : extended;
begin
  s := 0.0;
  for i:= 0 to N_opt do
    s := s + y[i]/x[i];
  s := s/(N_opt+1);
  p := 0.0;
  for i:= 0 to N_opt do
    p := p + power(abs(y[i]/x[i]-s),2.0);
  p := power(p,0.5);
  p := p/(N_opt+1);
  s_sum := p;
end;
procedure s_C2(var x,y:x_array; var s_sum: extended);
var
  i : longint;
  s,p : extended;
begin
  s := 0.0;
  for i:= 0 to N_opt do
    s := s + y[i]/x[i];
  s := s/(N_opt+1);
  p := 0.0;
  for i:= 0 to N_opt do
    p := p + power(abs(y[i]/x[i]-s),0.5);
  p := power(p,2.0);
  p := p/(N_opt+1);
  s_sum := p;
end;
procedure s_C3(var x,y:x_array; var s_sum: extended);
var
  i : longint;
  s,p : extended;
begin
  s := 0.0;
  for i:= 0 to N_opt do
    s := s + y[i]/x[i];
  s := s/(N_opt+1);
  p := 0.0;
  for i:= 0 to N_opt do
    p := p + power(abs(y[i]/x[i]-s),1.5);
  p := p/(N_opt+1);
  s_sum := p;
end;
procedure s_C4(var x,y:x_array; var s_sum: extended);
var
  i : longint;
  s,p : extended;
begin
  s := 0.0;
  for i:= 0 to N_opt do
    s := s + y[i]/x[i];
  s := s/(N_opt+1);

```

```

p := 0.0;
for i:= 0 to N_opt do
  p := p + x[i]*power(abs(y[i]/x[i]-s),2.0);
  p := p/(N_opt+1);
  s_sum := p;
end;
procedure s_C5(var x,y:x_array; var s_sum: extended);
var
  i : longint;
  s,p : extended;
begin
  s := 0.0;
  for i:= 0 to N_opt do
    s := s + y[i]/x[i];
  s := s/(N_opt+1);
  p := 0.0;
  for i:= 0 to N_opt do
    p := p + power(x[i],0.5)*power(abs(y[i]/x[i]-s),2.0);
  p := p/(N_opt+1);
  s_sum := p;
end;
procedure s_C6(var x,y:x_array; var s_sum: extended);
var
  i : longint;
  s,p : extended;
begin
  s := 0.0;
  for i:= 0 to N_opt do
    s := s + y[i]/x[i];
  s := s/(N_opt+1);
  p := 0.0;
  for i:= 0 to N do
    p := p + power(x[i],2.0)*power(abs(y[i]/x[i]-s),2.0);
  p := p/(N_opt+1);
  s_sum := p;
end;
procedure s_C7(var x,y:x_array; var s_sum: extended);
var
  i : longint;
  s1,s2,p : extended;
begin
  s1 := 0.0;
  s2 := 0.0;
  for i:= 0 to N_opt do begin
    s1 := s1 + y[i]/x[i];
    s2 := s2 + x[i]/y[i];
  end;
  s1 := s1/(N_opt+1);
  s2 := s2/(N_opt+1);
  p := 0.0;
  for i:= 0 to N_opt do
    p := p + power(abs(x[i]/y[i]-s2),2.0)*power(abs(y[i]/x[i]-s1),2.0);
  p := p/(N_opt+1);
  s_sum := p;
end;
procedure s_C8(var x,y:x_array; var s_sum: extended);
var
  i : longint;
  s1,s2,p : extended;
begin
  s1 := 0.0;
  s2 := 0.0;
  for i:= 0 to N_opt do begin
    s1 := s1 + y[i]/x[i];
    s2 := s2 + x[i]/y[i];
  end;
  s1 := s1/(N_opt+1);
  s2 := s2/(N_opt+1);
  p := 0.0;
  for i:= 0 to N_opt do
    p := p + power(abs(x[i]/y[i]-s2),0.5)*power(abs(y[i]/x[i]-s1),0.5);
  p := p/(N_opt+1);
  s_sum := p;
end;

```

```

procedure s_C9(var x,y:x_array; var s_sum: extended);
var
  i : longint;
  s1,s2,p : extended;
begin
  s1 := 0.0;
  s2 := 0.0;
  for i:= 0 to N_opt do begin
    s1 := s1 + y[i]/x[i];
    s2 := s2 + x[i]/y[i];
  end;
  s1 := s1/(N_opt+1);
  s2 := s2/(N_opt+1);
  p := 0.0;
  for i:= 0 to N_opt do
    p := p + power(abs(x[i]/y[i]-s2),0.125)*power(abs(y[i]/x[i]-s1),0.125);
  p := p/(N_opt+1);
  s_sum := p;
end;
procedure s_CA(var x,y:x_array; var s_sum: extended);
var
  i : longint;
  s1,s2 : extended;
  p1,p2 : extended;
begin
  s1 := 0.0;
  s2 := 0.0;
  for i:= 1 to N_opt do begin
    s1 := s1 + y[i]/x[i];
    s2 := s2 + x[i]/y[i];
  end;
  s1 := s1 /N_opt;
  s2 := s2 /N_opt;
  p1 := 0.0;
  p2 := 0.0;
  for i:= 1 to N_opt do begin
    p1 := p1 + power(abs(y[i]/x[i]-s1),2.0);
    p2 := p2 + power(abs(x[i]/y[i]-s2),2.0);
  end;
  s_sum := sqrt(p1*p2);
end;
procedure one_step(var v,c:v_array);
var
  c1:extended;//X,A,B :1,2,3
begin
  c1:=v[1]*power(c[2],v[4])*power(c[3],v[5])-v[2]*power(c[1],v[6]);
  c[1] := c[1]+dt*(c1-v[3]*power(c[1],v[7]));
  c[2] := c[2]-dt*c1;
  c[3] := c[3]-dt*c1;
end;
procedure get_mod(var v,c:v_array; var x:x_array);
var
  i : shortint;
  j : longint;
begin
  x[0] := c[1];
  for j := 1 to N_opt do begin
    one_step(v,c);
    x[j] := c[1];
    for i := 1 to N_const do
      if(c[i]<0)then begin
        //writeln('concentratia substantei ',i,' la iteratia ',j,' negativa!');
        c[i] := 0.0;
        //readln;//halt;
      end;
    end;
  end;
end;
procedure v_next(var i:i_array; var v0,vi,v1:v_array);
var
  j : shortint;
begin
  for j := 1 to N_vars do v1[j] := v0[j]*(1+vi[j]*(i[j]-1));
end;
procedure i_start(var i:i_array);

```

```
var
  j:shortint;
begin
  for j:= 0 to N_vars do i[j] := 0;
end;
function i_next(var i:i_array):boolean;
var
  j:shortint;
  t:shortint;
begin
  i[N_vars] := i[N_vars] + 1;
  for j:= N_vars downto 1 do begin
    t := i[j] div 3;
    i[j] := i[j] mod 3;
    i[j-1] := i[j-1] + t;
  end;
  if i[0]>0 then i_next := true else i_next := false;
end;
procedure get_exp(var x:x_array;fn:file_name);
var
  f_in:text;
  i:longint;
begin
  assign(f_in,fn);
  reset(f_in);
  i:=0;
  while(not(eof(f_in)))do begin
    readln(f_in,x[i]);
    i:=i+1;
  end;
  close(f_in);
end;
procedure get_ini(var x,v:v_array;fn:file_name);
var
  f_in:text;
  i:longint;
begin
  assign(f_in,fn);
  reset(f_in);
  i:=0;
  while(not(eof(f_in)))do begin
    readln(f_in,x[i]);
    v[i]:=dv;
    i:=i+1;
  end;
  close(f_in);
end;
procedure put_ini(var x:v_array;fn:file_name; step:longint);
var
  f_in:text;
  i:longint;
begin
  assign(f_in,fn);
  {$i-}
  reset(f_in);
  i:=ioresult;
  {$i+}
  if(i>0) then begin
    rewrite(f_in);
    close(f_in);
  end;
  append(f_in);
  write(f_in,step);
  for i:=0 to N_vars do write(f_in,x[i]);
  writeln(f_in);
  close(f_in);
end;
function m1(var x:x_array):extended;
var
  rez:extended;
  i:longint;
begin
  rez :=0.0;
  for i:=0 to N_opt do rez := rez + x[i];
```

```

    m1 := rez/(N_opt+1);
end;
function m2(var x,y:x_array):extended;
var
    rez:extended;
    i:longint;
begin
    rez :=0.0;
    for i:=0 to N_opt do rez := rez + x[i]*y[i];
    m2 := rez/(N_opt+1);
end;
function mye(var x,y:x_array; ex,ey:extended):extended;
var
    rez:extended;
    i:longint;
begin
    rez :=0.0;
    for i:=0 to N_opt do rez := rez + power(x[i],ex)*power(y[i],ey);
    mye := rez/(N_opt+1);
end;
function mxe(var x:x_array; ex:extended):extended;
var
    rez:extended;
    i:longint;
begin
    rez :=0.0;
    for i:=0 to N_opt do rez := rez + power(x[i],ex);
    mxe := rez/(N_opt+1);
end;
procedure ini_mod(var v:v_array);
begin
    v[1] := X0;
    v[2] := A0;
    v[3] := B0;
end;
procedure i_af(var i:i_array);
var
    j:shortint;
begin
    for j:= 1 to N_vars-1 do write(i[j], ' ');
    writeln(i[N_vars]);
end;
procedure v_af(var v:v_array; msg:file_name);
var
    j:shortint;
begin
    writeln(msg);
    for j:= 0 to N_vars-1 do write(v[j], ' ');
    writeln(v[N_vars]);
end;
procedure v_copy(var v1,v2:v_array);
var
    i : shortint;
begin
    for i := 0 to N_vars do v2[i] := v1[i];
end;
end.

```

```

program Cin;
{$APPTYPE CONSOLE}
uses
    SysUtils,
    math,
    functii;
var
    x_exp:x_array;
    x_mod:x_array;
    m_y0,m_y_,m_y1, m_y2, m_y3, my25,my05,my15 :extended;
    v_0:v_array;
    v v:v_array;
    v_i:i_array;
    v_1:v_array;
    v_c:v_array;//concentratii instantanee
    v_2:v_array;

```

```

step:longint;
stepf:longint;
begin
  get_exp(x_exp, 'Text1');
  m_y1 := m1(x_exp);
  m_y2 := m2(x_exp, x_exp);
  m_y0 := mxe(x_exp, -1.0);
  m_y_ := mxe(x_exp, -0.5);
  m_y3 := mxe(x_exp, 3.0);
  my25 := mxe(x_exp, 2.5);
  my05 := mxe(x_exp, 0.5);
  my15 := mxe(x_exp, 1.5);
  get_ini(v_0, v_v, 'Start');
  //put_ini(v_0, 'Itera', 0);
  put_ini(v_0, 'Itera1', 0);
  v_copy(v_0, v_2);
  step := 0;
  stepf := 0;
  repeat
    i_start(v_i);
    step := step + 1;
    repeat
      v_next(v_i, v_0, v_v, v_1);
      ini_mod(v_c);
      get_mod(v_1, v_c, x_mod);
      s_A0(x_mod, x_exp, m_y2, 0.00, 0.00, v_1[0]);
      //s_A1(x_mod, x_exp, m_y3, 0.00, 0.00, v_1[0]);
      //s_A2(x_mod, x_exp, my25, 0.00, 0.00, v_1[0]);
      //s_A3(x_mod, x_exp, m_y1, 0.0, 0.0, v_1[0]);
      //s_A4(x_mod, x_exp, my15, 0.0, 0.00, v_1[0]);
      //s_A5(x_mod, x_exp, m_y3, m_y1, 0.0, v_1[0]);
      //s_B0(x_mod, x_exp, m_y2, m_y1, 0.00, v_1[0]);
      //s_B1(x_mod, x_exp, m_y1, m_y2, m_y3, v_1[0]);
      //s_B2(x_mod, x_exp, my05, my15, my25, v_1[0]);
      //s_B3(x_mod, x_exp, m_y1, m_y0, 0.0, v_1[0]);
      //s_B4(x_mod, x_exp, my05, my15, m_y_, v_1[0]);
      //s_B5(x_mod, x_exp, m_y2, m_y1, m_y0, m_y3, v_1[0]);
      //s_C0(x_mod, x_exp, v_1[0]);
      //s_C1(x_mod, x_exp, v_1[0]);
      //s_C2(x_mod, x_exp, v_1[0]);
      //s_C3(x_mod, x_exp, v_1[0]);
      //s_C4(x_mod, x_exp, v_1[0]);
      //s_C5(x_mod, x_exp, v_1[0]);
      //s_C6(x_mod, x_exp, v_1[0]);
      //s_C7(x_mod, x_exp, v_1[0]);
      //s_C8(x_mod, x_exp, v_1[0]);
      //s_C9(x_mod, x_exp, v_1[0]);
      //s_CA(x_mod, x_exp, v_1[0]);
      if(v_1[0]<v_2[0]) then begin    ///
        v_copy(v_1, v_2);
      end;
    until i_next(v_i);
    //put_ini(v_2, 'Itera', step);
    if(step mod 100 = 0) then writeln(step, ' ', v_2[0]);
    if(v_2[0]<v_0[0]) then begin
      v_copy(v_2, v_0);
      stepf := stepf + 1;
      put_ini(v_2, 'Itera1', stepf);
    end;
  until(step>128000); //(v_2[0]>r_stop);    ///
  { TODO -oUser -cConsole Main : Insert code here }
end.

```

### Implementarea 1. Obținerea constantelor necunoscute ale modelelor cinetice

```

unit functii;
interface
uses math;
const
  dt=4e-5;
  N=7000;
  N_const=3;
  dv=0.01;
const
  y0=1.0;

```

```

y1=1.0;
y2=1.0;
y3=2.0;
type
  file_name=string[10];
  x_array=array[0..N]of extended;
  v_array=array[0..N_const]of extended;
  i_array=array[0..N_const]of shortint;
procedure s_CC(var x,y:x_array; n_e:longint; o_o_s: extended; var s_sum: extended);
procedure s_CB(var x,y:x_array; n_e:longint; o_o_s: extended; var s_sum: extended);
procedure s_CA(var x,y:x_array; n_e:longint; var s_sum: extended);
procedure s_A0(var x,y:x_array; n_e:longint; my2:extended; var s_sum: extended);
procedure s_B0(var x,y:x_array; n_e:longint; my2,my1:extended; var s_sum: extended);
  procedure get_mod(var v,c:v_array; var x:x_array; n_e:longint);
  procedure v_next(var i:i_array; var v0,vi,v1:v_array);
  procedure i_start(var i:i_array);
  function i_next(var i:i_array):boolean;
  procedure get_exp(var x:x_array;var n_e:longint; fn:file_name);
  procedure put_ini(var x:v_array;fn:file_name; step:longint);
  procedure one_step(var v,c:v_array);
  procedure v_copy(var v1,v2:v_array);
  function m1(var x:x_array; n_e:longint):extended;
  function m2(var x,y:x_array; n_e:longint):extended;
implementation
procedure s_CC(var x,y:x_array; n_e:longint; o_o_s: extended; var s_sum: extended);
  var
    i : longint;
    i_n : longint;
    n_s : longint;
    s1,s2,p1,p2 : extended;
  begin
    n_s := 6*n_e div 14;
    s1 := 0.0; s2 := 0.0; p1 := 0.0; p2 := 0.0; i_n := 0;
    for i:= 1 to n_s do if(y[i]<o_o_s) then begin
      s1 := s1 + y[i]/x[i];
      s2 := s2 + x[i]/y[i];
      i_n := i_n + 1;
    end;
    s1 := s1/i_n; s2 := s2/i_n;
    for i:= 1 to n_s do if(y[i]<o_o_s) then begin
      p1 := p1 + power(abs(y[i]/x[i]-s1),4.0);
      p2 := p2 + power(abs(x[i]/y[i]-s2),4.0);
    end;
    s_sum := power(p1*p2,0.5);
  end;
procedure s_CB(var x,y:x_array; n_e:longint; o_o_s: extended; var s_sum: extended);
  var
    i : longint;
    i_n : longint;
    s1,s2,p1,p2 : extended;
  begin
    s1 := 0.0; s2 := 0.0; p1 := 0.0; p2 := 0.0; i_n := 0;
    for i:= 1 to n_e do if(y[i]<o_o_s) then begin
      s1 := s1 + y[i]/x[i];
      s2 := s2 + x[i]/y[i];
      i_n := i_n + 1;
    end;
    s1 := s1/i_n; s2 := s2/i_n;
    for i:= 1 to n_e do if(y[i]<o_o_s) then begin
      p1 := p1 + power(abs(y[i]/x[i]-s1),4.0);
      p2 := p2 + power(abs(x[i]/y[i]-s2),4.0);
    end;
    s_sum := power(p1*p2,0.5);
  end;
procedure s_CA(var x,y:x_array; n_e:longint; var s_sum: extended);
  var
    i : longint;
    s1,s2,p1,p2 : extended;
  begin
    s1 := 0.0; s2 := 0.0; p1 := 0.0; p2 := 0.0;
    for i:= 1 to n_e do begin
      s1 := s1 + y[i]/x[i];
      s2 := s2 + x[i]/y[i];
    end;
  end;

```

```

s1 := s1/n_e;   s2 := s2/n_e;
for i:= 1 to n_e do begin
  p1 := p1 + power(abs(y[i]/x[i]-s1),8.0)/sqrt(i);
  p2 := p2 + power(abs(x[i]/y[i]-s2),8.0)/sqrt(i);
end;
s_sum := sqrt(p1*p2);
end;
procedure s_A0(var x,y:x_array; n_e: longint; my2:extended; var s_sum: extended);
var
  m_xy, m_x2 : extended;
begin//S = (E-aX)^2
  m_xy := m2(x,y,n_e);
  m_x2 := m2(x,x,n_e);
  s_sum := my2-m_xy*m_xy/m_x2;
end;
procedure s_B0(var x,y:x_array; n_e:longint; my2,my1:extended; var s_sum: extended);
var
  a, b, m_x, m_x2, m_xy : extended;
begin//S = (E-aX-b)^2
  m_x := m1(x,n_e);
  m_x2 := m2(x,x,n_e);
  m_xy := m2(x,y,n_e);
  a := (m_xy-m_x*my1)/(m_x2-m_x*m_x);
  b := my1-a*m_x;
  s_sum := my2 - 2.0*a*m_xy - 2.0*b*my1+a*a*m_x2 + 2.0*a*b*m_x + b*b;
end;
procedure one_step(var v,c:v_array);
begin//X,A,B :1,2,3
  c[0] := dt*(v[1]*power(c[2],y0)*power(c[3],y1)-v[2]*power(c[1],y2));
  c[1] := c[1]+c[0]-dt*v[3]*power(c[1],y3);
  c[2] := c[2]-c[0];
  c[3] := c[3]-c[0];
end;
procedure get_mod(var v,c:v_array; var x:x_array; n_e:longint);
var
  i : shortint;
  j : longint;
begin
  x[0] := c[1];
  for j := 1 to n_e do begin
    one_step(v,c);
    x[j] := c[1];
    for i := 1 to N_const do
      if(c[i]<0)then begin
        c[i] := 0.0;
      end;
    end;
  end;
end;
procedure v_next(var i:i_array; var v0,vi,v1:v_array);
var
  j : shortint;
begin
  for j := 1 to N_const do v1[j] := v0[j]*(1+vi[j]*(i[j]-1));
end;
procedure i_start(var i:i_array);
var
  j:shortint;
begin
  for j:= 0 to N_const do i[j] := 0;
end;
function i_next(var i:i_array):boolean;
var
  j:shortint;
  t:shortint;
begin
  i[N_const] := i[N_const] + 1;
  for j:= N_const downto 1 do begin
    t := i[j] div 3;
    i[j] := i[j] mod 3;
    i[j-1] := i[j-1] + t;
  end;
  if i[0]>0 then begin
    i_next := true;
    i[0] := 0;
  end;
end;

```

```

    end else i_next := false;
end;
procedure get_exp(var x:x_array;var n_e:longint; fn:file_name);
var
    f_in:text;
    i:longint;
begin
    assign(f_in,fn);
    reset(f_in);
    i:=0;
    while(not.eof(f_in))do begin
        readln(f_in,x[i]);
        i:=i+1;
    end;
    close(f_in);
    n_e := i-1;
end;
procedure put_ini(var x:v_array;fn:file_name; step:longint);
var
    f_in:text;
    i:longint;
begin
    assign(f_in,fn);
    {$i-}
    reset(f_in);
    i:=ioresult;
    {$i+}
    if(i>0) then begin
        rewrite(f_in);
        close(f_in);
    end;
    append(f_in);
    write(f_in,step);
    for i:=0 to N_const do write(f_in,x[i]);
    write(f_in,y0);
    write(f_in,y1);
    write(f_in,y2);
    write(f_in,y3);
    writeln(f_in);
    close(f_in);
end;
procedure v_copy(var v1,v2:v_array);
var
    i : shortint;
begin
    for i := 0 to N_const do v2[i] := v1[i];
end;
function m1(var x:x_array; n_e:longint):extended;
var
    rez:extended;
    i:longint;
begin
    rez :=0.0;
    for i:=0 to n_e do rez := rez + x[i];
    m1 := rez/(n_e+1);
end;
function m2(var x,y:x_array; n_e:longint):extended;
var
    rez:extended;
    i:longint;
begin
    rez :=0.0;
    for i:=0 to n_e do rez := rez + x[i]*y[i];
    m2 := rez/(n_e+1);
end;
end.

program Cin;
{$APPTYPE CONSOLE}
uses
    SysUtils,
    math,
    functii;
var

```

```

x_exp:x_array;
x_mod:x_array;
v_0:v_array;
v_v:v_array;
v_i:i_array;
v_1:v_array;
v_c:v_array;//concentratii instantanee
v_2:v_array;
stepf,step:longint;
n_exp:longint;
X0,A0,B0,e0:extended; //my1,my2: extended;
out_of_scale:extended;
begin
  get_exp(x_exp,n_exp,'Text05');
  A0 := 0.005;
  B0 := 0.005;
  out_of_scale := 1.7e-1;
  e0 := 1012.2;
  v_0[0] := 1e80;
  v_0[1] := 1.82e+3;
  v_0[2] := 8.5e-15;
  v_0[3] := 2.66e+5;
  X0 := x_exp[0]/e0;
  //my2:=m2(x_exp,x_exp,n_exp)//my1:=m1(x_exp,n_exp);
  put_ini(v_0,'Iteral',0);
  v_copy(v_0,v_2);
  step := 0;
  stepf:= 0;
  i_start(v_i);
  v_v[1] := dv; v_v[2] := dv; v_v[3] := dv;
  repeat
    repeat
      v_next(v_i,v_0,v_v,v_1);
      v_c[1] := X0;
      v_c[2] := A0-X0;
      v_c[3] := B0-X0;
      get_mod(v_1,v_c,x_mod,n_exp);
      s_CC(x_mod,x_exp,n_exp,out_of_scale,v_1[0]);
      //s_CB(x_mod,x_exp,n_exp,out_of_scale,v_1[0]);
      //s_CA(x_mod,x_exp,n_exp,v_1[0]);
      //s_A0(x_mod,x_exp,n_exp,my2,v_1[0]);
      //s_B0(x_mod,x_exp,n_exp,my2,my1,v_1[0]);
      if(v_1[0]<v_2[0]) then begin
        v_copy(v_1,v_2);
      end;
    until i_next(v_i);
    if (step mod 200 = 0) then writeln(step:5, ' ', v_2[0]);
    step := step + 1;
    if(v_2[0]<v_0[0]) then begin
      v_copy(v_2,v_0);
      stepf := stepf + 1;
      put_ini(v_2,'Iteral',stepf);
    end;
  until(step>128000);
end.

```

Pentru a implementa optimizarea fazei mobile la separarea cromatografică cu amestecuri de trei solvenți s-a creat un pachet de programe PHP (Pre Hypertext Processed) care asigură o maximă portabilitate. Astfel, programul de optimizare poate fi executat de pe orice calculator care este legat la Internet de la adresa:

[http://vl.academicdirect.org/molecular\\_dynamics/mobile\\_phase\\_opt/](http://vl.academicdirect.org/molecular_dynamics/mobile_phase_opt/)

Trei programe (op1.php, op2.php, op3.php) asigură interfața pentru introducerea datelor experimentale și selecția modelelor folosite.

Astfel, programul *op1.php* permite specificarea celor trei solvenți folosiți și a compușilor care se dorește a fi separați (dacă aceștia sunt cunoscuți). Aceste informații nu afectează modul de calcul pe care se bazează optimizarea, ci sunt folosiți numai pentru ușurarea manipulării interfeței programului și prezentarea rezultatelor optimizării.

Rezultatul alegerii este transmis programului *op2.php* care dintr-o listă de 10 compoziții ale fazei mobile experimente permite utilizatorului să aleagă exact acele experimente pe care le-a efectuat.

Programul *op3.php* conține ultima interfață pentru introducerea datelor măsurate. Aici pentru fiecare experiment se cere distanța pe care a migrat eluentul și pentru fiecare compus se cere distanța pe care a migrat acesta și lărgimea spotului cromatografic.

Alegerea modelului matematic și a parametrului cromatografic folosite este posibilă în orice combinație dintre modelul cu 6 și cel cu 7 termeni și respectiv funcție obiectiv, rezoluție sau factor de retenție.

Programul *op4.php* efectuează toate calculele solicitate și afișează rezultatele în forma:

- Nume parametru cromatografic;
- Ecuația modelării parametrului cromatografic;
- Valorile parametrului cromatografic ce rezultă din experiment din aplicarea formulelor de calcul ale acestuia, pentru fiecare experiment ales și fiecare compus, pereche de compuși sau sub-funcție obiectiv (vezi modelul matematic);
- Valorile parametrului cromatografic ce rezultă din modelare în aceeași succesiune ca pentru valorile ce rezultă din experiment;
- Lista valorilor prezise de model pentru valorile parametrului cromatografic pentru toate valorile posibile ale compoziției fazei mobile cu un increment de o unitate procentuală de compoziție;
- Compoziția optimă calculată de model și valoarea prezisă a parametrului cromatografic în acest punct;
- O cale de acces către un alt program (*graph.php*) care reprezintă grafic sub formă de suprafață de nivel dependența parametrului cromatografic prezis în funcție de compoziția fazei mobile folosind 4 specificații utilizator (care doi din cei trei solvenți sunt aleși pentru a reprezenta axele  $O_x$  și  $O_y$ , care este valoarea minimă a parametrului cromatografic are să apară pe graficul rezultat, și câte nuanțe intermediare de culoare între 2 culori de bază să fie folosite pentru reprezentarea suprafeței de nivel între valoarea minimă și valoarea maximă a

parametrului cromatografic prezis); programul produce un grafic în format PNG (Portable Network Graphics);

- O cale de acces către salvarea rezultatelor în format text.

Fișierele *data1.php*, *data2.php* și *data3.php* conțin tablouri uni- și bi- dimensionale a 3 experimente care pot fi folosite drept model în execuția programului de modelare.

Astfel, compușii, solvenții și distanțele de migrare ale eluenților sunt tablouri unidimensionale iar experimentele și rezultatele sunt tablouri bidimensionale. O notă aparte fac rezultatele, a căror implementare ca tablouri bidimensionale (compus vs. data) a fost preferată în favoarea celei naturale a acestora de tablouri tridimensionale (compus vs. experiment vs. data) pentru ușurarea manipulării acestora de către utilizator.

Transmiterea datelor între client (utilizator) și server (programe) se face cu precădere prin metoda POST, însă opțiunea de alegerea datelor model se face prin metoda GET.

Nucleul principal al aplicație de optimizare este realizat de modulul *z\_HPTLC\_Models.php*:

- Funcția *MX\_Model* întoarce un șir ale cărui valori sunt obținute din efectuarea înmulțirilor acolo unde este necesar conform modelului dat de ecuațiile (1) și (2);
- Funcția *MX\_Put* folosește rezultatul dat de funcția *MX\_Model* și valorile parametrului cromatografic pentru a construi sistemul de ecuații liniare dat de ecuația (11);
- Funcția *MX\_System* folosește rezultatul dat de funcția *MX\_Put* pentru a construi sistemul de ecuații liniare cu soluție unic determinată (12);
- Funcția *MX\_Gauss* rezolvă sistemul de ecuații liniare (12) dat de funcția *MX\_System* și întoarce valorile calculate ale coeficienților modelului (ecuația 13);
- Funcția *MX\_Coefs* integrează funcțiile *MX\_Put*, *MX\_System* și *MX\_Gauss* într-un modul care primește ca și date valorile parametrului cromatografic și valorile compoziției fazei mobile și produce valorile coeficienților modelului;
- Funcția *MX\_Est* efectuează predicția valorilor parametrului cromatografic folosind datele calculate ale coeficienților modelului și o compoziție dată a fazei mobile;
- Funcția *Worst\_RF* definește parametrul care caracterizează o separare modelată prin factorul de retenție ca parametru cromatografic; folosește un șir de valori calculate ale factorului de retenție pentru fiecare compus și întoarce ca valoare cea mai mică diferență care se înregistrează în acest șir;

**ET108/2006 – Et. Finală/2007 – Lucrare in extenso**

- Funcția *Worst\_RS* definește parametrul care caracterizează o separare modelată prin rezoluție ca parametru cromatografic; folosește un șir de valori calculate ale rezoluției o serie de perechi de compuși și întoarce ca valoare cea mai mică valoare din acest șir;
- Funcția *Worst\_OB* definește parametrul care caracterizează o separare modelată prin funcție obiectiv; are o singură dată de intrare, valoarea funcției obiectiv și o întoarce pe aceasta ca valoare;
- Funcția *f\_sm* implementează calculul separării medii dat de ecuația (6);
- Funcția *f\_rsa* implementează calculul rezoluției medii dat de ecuația (7);
- Funcția *f\_rrp* implementează calculul produsul ponderat cu media rezoluțiilor dat de ecuația (8);
- Funcția *f\_inf* implementează calculul factorului de calitate al separării calculat după metoda Logit dat de ecuația (9);
- Funcțiile *f\_obX* ( $X=1,2,\dots$ ) implementează diferite funcții obiectiv date de ecuația (10).

**Etapa 3, Activitatea 1. Testarea funcțiilor obiectiv**

Următoarele date și rezultate sunt din testarea funcțiilor obiectiv de determinare a constantelor necunoscute în cinetica reacțiilor:

Date - concentrații egale și egale cu $10^{-3}$ M, extincții în unități de curent (mA)							
0.00277	0.01308	0.02363	0.03645	0.04555	0.05381	0.05799	0.06328
0.00370	0.01308	0.02363	0.03645	0.04760	0.05381	0.05904	0.06328
0.00370	0.01213	0.02363	0.03645	0.04658	0.05381	0.05799	0.06328
0.00370	0.01308	0.02461	0.03745	0.04658	0.05381	0.05694	0.06328
0.00463	0.01403	0.02461	0.03745	0.04658	0.05381	0.05694	0.06435
0.00463	0.01403	0.02363	0.03745	0.04760	0.05485	0.05799	0.06328
0.00463	0.01403	0.02558	0.03745	0.04760	0.05485	0.05904	0.06435
0.00463	0.01498	0.02558	0.03745	0.04863	0.05485	0.05904	0.06435
0.00370	0.01498	0.02558	0.03846	0.04863	0.05381	0.05904	0.06328
0.00463	0.01498	0.02558	0.03846	0.04760	0.05381	0.05904	0.06435
0.00556	0.01593	0.02656	0.03946	0.04760	0.05381	0.05799	0.06328
0.00556	0.01498	0.02558	0.03946	0.04760	0.05485	0.05904	0.06435
0.00556	0.01593	0.02656	0.03946	0.04760	0.05485	0.05799	0.06222
0.00556	0.01689	0.02558	0.04047	0.04863	0.05485	0.05799	0.06328
0.00556	0.01593	0.02656	0.04047	0.04863	0.05485	0.05799	0.06435
0.00556	0.01593	0.02656	0.04047	0.04863	0.05485	0.05904	0.06435
0.00649	0.01689	0.02754	0.04047	0.04966	0.05589	0.06010	0.06435
0.00742	0.01784	0.02852	0.04148	0.04863	0.05485	0.06010	0.06328
0.00649	0.01689	0.02852	0.04148	0.04966	0.05589	0.06116	0.06328
0.00649	0.01784	0.02852	0.04148	0.04966	0.05381	0.06116	0.06435
0.00742	0.01689	0.02950	0.04148	0.04966	0.05589	0.05904	0.06435
0.00742	0.01784	0.02950	0.04148	0.04966	0.05589	0.06010	0.06435
0.00836	0.01880	0.02950	0.04250	0.04966	0.05485	0.06116	0.06435
0.00836	0.01880	0.02950	0.04250	0.05069	0.05589	0.06116	0.06328
0.00742	0.01880	0.03148	0.04250	0.05069	0.05589	0.06116	0.06328
0.00836	0.01880	0.03049	0.04250	0.05069	0.05589	0.06116	0.06542
0.00930	0.01977	0.03049	0.04351	0.05069	0.05589	0.06116	0.06435
0.00930	0.01977	0.03148	0.04351	0.05173	0.05589	0.06222	0.06542
0.00930	0.02073	0.03148	0.04351	0.05173	0.05589	0.06222	0.06435
0.00836	0.02073	0.03247	0.04453	0.05173	0.05589	0.06116	0.06435
0.00930	0.02073	0.03247	0.04453	0.05173	0.05694	0.06222	0.06542
0.00930	0.02073	0.03346	0.04351	0.05173	0.05694	0.06222	0.06542
0.01024	0.02170	0.03247	0.04351	0.05173	0.05694	0.06328	0.06542
0.01024	0.02170	0.03346	0.04453	0.05173	0.05694	0.06222	0.06435
0.00930	0.02170	0.03346	0.04453	0.05277	0.05799	0.06116	0.06435
0.01024	0.02266	0.03346	0.04555	0.05173	0.05694	0.06222	0.06542
0.01024	0.02266	0.03545	0.04555	0.05277	0.05799	0.06222	0.06542
0.01118	0.02266	0.03446	0.04555	0.05173	0.05799	0.06222	0.06542
0.01024	0.02363	0.03446	0.04658	0.05277	0.05799	0.06328	0.06542
0.01118	0.02266	0.03545	0.04658	0.05277	0.05694	0.06328	0.06542
0.01118	0.02363	0.03545	0.04658	0.05381	0.05904	0.06328	0.06542
0.01213	0.02363	0.03545	0.04658	0.05381	0.05799	0.06222	0.06435
0.01213	0.02363	0.03545	0.04658	0.05381	0.05904	0.06222	0.06542

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.06542	0.06542	0.06649	0.06864	0.06864	0.07080	0.07080	0.06972
0.06542	0.06649	0.06756	0.06864	0.06972	0.06972	0.07080	0.07080
0.06435	0.06649	0.06864	0.06972	0.06864	0.06972	0.07080	0.06972
0.06649	0.06649	0.06756	0.06864	0.06972	0.07080	0.06972	0.07080
0.06542	0.06649	0.06756	0.06864	0.06864	0.06972	0.06972	0.06972
0.06649	0.06649	0.06756	0.06972	0.06864	0.07080	0.07080	0.06972
0.06542	0.06542	0.06756	0.06756	0.06756	0.07080	0.07080	0.07080
0.06542	0.06649	0.06864	0.06756	0.06864	0.06972	0.07080	0.07080
0.06542	0.06649	0.06756	0.06756	0.06864	0.06972	0.06972	0.06972
0.06542	0.06542	0.06756	0.06649	0.06864	0.06864	0.06972	0.07080
0.06542	0.06542	0.06864	0.06756	0.06864	0.06972	0.07080	0.06972
0.06649	0.06542	0.06864	0.06756	0.06972	0.06864	0.07080	0.06972
0.06649	0.06542	0.06864	0.06864	0.06864	0.06864	0.07080	0.07080
0.06649	0.06542	0.06864	0.06756	0.06972	0.06864	0.07080	0.07080
0.06649	0.06649	0.06756	0.06756	0.06972	0.06972	0.07080	0.07188
0.06649	0.06649	0.06864	0.06756	0.06972	0.06864	0.06972	0.07080
0.06542	0.06649	0.06864	0.06756	0.06864	0.06864	0.07080	0.07080
0.06649	0.06649	0.06756	0.06649	0.06972	0.06972	0.06972	0.07080
0.06649	0.06649	0.06864	0.06649	0.06864	0.06864	0.06972	0.07080
0.06542	0.06756	0.06756	0.06756	0.06864	0.06864	0.07080	0.07080
0.06649	0.06649	0.06864	0.06649	0.06864	0.06756	0.07080	0.07080
0.06542	0.06649	0.06756	0.06756	0.06972	0.06864	0.07080	0.06972
0.06649	0.06649	0.06864	0.06756	0.06972	0.06864	0.07188	0.06972
0.06542	0.06649	0.06864	0.06864	0.06972	0.06864	0.06972	0.06972
0.06649	0.06649	0.06864	0.06756	0.06972	0.06864	0.07080	0.06972
0.06756	0.06649	0.06756	0.06756	0.06864	0.06972	0.07188	0.07080
0.06649	0.06542	0.06864	0.06864	0.06864	0.06864	0.07080	0.07080
0.06649	0.06756	0.06864	0.06756	0.06864	0.07080	0.07080	0.06972
0.06756	0.06542	0.06972	0.06649	0.06864	0.06756	0.07080	0.07080
0.06756	0.06649	0.06972	0.06864	0.06864	0.06972	0.07080	0.06972
0.06649	0.06649	0.06972	0.06756	0.06864	0.06864	0.07188	0.07080
0.06649	0.06649	0.06972	0.06756	0.06864	0.07080	0.07080	0.07080
0.06649	0.06649	0.06864	0.06649	0.06864	0.06972	0.07080	0.06972
0.06542	0.06649	0.06864	0.06864	0.06972	0.06972	0.07188	0.06972
0.06542	0.06649	0.06972	0.06864	0.06972	0.06972	0.07080	0.06972
0.06649	0.06649	0.06864	0.06864	0.06972	0.06972	0.07188	0.07080
0.06542	0.06649	0.06864	0.06864	0.06972	0.06864	0.07188	0.07080
0.06542	0.06756	0.06756	0.06864	0.06972	0.06864	0.07080	0.07080
0.06649	0.06649	0.06864	0.06864	0.06972	0.06972	0.07080	0.06972
0.06649	0.06649	0.06756	0.06864	0.07080	0.07080	0.06972	0.07080
0.06542	0.06756	0.06864	0.06864	0.07080	0.07080	0.07080	0.06972
0.06649	0.06756	0.06972	0.06756	0.06972	0.06972	0.07080	0.07080
0.06542	0.06649	0.06864	0.06864	0.07080	0.07080	0.06972	0.07080
0.06649	0.06649	0.06864	0.06864	0.06972	0.06972	0.07080	0.07080
0.06649	0.06756	0.06864	0.06756	0.06972	0.07080	0.07080	0.06972
0.06649	0.06756	0.06864	0.06864	0.06864	0.07080	0.07080	0.07080
0.06542	0.06756	0.06864	0.06864	0.06972	0.07080	0.06972	0.07080
0.06649	0.06756	0.06864	0.06972	0.06972	0.07080	0.06972	0.07080

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.07080	0.07188	0.07406	0.07515	0.07297	0.07406	0.07406	0.07515
0.07080	0.07297	0.07406	0.07515	0.07406	0.07515	0.07515	0.07515
0.07080	0.07188	0.07406	0.07625	0.07406	0.07515	0.07406	0.07515
0.07188	0.07297	0.07297	0.07625	0.07297	0.07515	0.07406	0.07515
0.07188	0.07297	0.07406	0.07515	0.07297	0.07515	0.07515	0.07515
0.07188	0.07297	0.07406	0.07515	0.07406	0.07515	0.07297	0.07515
0.07080	0.07188	0.07406	0.07625	0.07406	0.07406	0.07515	0.07515
0.07188	0.07297	0.07406	0.07625	0.07406	0.07515	0.07406	0.07406
0.07188	0.07188	0.07515	0.07625	0.07406	0.07515	0.07515	0.07515
0.07188	0.07297	0.07406	0.07515	0.07406	0.07406	0.07406	0.07515
0.07188	0.07297	0.07406	0.07406	0.07515	0.07515	0.07406	0.07406
0.07297	0.07297	0.07406	0.07515	0.07406	0.07406	0.07515	0.07515
0.07297	0.07297	0.07297	0.07515	0.07406	0.07515	0.07515	0.07406
0.07080	0.07297	0.07406	0.07515	0.07297	0.07406	0.07406	0.07406
0.07080	0.07297	0.07406	0.07406	0.07297	0.07406	0.07406	0.07515
0.07188	0.07188	0.07406	0.07406	0.07515	0.07406	0.07406	0.07515
0.07188	0.07297	0.07406	0.07515	0.07406	0.07406	0.07406	0.07515
0.07080	0.07188	0.07406	0.07515	0.07406	0.07515	0.07406	0.07406
0.07188	0.07406	0.07406	0.07406	0.07406	0.07515	0.07625	0.07406
0.07188	0.07297	0.07406	0.07515	0.07406	0.07406	0.07515	0.07406
0.07297	0.07406	0.07406	0.07515	0.07406	0.07406	0.07515	0.07406
0.07297	0.07406	0.07515	0.07515	0.07406	0.07406	0.07406	0.07406
0.07297	0.07406	0.07515	0.07515	0.07406	0.07515	0.07515	0.07406
0.07297	0.07297	0.07515	0.07297	0.07406	0.07406	0.07515	0.07515
0.07297	0.07297	0.07515	0.07406	0.07406	0.07406	0.07406	0.07297
0.07297	0.07406	0.07515	0.07406	0.07406	0.07515	0.07515	0.07406
0.07297	0.07297	0.07515	0.07406	0.07515	0.07406	0.07515	0.07297
0.07188	0.07297	0.07515	0.07406	0.07406	0.07515	0.07515	0.07406
0.07188	0.07297	0.07515	0.07406	0.07515	0.07406	0.07515	0.07406
0.07188	0.07297	0.07515	0.07406	0.07406	0.07515	0.07406	0.07406
0.07188	0.07297	0.07515	0.07406	0.07515	0.07406	0.07406	0.07297
0.07297	0.07406	0.07625	0.07406	0.07406	0.07515	0.07406	0.07297
0.07297	0.07406	0.07625	0.07406	0.07406	0.07406	0.07515	0.07297
0.07188	0.07406	0.07625	0.07406	0.07406	0.07515	0.07406	0.07406
0.07188	0.07297	0.07515	0.07406	0.07406	0.07406	0.07406	0.07406
0.07188	0.07188	0.07515	0.07406	0.07406	0.07515	0.07406	0.07297
0.07080	0.07406	0.07625	0.07406	0.07515	0.07515	0.07515	0.07297
0.07188	0.07297	0.07406	0.07406	0.07515	0.07515	0.07406	0.07188
0.07188	0.07297	0.07515	0.07406	0.07515	0.07515	0.07406	0.07297
0.07080	0.07297	0.07625	0.07406	0.07515	0.07515	0.07515	0.07297
0.07188	0.07406	0.07515	0.07406	0.07625	0.07515	0.07515	0.07297
0.07080	0.07297	0.07734	0.07406	0.07515	0.07515	0.07515	0.07297
0.07188	0.07297	0.07515	0.07406	0.07515	0.07515	0.07406	0.07297
0.07080	0.07406	0.07515	0.07406	0.07515	0.07515	0.07515	0.07297
0.07188	0.07406	0.07515	0.07297	0.07515	0.07406	0.07406	0.07297
0.07188	0.07406	0.07515	0.07406	0.07515	0.07515	0.07515	0.07297
0.07188	0.07297	0.07515	0.07406	0.07515	0.07297	0.07515	0.07188
0.07297	0.07406	0.07625	0.07297	0.07406	0.07406	0.07515	0.07188

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.07297	0.06864	0.06435	0.06010	0.05485	0.05173	0.04863	0.04555
0.07297	0.06864	0.06435	0.06010	0.05485	0.05173	0.04863	0.04658
0.07080	0.06864	0.06328	0.05904	0.05381	0.05173	0.04863	0.04658
0.07188	0.06864	0.06328	0.05799	0.05381	0.05173	0.04760	0.04658
0.07188	0.06756	0.06222	0.05799	0.05381	0.05173	0.04863	0.04658
0.07080	0.06864	0.06328	0.05904	0.05381	0.05069	0.04863	0.04555
0.07188	0.06756	0.06222	0.05904	0.05381	0.05173	0.04863	0.04658
0.07297	0.06864	0.06328	0.05799	0.05381	0.05069	0.04863	0.04555
0.07080	0.06972	0.06222	0.05904	0.05381	0.05069	0.04760	0.04555
0.07080	0.06864	0.06435	0.06010	0.05381	0.05069	0.04863	0.04555
0.07080	0.06756	0.06435	0.05799	0.05381	0.04966	0.04863	0.04555
0.07080	0.06756	0.06222	0.05904	0.05381	0.05173	0.04863	0.04555
0.07080	0.06756	0.06222	0.05799	0.05277	0.05069	0.04760	0.04555
0.07080	0.06864	0.06222	0.05799	0.05277	0.05173	0.04760	0.04555
0.07080	0.06756	0.06222	0.05799	0.05277	0.05069	0.04760	0.04555
0.07080	0.06756	0.06222	0.05694	0.05381	0.05069	0.04658	0.04555
0.07080	0.06756	0.06116	0.05799	0.05381	0.05173	0.04760	0.04555
0.06972	0.06649	0.06116	0.05799	0.05277	0.05069	0.04760	0.04555
0.07080	0.06649	0.06222	0.05694	0.05277	0.05069	0.04760	0.04555
0.07080	0.06649	0.06222	0.05799	0.05277	0.04966	0.04760	0.04453
0.06972	0.06649	0.06116	0.05799	0.05173	0.05069	0.04760	0.04555
0.07080	0.06649	0.06222	0.05589	0.05277	0.04966	0.04658	0.04555
0.06972	0.06649	0.06116	0.05799	0.05381	0.04966	0.04760	0.04453
0.07080	0.06649	0.06116	0.05589	0.05381	0.04966	0.04760	0.04453
0.06972	0.06649	0.06116	0.05694	0.05277	0.04966	0.04658	0.04555
0.06864	0.06756	0.06116	0.05694	0.05277	0.04966	0.04658	0.04453
0.06972	0.06649	0.06116	0.05694	0.05277	0.04966	0.04760	0.04555
0.06972	0.06542	0.06116	0.05694	0.05173	0.04863	0.04760	0.04555
0.06972	0.06649	0.06116	0.05694	0.05277	0.04966	0.04760	0.04555
0.06972	0.06649	0.06010	0.05589	0.05277	0.04966	0.04658	0.04453
0.06972	0.06542	0.06116	0.05589	0.05277	0.04966	0.04658	0.04453
0.06972	0.06542	0.06116	0.05589	0.05277	0.04863	0.04658	0.04351
0.06972	0.06542	0.06116	0.05589	0.05277	0.04966	0.04760	0.04453
0.06972	0.06542	0.06116	0.05589	0.05277	0.04966	0.04658	0.04555
0.06972	0.06542	0.06116	0.05589	0.05277	0.04966	0.04658	0.04351
0.06972	0.06542	0.06010	0.05589	0.05173	0.04863	0.04658	0.04453
0.06972	0.06542	0.06010	0.05589	0.05173	0.04966	0.04658	0.04453
0.06972	0.06542	0.06010	0.05589	0.05173	0.04863	0.04760	0.04453
0.06864	0.06542	0.06010	0.05589	0.05173	0.04966	0.04658	0.04453
0.06972	0.06542	0.06116	0.05485	0.05173	0.04966	0.04658	0.04453
0.06864	0.06435	0.06116	0.05485	0.05173	0.04863	0.04658	0.04453
0.06864	0.06435	0.06010	0.05485	0.05173	0.04966	0.04658	0.04453
0.06972	0.06542	0.06010	0.05485	0.05173	0.04966	0.04555	0.04351
0.06864	0.06435	0.06010	0.05589	0.05173	0.04863	0.04658	0.04453
0.06864	0.06435	0.06010	0.05485	0.05173	0.04863	0.04658	0.04351
0.06972	0.06328	0.06010	0.05381	0.05069	0.04966	0.04555	0.04453
0.06864	0.06435	0.05904	0.05485	0.05277	0.04863	0.04658	0.04351
0.06864	0.06328	0.05799	0.05485	0.05173	0.04760	0.04658	0.04351

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.04351	0.04148	0.03946	0.03745	0.03645	0.03446	0.03446	0.03148
0.04351	0.04250	0.03946	0.03846	0.03545	0.03446	0.03446	0.03247
0.04351	0.04250	0.03946	0.03745	0.03545	0.03545	0.03346	0.03247
0.04351	0.04047	0.03946	0.03745	0.03545	0.03446	0.03346	0.03247
0.04351	0.04148	0.04047	0.03745	0.03645	0.03346	0.03346	0.03247
0.04250	0.04148	0.03946	0.03946	0.03545	0.03446	0.03346	0.03247
0.04351	0.04148	0.03846	0.03745	0.03545	0.03545	0.03346	0.03148
0.04250	0.04148	0.03946	0.03846	0.03645	0.03446	0.03346	0.03148
0.04250	0.04148	0.03946	0.03846	0.03545	0.03545	0.03346	0.03247
0.04351	0.04250	0.03946	0.03846	0.03545	0.03446	0.03346	0.03247
0.04250	0.04047	0.03946	0.03745	0.03446	0.03446	0.03247	0.03148
0.04351	0.04148	0.03846	0.03745	0.03545	0.03446	0.03346	0.03247
0.04250	0.04148	0.03946	0.03745	0.03545	0.03446	0.03346	0.03148
0.04351	0.04148	0.03846	0.03745	0.03645	0.03446	0.03346	0.03148
0.04351	0.04148	0.03846	0.03745	0.03645	0.03446	0.03247	0.03148
0.04351	0.04047	0.03846	0.03745	0.03446	0.03446	0.03346	0.03247
0.04250	0.04148	0.03946	0.03745	0.03545	0.03446	0.03346	0.03247
0.04250	0.04148	0.03946	0.03745	0.03545	0.03446	0.03247	0.03247
0.04250	0.04148	0.03846	0.03745	0.03545	0.03446	0.03247	0.03247
0.04351	0.04250	0.03946	0.03846	0.03545	0.03346	0.03346	0.03247
0.04351	0.04148	0.03846	0.03745	0.03545	0.03446	0.03148	0.03247
0.04250	0.04148	0.03846	0.03745	0.03446	0.03545	0.03247	0.03247
0.04250	0.04148	0.03846	0.03745	0.03545	0.03446	0.03247	0.03346
0.04250	0.04047	0.03846	0.03745	0.03645	0.03545	0.03247	0.03148
0.04351	0.04148	0.03745	0.03745	0.03545	0.03545	0.03247	0.03148
0.04250	0.04047	0.03846	0.03745	0.03545	0.03446	0.03346	0.03247
0.04250	0.04148	0.03846	0.03745	0.03545	0.03446	0.03247	0.03247
0.04250	0.04047	0.03745	0.03745	0.03545	0.03446	0.03247	0.03247
0.04250	0.04047	0.03745	0.03745	0.03545	0.03446	0.03247	0.03247
0.04351	0.04148	0.03846	0.03745	0.03545	0.03446	0.03247	0.03148
0.04250	0.04047	0.03745	0.03745	0.03446	0.03446	0.03148	0.03148
0.04250	0.04047	0.03745	0.03745	0.03545	0.03545	0.03247	0.03247
0.04250	0.04047	0.03846	0.03645	0.03446	0.03545	0.03247	0.03247
0.04148	0.04047	0.03846	0.03645	0.03545	0.03446	0.03247	0.03247
0.04250	0.04047	0.03745	0.03645	0.03545	0.03446	0.03247	0.03247
0.04250	0.04047	0.03846	0.03645	0.03545	0.03446	0.03247	0.03148
0.04250	0.04047	0.03745	0.03645	0.03446	0.03446	0.03247	0.03247
0.04250	0.04047	0.03846	0.03645	0.03545	0.03346	0.03247	0.03148
0.04148	0.03946	0.03846	0.03645	0.03446	0.03346	0.03247	0.03247
0.04148	0.04148	0.03846	0.03645	0.03446	0.03446	0.03247	0.03247
0.04250	0.04047	0.03846	0.03745	0.03446	0.03346	0.03247	0.03148
0.04148	0.04047	0.03846	0.03745	0.03545	0.03346	0.03247	0.03247
0.04148	0.04047	0.03846	0.03745	0.03346	0.03346	0.03148	0.03049
0.04250	0.04047	0.03745	0.03645	0.03545	0.03346	0.03148	0.03148
0.04148	0.04047	0.03846	0.03645	0.03446	0.03446	0.03148	0.03148
0.04148	0.04047	0.03846	0.03745	0.03446	0.03346	0.03247	0.03247
0.04148	0.04047	0.03846	0.03645	0.03446	0.03346	0.03247	0.03148
0.04250	0.03846	0.03846	0.03645	0.03545	0.03346	0.03247	0.03148
0.04148	0.03946	0.03846	0.03645	0.03446	0.03346	0.03247	0.03148

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.03148	0.03049	0.02950	0.02754	0.02852	0.02656	0.02558	0.02558
0.03148	0.03049	0.02950	0.02754	0.02754	0.02558	0.02754	0.02558
0.03049	0.03049	0.02950	0.02852	0.02754	0.02558	0.02656	0.02558
0.03247	0.02950	0.02950	0.02852	0.02754	0.02558	0.02558	0.02461
0.03148	0.02950	0.02950	0.02656	0.02754	0.02656	0.02754	0.02461
0.03148	0.03049	0.02852	0.02852	0.02754	0.02656	0.02656	0.02461
0.03148	0.03049	0.02950	0.02852	0.02754	0.02656	0.02558	0.02461
0.03148	0.02852	0.02852	0.02754	0.02754	0.02558	0.02558	0.02461
0.02950	0.02950	0.02852	0.02754	0.02754	0.02656	0.02656	0.02461
0.03247	0.02950	0.02950	0.02852	0.02656	0.02656	0.02558	0.02461
0.03049	0.03049	0.02950	0.02852	0.02852	0.02656	0.02558	0.02363
0.03148	0.02950	0.02950	0.02852	0.02656	0.02656	0.02656	0.02461
0.03148	0.02950	0.02852	0.02852	0.02852	0.02558	0.02461	0.02461
0.03148	0.02950	0.02852	0.02754	0.02754	0.02656	0.02558	0.02558
0.03049	0.02950	0.02852	0.02754	0.02754	0.02656	0.02558	0.02461
0.03049	0.03049	0.02852	0.02852	0.02656	0.02656	0.02461	0.02461
0.03049	0.03049	0.02852	0.02852	0.02656	0.02656	0.02558	0.02558
0.03049	0.02950	0.02950	0.02852	0.02754	0.02656	0.02558	0.02558
0.03049	0.02950	0.02852	0.02852	0.02656	0.02656	0.02558	0.02461
0.03049	0.03049	0.02852	0.02852	0.02754	0.02754	0.02558	0.02461
0.03148	0.03049	0.02852	0.02852	0.02656	0.02656	0.02558	0.02558
0.03148	0.02950	0.02950	0.02754	0.02656	0.02754	0.02461	0.02558
0.02950	0.03049	0.02852	0.02852	0.02656	0.02656	0.02558	0.02558
0.03049	0.03049	0.02754	0.02852	0.02656	0.02656	0.02461	0.02461
0.03148	0.03049	0.02852	0.02852	0.02656	0.02754	0.02558	0.02461
0.03049	0.02950	0.02852	0.02754	0.02656	0.02558	0.02558	0.02461
0.02950	0.02950	0.02852	0.02754	0.02656	0.02656	0.02558	0.02461
0.02950	0.03049	0.02852	0.02754	0.02656	0.02656	0.02363	0.02461
0.03049	0.02852	0.02852	0.02852	0.02656	0.02656	0.02558	0.02558
0.02950	0.02950	0.02852	0.02754	0.02558	0.02656	0.02558	0.02461
0.03049	0.02950	0.02852	0.02852	0.02558	0.02656	0.02558	0.02461
0.03049	0.02950	0.02852	0.02852	0.02656	0.02656	0.02461	0.02461
0.03049	0.03049	0.02852	0.02754	0.02656	0.02558	0.02558	0.02461
0.03049	0.03049	0.02852	0.02852	0.02656	0.02558	0.02461	0.02461
0.02950	0.02950	0.02852	0.02754	0.02656	0.02656	0.02558	0.02558
0.03049	0.02950	0.02852	0.02754	0.02656	0.02656	0.02461	0.02558
0.03049	0.02950	0.02852	0.02754	0.02656	0.02558	0.02461	0.02558
0.03049	0.03049	0.02754	0.02754	0.02754	0.02558	0.02461	0.02461
0.02950	0.02950	0.02754	0.02754	0.02754	0.02656	0.02558	0.02656
0.03049	0.02950	0.02852	0.02754	0.02656	0.02558	0.02558	0.02558
0.02950	0.03049	0.02852	0.02754	0.02754	0.02754	0.02461	0.02461
0.03049	0.02950	0.02852	0.02754	0.02754	0.02558	0.02461	0.02461
0.02950	0.02950	0.02754	0.02852	0.02656	0.02558	0.02461	0.02558
0.02950	0.02852	0.02852	0.02754	0.02656	0.02656	0.02461	0.02461
0.02950	0.02950	0.02852	0.02754	0.02558	0.02754	0.02461	0.02461
0.02950	0.02950	0.02852	0.02656	0.02558	0.02656	0.02461	0.02461
0.02950	0.02950	0.02852	0.02852	0.02656	0.02656	0.02558	0.02558
0.03049	0.02950	0.02852	0.02754	0.02558	0.02558	0.02461	0.02558



*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.02073	0.01977	0.01977	0.01977	0.01977	0.01880	0.01880	0.01784
0.02073	0.02073	0.01977	0.01977	0.01977	0.01977	0.01880	0.01784
0.02170	0.02073	0.02073	0.02073	0.01977	0.01880	0.01977	0.01784
0.02170	0.02073	0.02073	0.01977	0.01977	0.01977	0.01977	0.01880
0.02073	0.01977	0.01977	0.01977	0.01880	0.01880	0.01880	0.01977
0.02170	0.02073	0.02073	0.01977	0.01977	0.01977	0.01880	0.01784
0.02170	0.01977	0.02073	0.01977	0.01977	0.01880	0.01880	0.01784
0.01977	0.02073	0.02073	0.01880	0.01880	0.01880	0.01880	0.01880
0.02073	0.01977	0.01977	0.01977	0.01977	0.01880	0.01880	0.01880
0.02073	0.01880	0.02073	0.01880	0.01977	0.01977	0.01880	0.01880
0.02170	0.01977	0.01977	0.01977	0.01977	0.01880	0.01880	0.01784
0.02073	0.02073	0.02073	0.01977	0.01880	0.01880	0.01880	0.01880
0.02073	0.02073	0.02073	0.01977	0.01880	0.01977	0.01880	0.01880
0.02073	0.01977	0.02073	0.01977	0.01977	0.01880	0.01977	0.01880
0.02073	0.02073	0.02073	0.01880	0.01977	0.01880	0.01880	0.01880
0.02073	0.02073	0.02073	0.01977	0.01977	0.01880	0.01880	0.01880
0.02073	0.02073	0.02073	0.01977	0.01977	0.01784	0.01880	0.01880
0.02073	0.01977	0.02073	0.01977	0.01880	0.01880	0.01880	0.01880
0.02073	0.01977	0.02073	0.01977	0.01977	0.01880	0.01880	0.01880
0.02073	0.01977	0.02073	0.01880	0.02073	0.01880	0.01880	0.01880
0.02170	0.02073	0.01977	0.01977	0.01977	0.01880	0.01880	0.01880
0.02170	0.01977	0.02073	0.01977	0.01977	0.01784	0.01880	0.01784
0.02073	0.01977	0.01977	0.01880	0.01977	0.01880	0.01880	0.01784
0.02170	0.01977	0.01977	0.01977	0.01977	0.01880	0.01880	0.01784
0.02073	0.01977	0.02073	0.01977	0.01977	0.01880	0.01977	0.01784
0.02170	0.01977	0.01977	0.01880	0.01977	0.01880	0.01880	0.01784
0.02073	0.01977	0.02073	0.01977	0.01977	0.01880	0.01880	0.01784
0.02073	0.01977	0.01977	0.01880	0.01977	0.01784	0.01880	0.01784
0.02073	0.01977	0.01880	0.01880	0.01880	0.01880	0.01880	0.01784
0.02073	0.01977	0.01977	0.01977	0.01880	0.01784	0.01977	0.01784
0.02073	0.01977	0.02073	0.01880	0.01977	0.01880	0.01880	0.01784
0.02073	0.02073	0.01977	0.01977	0.01977	0.01880	0.01977	0.01784
0.02073	0.02073	0.01977	0.01880	0.01977	0.01880	0.01784	0.01880
0.02073	0.01977	0.01977	0.01977	0.01977	0.01880	0.01880	0.01880
0.02073	0.02073	0.02073	0.01977	0.01880	0.01880	0.01880	0.01784
0.02073	0.02073	0.02073	0.01977	0.01880	0.01977	0.01880	0.01784
0.02073	0.02073	0.01977	0.01977	0.01880	0.01880	0.01880	0.01784
0.02073	0.02073	0.01977	0.01977	0.01977	0.01880	0.01880	0.01880
0.01977	0.01977	0.01977	0.01977	0.01977	0.01880	0.01977	0.01784
0.02073	0.02073	0.01880	0.01977	0.01977	0.01880	0.01880	0.01784
0.01977	0.02073	0.01977	0.01977	0.01977	0.01977	0.01880	0.01880
0.02073	0.02073	0.01977	0.01977	0.01977	0.01880	0.01880	0.01784
0.02073	0.01977	0.01977	0.01977	0.01977	0.01880	0.01880	0.01784
0.02073	0.01977	0.01977	0.01977	0.01977	0.01880	0.01880	0.01784
0.02073	0.02073	0.01977	0.01977	0.01784	0.01880	0.01880	0.01784
0.02073	0.02073	0.02073	0.01880	0.01977	0.01880	0.01784	0.01784
0.02073	0.01977	0.01977	0.01880	0.01880	0.01880	0.01784	0.01784



*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.01689	0.01689	0.01498	0.01689	0.01498	0.01498	0.01498	0.01593
0.01593	0.01593	0.01593	0.01593	0.01498	0.01498	0.01498	0.01498
0.01689	0.01689	0.01498	0.01498	0.01403	0.01593	0.01403	0.01498
0.01689	0.01689	0.01498	0.01689	0.01593	0.01498	0.01403	0.01498
0.01689	0.01689	0.01689	0.01593	0.01498	0.01498	0.01498	0.01498
0.01593	0.01689	0.01593	0.01689	0.01498	0.01498	0.01498	0.01498
0.01689	0.01689	0.01498	0.01593	0.01498	0.01498	0.01403	0.01498
0.01593	0.01593	0.01498	0.01593	0.01498	0.01593	0.01498	0.01498
0.01593	0.01689	0.01593	0.01593	0.01593	0.01593	0.01498	0.01498
0.01689	0.01689	0.01593	0.01593	0.01498	0.01593	0.01498	0.01498
0.01593	0.01593	0.01593	0.01593	0.01593	0.01498	0.01403	0.01498
0.01689	0.01593	0.01593	0.01498	0.01403	0.01593	0.01498	0.01498
0.01593	0.01593	0.01689	0.01689	0.01593	0.01593	0.01403	0.01498
0.01593	0.01689	0.01593	0.01689	0.01498	0.01498	0.01498	0.01403
0.01593	0.01689	0.01593	0.01593	0.01403	0.01498	0.01403	0.01593
0.01593	0.01689	0.01498	0.01498	0.01498	0.01498	0.01498	0.01498
0.01689	0.01689	0.01593	0.01593	0.01498	0.01498	0.01498	0.01498
0.01689	0.01689	0.01593	0.01593	0.01498	0.01498	0.01498	0.01498
0.01593	0.01593	0.01498	0.01498	0.01498	0.01498	0.01403	0.01403
0.01689	0.01593	0.01689	0.01689	0.01498	0.01593	0.01403	0.01498
0.01593	0.01593	0.01498	0.01593	0.01498	0.01498	0.01403	0.01498
0.01593	0.01593	0.01689	0.01593	0.01498	0.01498	0.01593	0.01498
0.01593	0.01498	0.01498	0.01593	0.01498	0.01498	0.01498	0.01498
0.01593	0.01593	0.01593	0.01498	0.01498	0.01498	0.01403	0.01498
0.01689	0.01593	0.01593	0.01593	0.01498	0.01498	0.01498	0.01498
0.01689	0.01689	0.01498	0.01593	0.01498	0.01498	0.01498	0.01498
0.01689	0.01689	0.01593	0.01498	0.01593	0.01498	0.01498	0.01498
0.01593	0.01593	0.01593	0.01593	0.01593	0.01498	0.01593	0.01593
0.01689	0.01689	0.01593	0.01593	0.01593	0.01498	0.01593	0.01403
0.01593	0.01593	0.01593	0.01593	0.01498	0.01593	0.01498	0.01498
0.01784	0.01498	0.01689	0.01593	0.01498	0.01593	0.01498	0.01403
0.01593	0.01593	0.01498	0.01498	0.01498	0.01498	0.01498	0.01403
0.01689	0.01593	0.01593	0.01593	0.01498	0.01593	0.01498	0.01593
0.01593	0.01593	0.01593	0.01593	0.01498	0.01498	0.01498	0.01498
0.01689	0.01593	0.01593	0.01593	0.01593	0.01498	0.01498	0.01593
0.01689	0.01593	0.01498	0.01593	0.01593	0.01498	0.01498	0.01498
0.01689	0.01498	0.01593	0.01593	0.01689	0.01498	0.01498	0.01498
0.01689	0.01498	0.01593	0.01498	0.01593	0.01498	0.01498	0.01498
0.01593	0.01593	0.01689	0.01498	0.01593	0.01498	0.01498	0.01498
0.01593	0.01498	0.01593	0.01498	0.01593	0.01498	0.01498	0.01498
0.01689	0.01593	0.01593	0.01498	0.01498	0.01498	0.01498	0.01403
0.01593	0.01593	0.01689	0.01498	0.01593	0.01593	0.01403	0.01403
0.01689	0.01593	0.01593	0.01593	0.01593	0.01498	0.01498	0.01403
0.01689	0.01593	0.01593	0.01498	0.01498	0.01689	0.01498	0.01403
0.01689	0.01593	0.01593	0.01593	0.01593	0.01498	0.01593	0.01403
0.01593	0.01593	0.01593	0.01498	0.01593	0.01593	0.01498	0.01403
0.01593	0.01498	0.01593	0.01498	0.01593	0.01498	0.01498	0.01498
0.01498	0.01593	0.01689	0.01498	0.01593	0.01498	0.01498	0.01403







*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.01213	0.01118	0.01118	0.01118	0.01213	0.01024	0.01024	0.01024
0.01213	0.01118	0.01213	0.01024	0.01118	0.01213	0.01024	0.01118
0.01213	0.01118	0.01118	0.01024	0.01118	0.01024	0.01118	0.01024
0.01118	0.01118	0.01213	0.01024	0.01118	0.01024	0.01024	0.01024
0.01213	0.01118	0.01213	0.01118	0.01213	0.01118	0.01118	0.01024
0.01213	0.01024	0.01118	0.01024	0.01213	0.01118	0.01118	0.01118
0.01213	0.01118	0.01213	0.01118	0.01024	0.01118	0.01118	0.01118
0.01118	0.01118	0.01118	0.01024	0.01118	0.01118	0.01118	0.01024
0.01213	0.01118	0.01118	0.01024	0.01118	0.01024	0.01118	0.01024
0.01118	0.01118	0.01213	0.01118	0.01118	0.01118	0.01024	0.01118
0.01213	0.01118	0.01118	0.01118	0.01024	0.01118	0.01118	0.01024
0.01213	0.01024	0.01024	0.01118	0.01213	0.01024	0.01213	0.01118
0.01213	0.01024	0.01118	0.01024	0.01213	0.01024	0.01118	0.01024
0.01118	0.01118	0.01118	0.01118	0.01118	0.01024	0.01118	0.01024
0.01213	0.01024	0.01118	0.01024	0.01308	0.01024	0.01024	0.01024
0.01118	0.01118	0.01118	0.01024	0.01118	0.01024	0.01118	0.00930
0.01118	0.01118	0.01213	0.01118	0.01213	0.01118	0.01118	0.01024
0.01118	0.01024	0.01213	0.01024	0.01213	0.01118	0.01024	0.01024
0.01118	0.01118	0.01118	0.01118	0.01118	0.00930	0.01024	0.01118
0.01118	0.01024	0.01118	0.01024	0.01118	0.01024	0.01024	0.01024
0.01213	0.01118	0.01118	0.01024	0.01024	0.01024	0.01024	0.01024
0.01213	0.01118	0.01213	0.01024	0.01024	0.01024	0.01118	0.01024
0.01213	0.01118	0.01024	0.01024	0.01024	0.01118	0.01024	0.01024
0.01118	0.01118	0.01118	0.01024	0.01118	0.01024	0.01213	0.01024
0.01118	0.01118	0.01213	0.01024	0.01118	0.01118	0.01118	0.01024
0.01118	0.01118	0.01118	0.01118	0.01118	0.01118	0.01118	0.01024
0.01213	0.01118	0.01118	0.01118	0.01118	0.01024	0.01118	0.01024
0.01118	0.01118	0.01118	0.01118	0.01118	0.01024	0.01118	0.01118
0.01118	0.01024	0.01118	0.01118	0.01213	0.01118	0.01118	0.01024
0.01118	0.01118	0.01213	0.01118	0.01213	0.01024	0.01118	0.01024
0.01118	0.01024	0.01118	0.01118	0.01118	0.01118	0.01118	0.01118
0.01213	0.01024	0.01118	0.01024	0.01118	0.01118	0.01118	0.01118
0.01118	0.01213	0.01118	0.01118	0.01024	0.01024	0.01024	0.01024
0.01118	0.01213	0.01024	0.01024	0.01118	0.01118	0.01213	0.01024
0.01118	0.01024	0.01118	0.01118	0.01213	0.01118	0.01024	0.01024
0.01213	0.01118	0.01118	0.01118	0.01024	0.01118	0.01118	0.01024
0.01118	0.01118	0.01118	0.01118	0.01118	0.01118	0.01118	0.01024
0.01213	0.01118	0.01118	0.01118	0.01118	0.01024	0.01118	0.01024
0.01118	0.01024	0.01118	0.01118	0.01024	0.01118	0.01118	0.01024
0.01024	0.01118	0.01118	0.01118	0.01118	0.01118	0.01024	0.01024
0.01118	0.01118	0.01118	0.01118	0.01118	0.01024	0.01118	0.01118
0.01118	0.01213	0.01118	0.01118	0.01024	0.01024	0.01024	0.01024
0.01118	0.01024	0.01118	0.01118	0.01118	0.01118	0.01024	0.01024
0.01024	0.01118	0.01118	0.01118	0.01118	0.01024	0.01118	0.01118
0.01118	0.01118	0.01118	0.01118	0.01213	0.01024	0.01024	0.01024
0.01118	0.01118	0.01118	0.01213	0.01024	0.01118	0.01024	0.01024
0.01118	0.01213	0.01118	0.01118	0.01118	0.01118	0.01118	0.01024

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.01118	0.01024	0.01118	0.01024	0.01024	0.01024	0.00930	0.00930
0.01024	0.01024	0.01024	0.01024	0.01024	0.01118	0.00930	0.01024
0.01024	0.01024	0.01118	0.01024	0.01024	0.01118	0.01024	0.01024
0.01024	0.01024	0.01024	0.01024	0.01024	0.01024	0.01024	0.01024
0.01024	0.01024	0.00930	0.01118	0.01024	0.01024	0.01024	0.01024
0.01118	0.01118	0.01024	0.01024	0.01024	0.01024	0.01024	0.01024
0.01024	0.01024	0.00930	0.01024	0.01024	0.01118	0.01118	0.01024
0.01024	0.01024	0.01118	0.01118	0.01024	0.01118	0.00930	0.01024
0.01118	0.01024	0.01118	0.01024	0.00930	0.01118	0.00930	0.01024
0.01118	0.01118	0.01118	0.01118	0.00930	0.01024	0.01024	0.01024
0.01024	0.01024	0.01024	0.01024	0.01118	0.01118	0.01024	0.01024
0.01118	0.01024	0.01024	0.01024	0.01024	0.00930	0.00930	0.00930
0.01024	0.01118	0.01024	0.01024	0.01118	0.01024	0.01024	0.00930
0.01024	0.01118	0.01118	0.00930	0.01024	0.01024	0.01024	0.01024
0.01118	0.01024	0.01118	0.00930	0.01024	0.01118	0.01118	0.00930
0.00930	0.00930	0.01118	0.01024	0.01118	0.01024	0.01024	0.01118
0.01024	0.01024	0.01024	0.01024	0.01024	0.01024	0.01024	0.00930
0.01118	0.01024	0.01024	0.01024	0.01024	0.01024	0.01024	0.00930
0.01118	0.01024	0.01118	0.01024	0.01024	0.01024	0.01024	0.01024
0.01118	0.01118	0.01118	0.01024	0.01118	0.01024	0.01024	0.01024
0.01118	0.01024	0.01024	0.01024	0.01024	0.01024	0.01024	0.00930
0.01118	0.01024	0.01118	0.00930	0.01118	0.00930	0.01024	0.01024
0.01118	0.01024	0.01118	0.01024	0.01024	0.01024	0.01118	0.00930
0.01024	0.00930	0.01024	0.01024	0.01024	0.01024	0.01024	0.00930
0.01024	0.01024	0.01024	0.01024	0.01024	0.01024	0.01118	0.00930
0.01118	0.01118	0.01118	0.00930	0.01024	0.00930	0.01024	0.00930
0.01024	0.01024	0.01024	0.00930	0.00930	0.00930	0.01024	0.00930
0.00930	0.01024	0.01024	0.01024	0.01024	0.01024	0.01024	0.00930
0.01024	0.01024	0.01024	0.01024	0.01024	0.00930	0.01024	0.01024
0.01118	0.01024	0.01118	0.01024	0.01024	0.01118	0.01024	0.00930
0.01024	0.01024	0.01118	0.00930	0.01118	0.00930	0.01118	0.00930
0.01024	0.00930	0.01024	0.01024	0.01118	0.00930	0.01024	0.01024
0.01118	0.01024	0.01024	0.01024	0.01024	0.01024	0.01024	0.01024
0.01118	0.01024	0.01118	0.01024	0.01024	0.01024	0.01024	0.00930
0.01118	0.01024	0.01024	0.00930	0.01024	0.00930	0.01024	0.00930
0.01118	0.01024	0.01024	0.01024	0.01024	0.01024	0.00930	0.01024
0.01024	0.01024	0.01118	0.01024	0.01024	0.01024	0.01024	0.00930
0.01024	0.01118	0.01118	0.01024	0.01118	0.01024	0.01024	0.00930
0.01118	0.01024	0.01118	0.01024	0.01118	0.01024	0.01024	0.00930
0.01118	0.01118	0.01024	0.01024	0.01118	0.01024	0.01118	0.00836
0.01024	0.01024	0.01118	0.01024	0.01024	0.00930	0.00930	0.00930
0.01118	0.01024	0.01024	0.01024	0.01024	0.01024	0.01024	0.00930
0.01118	0.01024	0.01118	0.01024	0.01024	0.01024	0.01024	0.00930
0.01024	0.01024	0.01024	0.01024	0.01024	0.00930	0.00930	0.01024
0.01213	0.01024	0.01118	0.01024	0.01118	0.00930	0.01024	0.00930
0.01118	0.01024	0.01024	0.01118	0.01118	0.01024	0.01118	0.00930
0.01118	0.01118	0.01118	0.01024	0.01024	0.01024	0.01024	0.00930
0.01024	0.01118	0.01024	0.01024	0.01024	0.00930	0.01024	0.00930





*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.00930	0.00836	0.00836	0.00836	0.00836	0.00930	0.00836	0.00836
0.00836	0.00930	0.00836	0.00930	0.00930	0.00930	0.00836	0.00930
0.00836	0.00930	0.00930	0.00836	0.00930	0.00742	0.00836	0.00930
0.00930	0.00836	0.00836	0.00836	0.00742	0.00836	0.00930	0.00930
0.00836	0.00836	0.00930	0.00930	0.00930	0.00930	0.00742	0.00930
0.00836	0.00836	0.00930	0.00930	0.00930	0.00930	0.00836	0.00836
0.00836	0.00836	0.00836	0.00930	0.00930	0.00742	0.00930	0.00930
0.00930	0.00836	0.00930	0.00836	0.00836	0.00836	0.00836	0.00836
0.00836	0.00836	0.00836	0.00930	0.00836	0.00836	0.00930	0.00930
0.00836	0.00836	0.00930	0.00930	0.00836	0.00836	0.00930	0.00930
0.00930	0.00836	0.00930	0.00836	0.00930	0.00836	0.00836	0.00930
0.00930	0.00836	0.00930	0.00836	0.00836	0.00930	0.00930	0.00930
0.00742	0.00930	0.00930	0.00836	0.00836	0.00836	0.00836	0.00930
0.00930	0.00836	0.00930	0.00930	0.00930	0.00836	0.00930	0.00930
0.00930	0.00930	0.00836	0.00836	0.00836	0.01024	0.00930	0.00836
0.00836	0.00930	0.00930	0.00836	0.00742	0.00930	0.00836	0.00836
0.00836	0.00930	0.00836	0.00836	0.00836	0.00742	0.00930	0.00930
0.00930	0.00930	0.00930	0.00930	0.00930	0.00836	0.00836	0.00930
0.00930	0.00836	0.00930	0.00836	0.00836	0.00836	0.00930	0.00930
0.00836	0.00930	0.00930	0.00930	0.00836	0.00836	0.00930	0.00836
0.00930	0.00836	0.00930	0.00836	0.00742	0.00836	0.00930	0.00836
0.00836	0.00836	0.00930	0.00930	0.00836	0.00836	0.00930	
0.00836	0.00836	0.00930	0.00836	0.00836	0.00930	0.00930	
0.00930	0.00836	0.00930	0.00836	0.00836	0.00930	0.01024	

Date - concentrații egale și egale cu  $5 \cdot 10^{-3}$  M, extincții în unități de curent (mA)

0.00196	0.01090	0.02726	0.05081	0.06878	0.08513	0.09843	0.11596
0.00295	0.01090	0.02726	0.05081	0.06993	0.08513	0.09843	0.11596
0.00393	0.01190	0.02935	0.05191	0.07223	0.08752	0.09843	0.11596
0.00295	0.01291	0.02935	0.05191	0.07223	0.08752	0.10089	0.11724
0.00492	0.01392	0.02935	0.05191	0.07223	0.08632	0.10089	0.11724
0.00492	0.01291	0.03040	0.05302	0.07339	0.08872	0.10213	0.11724
0.00591	0.01392	0.03145	0.05302	0.07455	0.08992	0.10337	0.11596
0.00591	0.01493	0.03145	0.05412	0.07805	0.09233	0.10337	0.11724
0.00790	0.01595	0.03250	0.05746	0.07571	0.09113	0.10461	0.11982
0.00790	0.01696	0.03250	0.05858	0.07688	0.09113	0.10586	0.12111
0.00790	0.01696	0.03356	0.05858	0.07688	0.09233	0.10586	0.11982
0.00890	0.01798	0.03356	0.05970	0.07922	0.09233	0.10586	0.12240
0.00890	0.01900	0.03568	0.05970	0.08040	0.09355	0.10711	0.12111
0.00790	0.02003	0.03674	0.06308	0.08040	0.09476	0.10836	0.12240
0.00890	0.02105	0.03781	0.06195	0.07922	0.09476	0.10836	0.12500
0.00890	0.02003	0.03781	0.06422	0.07922	0.09355	0.10962	0.12500
0.00990	0.02105	0.03995	0.06422	0.07922	0.09598	0.10962	0.12370
0.01090	0.02105	0.04102	0.06535	0.07922	0.09598	0.11088	0.12500
0.01090	0.02414	0.04318	0.06649	0.08040	0.09598	0.11215	0.12631
0.01090	0.02414	0.04426	0.06535	0.08040	0.09720	0.11342	0.12631
0.01090	0.02518	0.04534	0.06763	0.08158	0.09843	0.11342	0.12762
0.00990	0.02414	0.04752	0.06763	0.08276	0.09843	0.11596	0.13026
0.01090	0.02622	0.04862	0.06763	0.08394	0.09843	0.11469	0.12894

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.13158	0.15611	0.17472	0.19571	0.19879	0.20659	0.21294	0.21776
0.13291	0.15471	0.17619	0.19571	0.19879	0.20659	0.21134	0.21615
0.13424	0.15471	0.17766	0.19417	0.19725	0.20817	0.21294	0.21615
0.13424	0.15471	0.17619	0.19265	0.19725	0.20659	0.21134	0.21615
0.13424	0.15471	0.17619	0.19113	0.19725	0.20817	0.21134	0.21615
0.13557	0.15331	0.17619	0.18961	0.19725	0.20817	0.21134	0.21615
0.13557	0.15751	0.17619	0.18961	0.19725	0.20817	0.20975	0.21615
0.13691	0.15892	0.17766	0.19113	0.19725	0.20817	0.21134	0.21615
0.13825	0.16175	0.17766	0.19265	0.19879	0.20817	0.20975	0.21615
0.13825	0.16175	0.17914	0.19417	0.19725	0.20817	0.21294	0.21615
0.13960	0.16175	0.17914	0.19113	0.19879	0.20817	0.21134	0.21615
0.13960	0.16317	0.18062	0.19265	0.20189	0.20975	0.21134	0.21454
0.13825	0.16317	0.18210	0.19265	0.20189	0.21134	0.20975	0.21615
0.13825	0.16317	0.18210	0.19265	0.20189	0.20975	0.21294	0.21615
0.13960	0.16317	0.18210	0.19417	0.20346	0.20817	0.21134	0.21615
0.13960	0.16603	0.18210	0.19417	0.20189	0.20817	0.20975	0.21776
0.13960	0.16603	0.18359	0.19571	0.20034	0.20659	0.21134	0.21776
0.14095	0.16603	0.18359	0.19725	0.20189	0.20659	0.21134	0.21615
0.14095	0.16603	0.18509	0.19571	0.20346	0.20659	0.21134	0.21134
0.14095	0.16603	0.18509	0.19571	0.20346	0.20817	0.21134	0.21294
0.14095	0.16891	0.18659	0.19571	0.20659	0.20975	0.21134	0.21134
0.14231	0.16747	0.18810	0.19571	0.20502	0.20975	0.21134	0.21294
0.14231	0.16747	0.18810	0.19725	0.20346	0.20975	0.20975	0.21294
0.14503	0.16747	0.18961	0.19725	0.20502	0.21134	0.20975	0.21294
0.14231	0.16891	0.18961	0.19571	0.20346	0.21294	0.20817	0.21294
0.14231	0.16747	0.18810	0.19725	0.20346	0.21134	0.20975	0.21294
0.14231	0.16891	0.19113	0.19571	0.20346	0.21294	0.20975	0.21134
0.14231	0.16891	0.19113	0.19879	0.20346	0.21134	0.20975	0.21294
0.14231	0.16891	0.18961	0.20034	0.20346	0.21134	0.21134	0.21294
0.14367	0.16891	0.18961	0.19879	0.20502	0.21294	0.20975	0.21134
0.14367	0.16747	0.18961	0.20034	0.20346	0.21294	0.21294	0.21134
0.14503	0.16747	0.18961	0.20034	0.20346	0.21294	0.21134	0.21134
0.14640	0.16603	0.18961	0.19879	0.20189	0.21134	0.21134	0.21134
0.14503	0.16747	0.18961	0.19879	0.20034	0.21294	0.21134	0.21134
0.14640	0.16747	0.18961	0.19879	0.20346	0.21294	0.21294	0.20975
0.14640	0.16891	0.18961	0.19879	0.20502	0.21134	0.21134	0.21134
0.14778	0.17181	0.19265	0.19879	0.20659	0.21134	0.21134	0.21134
0.14640	0.17181	0.19265	0.20034	0.20659	0.20817	0.20975	0.21454
0.14778	0.17181	0.19265	0.19725	0.20346	0.20502	0.21294	0.21294
0.14778	0.17181	0.19113	0.19879	0.20659	0.20502	0.21454	0.21294
0.14778	0.17181	0.19113	0.19725	0.20817	0.20659	0.21454	0.21615
0.14915	0.17326	0.19265	0.19725	0.20817	0.20659	0.21454	0.21454
0.15053	0.17181	0.19417	0.19725	0.20659	0.20659	0.21615	0.21615
0.15192	0.17181	0.19417	0.19725	0.20659	0.20817	0.21294	0.21615
0.15331	0.17326	0.19571	0.19725	0.20502	0.20975	0.21615	0.21776
0.15331	0.17472	0.19571	0.19879	0.20659	0.20975	0.21776	0.21776
0.15471	0.17326	0.19571	0.19725	0.20817	0.20975	0.21776	0.21615
0.15471	0.17472	0.19571	0.19725	0.20659	0.21134	0.21615	0.21615

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.21615	0.21294	0.21294	0.20659	0.20189	0.19725	0.19417	0.18810
0.21454	0.21294	0.20975	0.20817	0.20346	0.19879	0.19265	0.18659
0.21615	0.21134	0.20975	0.20659	0.20346	0.20034	0.19417	0.18659
0.21615	0.21294	0.20975	0.20817	0.20034	0.20034	0.19417	0.18509
0.21776	0.21294	0.20817	0.20659	0.20346	0.20034	0.19417	0.18810
0.21615	0.21134	0.20975	0.20659	0.20189	0.20189	0.19265	0.18509
0.21938	0.20975	0.20817	0.20659	0.20189	0.20034	0.19265	0.18659
0.21776	0.20975	0.20975	0.20659	0.20034	0.20034	0.19265	0.18509
0.21938	0.21134	0.20975	0.20659	0.20034	0.19879	0.19265	0.18509
0.22100	0.21134	0.20817	0.20502	0.20189	0.19725	0.19113	0.18359
0.21938	0.21134	0.20975	0.20502	0.20346	0.19725	0.19417	0.18509
0.22100	0.21294	0.20975	0.20817	0.20346	0.19725	0.19417	0.18359
0.21776	0.21615	0.20817	0.20659	0.20346	0.19571	0.19417	0.18359
0.21615	0.21294	0.20975	0.20659	0.20346	0.19571	0.19113	0.18359
0.21615	0.21454	0.20975	0.20659	0.20502	0.19571	0.19265	0.18359
0.21938	0.21294	0.20817	0.20659	0.20502	0.19571	0.18961	0.18509
0.21938	0.21134	0.20975	0.20659	0.20346	0.19265	0.19113	0.18359
0.21938	0.21134	0.20817	0.20659	0.20346	0.19417	0.19113	0.18359
0.21938	0.20975	0.20975	0.20659	0.20189	0.19113	0.19113	0.18359
0.21938	0.20975	0.20975	0.20659	0.20034	0.19113	0.19113	0.18509
0.21615	0.20975	0.20975	0.20817	0.19879	0.19265	0.19113	0.18359
0.21615	0.20975	0.20975	0.20659	0.20034	0.19417	0.19113	0.18359
0.21454	0.20817	0.21134	0.20817	0.20034	0.19417	0.19113	0.18359
0.21454	0.20975	0.21134	0.20817	0.20034	0.19417	0.19265	0.18359
0.21454	0.20975	0.21134	0.20659	0.20034	0.19571	0.19113	0.18210
0.21454	0.21134	0.20975	0.20817	0.20034	0.19417	0.18961	0.18210
0.21454	0.20975	0.20975	0.20817	0.20189	0.19417	0.18961	0.18210
0.21454	0.20817	0.20975	0.20817	0.20346	0.19417	0.18961	0.18062
0.21454	0.20975	0.20817	0.20659	0.20346	0.19417	0.18961	0.18062
0.21615	0.20975	0.21134	0.20817	0.20502	0.19417	0.18810	0.18062
0.21454	0.20975	0.21134	0.20659	0.20502	0.19571	0.18810	0.18210
0.21294	0.20817	0.21294	0.20659	0.20502	0.19571	0.18509	0.17914
0.21134	0.20975	0.21294	0.20659	0.20659	0.19571	0.18810	0.18210
0.21134	0.20975	0.21134	0.20502	0.20502	0.19571	0.18810	0.18062
0.20975	0.20975	0.21134	0.20502	0.20346	0.19571	0.18810	0.17914
0.21294	0.20975	0.21134	0.20659	0.20659	0.19571	0.18961	0.18062
0.21294	0.20975	0.21294	0.20502	0.20502	0.19725	0.18961	0.17914
0.21294	0.20817	0.21134	0.20346	0.20346	0.19725	0.18961	0.18062
0.21294	0.20975	0.20975	0.20189	0.20346	0.19571	0.18810	0.17914
0.21454	0.21294	0.20975	0.20346	0.20189	0.19571	0.18810	0.17914
0.21294	0.21294	0.20975	0.20346	0.20346	0.19571	0.18961	0.17914
0.21294	0.21294	0.20975	0.20346	0.20034	0.19417	0.18961	0.17914
0.21454	0.21134	0.20817	0.20346	0.19879	0.19571	0.18810	0.17914
0.21294	0.21134	0.20817	0.20346	0.19879	0.19417	0.18810	0.17914
0.21294	0.21294	0.20659	0.20189	0.19571	0.19571	0.18810	0.17914
0.21454	0.21134	0.20817	0.20189	0.19725	0.19417	0.18810	0.17914
0.21454	0.21134	0.20659	0.20346	0.19417	0.19417	0.18659	0.17914
0.21454	0.21134	0.20659	0.20189	0.19571	0.19417	0.18810	0.17914

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.17914	0.16891	0.15053	0.12500	0.09843	0.08632	0.07455	0.06763
0.17766	0.17036	0.15192	0.12500	0.09843	0.08632	0.07223	0.06763
0.17766	0.17036	0.15053	0.12370	0.09720	0.08513	0.07455	0.06649
0.17766	0.17036	0.15053	0.12370	0.09720	0.08632	0.07339	0.06649
0.17766	0.16891	0.15053	0.12240	0.09598	0.08513	0.07223	0.06763
0.17766	0.17036	0.14915	0.12240	0.09720	0.08513	0.07223	0.06649
0.17766	0.17036	0.15053	0.12240	0.09598	0.08513	0.07339	0.06649
0.17914	0.17036	0.14915	0.12111	0.09720	0.08513	0.07223	0.06649
0.17619	0.16891	0.14778	0.12111	0.09598	0.08513	0.07223	0.06649
0.17766	0.16891	0.14778	0.11982	0.09476	0.08394	0.07339	0.06535
0.17766	0.16891	0.14778	0.11982	0.09476	0.08513	0.07223	0.06535
0.17766	0.17036	0.14778	0.11853	0.09476	0.08394	0.07223	0.06535
0.17619	0.16891	0.14503	0.11724	0.09598	0.08276	0.07223	0.06535
0.17766	0.16747	0.14640	0.11724	0.09476	0.08394	0.07223	0.06535
0.17619	0.16747	0.14503	0.11724	0.09476	0.08276	0.07223	0.06422
0.17472	0.16747	0.14503	0.11596	0.09355	0.08276	0.07108	0.06535
0.17619	0.16747	0.14367	0.11596	0.09355	0.08158	0.07108	0.06535
0.17472	0.16747	0.14231	0.11469	0.09355	0.08276	0.07108	0.06535
0.17619	0.16747	0.14231	0.11469	0.09233	0.08040	0.07223	0.06535
0.17326	0.16603	0.14231	0.11342	0.09233	0.08040	0.06993	0.06535
0.17472	0.16603	0.14095	0.11342	0.09233	0.08158	0.06993	0.06422
0.17326	0.16460	0.14095	0.11342	0.09233	0.08158	0.06993	0.06422
0.17766	0.16460	0.14095	0.11215	0.09113	0.07922	0.06993	0.06422
0.17472	0.16460	0.14095	0.11088	0.09113	0.07922	0.07108	0.06422
0.17619	0.16460	0.13960	0.11088	0.09113	0.07922	0.06993	0.06422
0.17619	0.16317	0.13825	0.10962	0.09233	0.08040	0.06993	0.06422
0.17472	0.16317	0.13960	0.11088	0.09233	0.08040	0.06993	0.06422
0.17619	0.16175	0.13825	0.10836	0.09113	0.08040	0.06993	0.06422
0.17472	0.16033	0.13825	0.10836	0.09113	0.07922	0.06993	0.06422
0.17472	0.16033	0.13691	0.10711	0.09113	0.07805	0.06993	0.06422
0.17619	0.16033	0.13691	0.10711	0.08992	0.07922	0.06763	0.06308
0.17472	0.16033	0.13557	0.10711	0.08992	0.07805	0.06993	0.06308
0.17326	0.15892	0.13557	0.10711	0.08992	0.07805	0.06878	0.06308
0.17472	0.15892	0.13424	0.10586	0.08872	0.07805	0.06878	0.06308
0.17181	0.15892	0.13424	0.10586	0.08872	0.07688	0.06993	0.06308
0.17326	0.15611	0.13291	0.10461	0.08872	0.07571	0.06878	0.06308
0.17326	0.15611	0.13158	0.10461	0.08992	0.07688	0.06878	0.06083
0.17036	0.15611	0.13291	0.10337	0.08872	0.07571	0.06878	0.06195
0.17181	0.15471	0.13291	0.10337	0.08872	0.07571	0.06878	0.06195
0.17181	0.15611	0.13026	0.10213	0.08872	0.07571	0.06763	0.06083
0.17181	0.15471	0.13158	0.10213	0.08752	0.07571	0.06993	0.06083
0.17181	0.15471	0.13026	0.10213	0.08872	0.07571	0.06763	0.06083
0.17181	0.15611	0.13026	0.10089	0.08872	0.07455	0.06878	0.06083
0.17181	0.15331	0.12894	0.09966	0.08752	0.07571	0.06878	0.06083
0.17181	0.15331	0.12762	0.09843	0.08752	0.07455	0.06763	0.06195
0.17181	0.15192	0.12894	0.09966	0.08752	0.07455	0.06763	0.06083
0.17036	0.15471	0.12631	0.09966	0.08632	0.07339	0.06878	0.06195
0.16891	0.15331	0.12631	0.09843	0.08752	0.07339	0.06649	0.06083

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.06083	0.05635	0.04971	0.04643	0.04318	0.03995	0.03674	0.03674
0.06083	0.05523	0.04862	0.04643	0.04210	0.03995	0.03781	0.03674
0.06083	0.05635	0.04971	0.04643	0.04210	0.04102	0.03674	0.03568
0.06083	0.05635	0.04862	0.04752	0.04318	0.04102	0.03674	0.03568
0.06083	0.05523	0.04971	0.04643	0.04210	0.04102	0.03674	0.03674
0.05970	0.05412	0.04971	0.04534	0.04210	0.03888	0.03674	0.03674
0.05970	0.05523	0.04971	0.04534	0.04210	0.03995	0.03781	0.03674
0.05970	0.05523	0.04971	0.04643	0.04210	0.04102	0.03781	0.03674
0.05970	0.05523	0.04971	0.04534	0.04210	0.03995	0.03781	0.03674
0.05970	0.05412	0.04862	0.04534	0.04210	0.04102	0.03781	0.03674
0.05970	0.05523	0.04862	0.04534	0.04210	0.04102	0.03781	0.03674
0.05970	0.05523	0.04862	0.04534	0.04210	0.03995	0.03674	0.03674
0.05970	0.05412	0.04862	0.04534	0.04210	0.04102	0.03781	0.03674
0.05970	0.05523	0.04862	0.04534	0.04210	0.03995	0.03674	0.03462
0.05858	0.05302	0.04862	0.04534	0.04102	0.03995	0.03674	0.03568
0.05746	0.05412	0.04862	0.04534	0.04210	0.03995	0.03781	0.03674
0.05970	0.05412	0.04862	0.04534	0.04210	0.03995	0.03781	0.03674
0.05970	0.05412	0.04862	0.04643	0.04102	0.03995	0.03674	0.03674
0.05858	0.05412	0.04862	0.04426	0.04210	0.03888	0.03781	0.03568
0.05858	0.05412	0.04752	0.04534	0.04210	0.03888	0.03781	0.03674
0.05858	0.05302	0.04752	0.04426	0.04102	0.03888	0.03674	0.03674
0.05858	0.05412	0.04752	0.04534	0.04210	0.03995	0.03781	0.03568
0.05858	0.05191	0.04752	0.04534	0.04102	0.03888	0.03781	0.03568
0.05858	0.05302	0.04752	0.04534	0.04210	0.03995	0.03781	0.03568
0.05746	0.05302	0.04752	0.04426	0.04102	0.03888	0.03674	0.03568
0.05858	0.05302	0.04752	0.04426	0.04102	0.03995	0.03674	0.03568
0.05746	0.05302	0.04752	0.04426	0.04102	0.03888	0.03674	0.03674
0.05858	0.05302	0.04752	0.04318	0.04102	0.03995	0.03674	0.03568
0.05746	0.05302	0.04752	0.04426	0.03995	0.03888	0.03674	0.03568
0.05746	0.05191	0.04752	0.04534	0.04102	0.03888	0.03674	0.03462
0.05746	0.05191	0.04752	0.04426	0.04102	0.03888	0.03674	0.03568
0.05746	0.05191	0.04752	0.04426	0.04102	0.03888	0.03674	0.03674
0.05746	0.05191	0.04643	0.04426	0.04102	0.03888	0.03781	0.03568
0.05746	0.05191	0.04752	0.04318	0.03995	0.03888	0.03674	0.03568
0.05746	0.05081	0.04643	0.04426	0.04102	0.03781	0.03781	0.03462
0.05635	0.05191	0.04643	0.04318	0.04102	0.03888	0.03568	0.03568
0.05635	0.05081	0.04752	0.04426	0.04102	0.03888	0.03568	0.03674
0.05635	0.05081	0.04643	0.04426	0.04102	0.03888	0.03674	0.03674
0.05746	0.05081	0.04643	0.04318	0.03995	0.03781	0.03674	0.03568
0.05635	0.05081	0.04643	0.04426	0.04102	0.03995	0.03568	0.03674
0.05635	0.05081	0.04534	0.04318	0.04102	0.03888	0.03674	0.03674
0.05523	0.05191	0.04643	0.04318	0.04102	0.03888	0.03674	0.03568
0.05523	0.05081	0.04643	0.04210	0.04102	0.03888	0.03568	0.03462
0.05635	0.05081	0.04643	0.04426	0.03995	0.03888	0.03674	0.03674
0.05635	0.05081	0.04643	0.04318	0.04102	0.03781	0.03674	0.03674
0.05635	0.05081	0.04643	0.04318	0.03888	0.03781	0.03674	0.03462
0.05523	0.04971	0.04643	0.04210	0.04102	0.03888	0.03674	0.03462
0.05523	0.04971	0.04643	0.04318	0.04102	0.03781	0.03568	0.03568

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.03568	0.03356	0.03356	0.03250	0.03145	0.03040	0.02935	0.02935
0.03568	0.03356	0.03356	0.03356	0.03145	0.03040	0.03040	0.02935
0.03568	0.03462	0.03356	0.03145	0.03040	0.02935	0.02935	0.02830
0.03462	0.03356	0.03356	0.03250	0.03250	0.03040	0.03040	0.02935
0.03462	0.03356	0.03356	0.03145	0.03145	0.03040	0.02935	0.02935
0.03462	0.03462	0.03250	0.03250	0.03145	0.03145	0.02935	0.02935
0.03568	0.03462	0.03250	0.03250	0.03250	0.03040	0.02935	0.02935
0.03462	0.03462	0.03356	0.03250	0.03145	0.03040	0.02935	0.02935
0.03462	0.03356	0.03356	0.03250	0.03145	0.03040	0.03040	0.02935
0.03568	0.03462	0.03250	0.03040	0.03250	0.02935	0.03040	0.02935
0.03568	0.03462	0.03356	0.03250	0.03040	0.03040	0.03040	0.02935
0.03462	0.03462	0.03356	0.03145	0.03145	0.03040	0.02935	0.02830
0.03568	0.03462	0.03250	0.03250	0.03145	0.03040	0.02935	0.02935
0.03462	0.03356	0.03356	0.03145	0.03145	0.03040	0.03040	0.02935
0.03462	0.03462	0.03250	0.03250	0.03040	0.03040	0.02935	0.02935
0.03462	0.03356	0.03356	0.03250	0.03040	0.03040	0.02935	0.02830
0.03462	0.03462	0.03250	0.03250	0.03145	0.03040	0.02935	0.02830
0.03462	0.03356	0.03250	0.03250	0.03040	0.03040	0.02935	0.02830
0.03462	0.03462	0.03356	0.03145	0.03040	0.03040	0.02935	0.02830
0.03462	0.03356	0.03250	0.03250	0.03040	0.03040	0.03040	0.02830
0.03462	0.03356	0.03250	0.03145	0.03145	0.03040	0.02935	0.02830
0.03462	0.03356	0.03356	0.03250	0.03040	0.03040	0.02935	0.02830
0.03356	0.03356	0.03356	0.03250	0.03040	0.03040	0.02935	0.02935
0.03462	0.03462	0.03250	0.03250	0.03145	0.03040	0.02935	0.02935
0.03462	0.03462	0.03250	0.03250	0.03040	0.03040	0.02935	0.02935
0.03462	0.03462	0.03250	0.03250	0.03040	0.03040	0.02935	0.02830
0.03462	0.03356	0.03250	0.03145	0.03040	0.03040	0.02935	0.02830
0.03356	0.03356	0.03250	0.03145	0.03040	0.03040	0.02830	0.02935
0.03462	0.03356	0.03356	0.03145	0.03040	0.03040	0.02935	0.02935
0.03356	0.03356	0.03250	0.03250	0.03040	0.03040	0.02935	0.02935
0.03462	0.03462	0.03250	0.03250	0.03145	0.03040	0.02935	0.02830
0.03356	0.03356	0.03356	0.03250	0.03040	0.03040	0.02935	0.02830
0.03462	0.03356	0.03250	0.03250	0.03040	0.03040	0.02935	0.02830
0.03462	0.03462	0.03250	0.03250	0.03040	0.03040	0.02935	0.02726
0.03462	0.03462	0.03250	0.03145	0.03040	0.02935	0.02935	0.02935
0.03356	0.03356	0.03250	0.03250	0.03040	0.03040	0.02830	0.02935
0.03462	0.03356	0.03250	0.03145	0.03040	0.02935	0.02935	0.02830
0.03462	0.03356	0.03250	0.03145	0.03040	0.03040	0.02935	0.02935
0.03462	0.03356	0.03250	0.03250	0.03040	0.03040	0.02935	0.02935
0.03356	0.03356	0.03250	0.03145	0.03040	0.03040	0.02935	0.02830
0.03462	0.03356	0.03250	0.03250	0.03040	0.03040	0.02935	0.02830
0.03462	0.03356	0.03250	0.03250	0.03040	0.03040	0.02935	0.02830
0.03356	0.03356	0.03145	0.03250	0.03040	0.03040	0.02935	0.02830
0.03462	0.03356	0.03250	0.03145	0.03040	0.02935	0.02935	0.02830
0.03356	0.03356	0.03250	0.03250	0.03040	0.03040	0.02935	0.02830
0.03462	0.03356	0.03250	0.03250	0.02935	0.03040	0.02935	0.02830
0.03462	0.03356	0.03145	0.03250	0.03040	0.02935	0.02830	0.02935
0.03356	0.03356	0.03250	0.03145	0.03040	0.03040	0.02830	0.02726
0.03356	0.03250	0.03250	0.03145	0.03040	0.02935	0.02935	0.02935

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.02935	0.02726	0.02726	0.02518	0.02622	0.02518	0.02518	0.02414
0.02830	0.02726	0.02622	0.02622	0.02518	0.02518	0.02518	0.02414
0.02830	0.02726	0.02622	0.02622	0.02622	0.02518	0.02414	0.02311
0.02830	0.02726	0.02622	0.02622	0.02518	0.02414	0.02518	0.02311
0.02830	0.02726	0.02622	0.02518	0.02518	0.02414	0.02414	0.02311
0.02830	0.02830	0.02726	0.02414	0.02622	0.02518	0.02518	0.02518
0.02830	0.02726	0.02622	0.02518	0.02518	0.02518	0.02518	0.02414
0.02830	0.02726	0.02726	0.02518	0.02518	0.02414	0.02518	0.02311
0.02830	0.02622	0.02726	0.02622	0.02518	0.02518	0.02518	0.02414
0.02935	0.02726	0.02622	0.02518	0.02622	0.02414	0.02414	0.02414
0.02935	0.02830	0.02622	0.02622	0.02518	0.02518	0.02414	0.02414
0.02726	0.02726	0.02726	0.02518	0.02622	0.02518	0.02518	0.02311
0.02830	0.02726	0.02622	0.02622	0.02622	0.02518	0.02518	0.02414
0.02830	0.02726	0.02622	0.02726	0.02622	0.02518	0.02518	0.02414
0.02726	0.02726	0.02622	0.02622	0.02622	0.02518	0.02414	0.02414
0.02830	0.02726	0.02622	0.02518	0.02518	0.02518	0.02518	0.02414
0.02726	0.02622	0.02622	0.02622	0.02622	0.02414	0.02414	0.02414
0.02830	0.02726	0.02622	0.02622	0.02518	0.02414	0.02414	0.02311
0.02726	0.02726	0.02726	0.02518	0.02622	0.02518	0.02414	0.02311
0.02726	0.02622	0.02622	0.02622	0.02622	0.02518	0.02414	0.02414
0.02726	0.02830	0.02622	0.02622	0.02518	0.02414	0.02414	0.02414
0.02726	0.02726	0.02622	0.02622	0.02622	0.02518	0.02414	0.02311
0.02726	0.02726	0.02622	0.02518	0.02518	0.02518	0.02311	0.02414
0.02622	0.02726	0.02622	0.02518	0.02622	0.02518	0.02414	0.02311
0.02726	0.02622	0.02622	0.02622	0.02518	0.02518	0.02414	0.02414
0.02830	0.02726	0.02622	0.02622	0.02518	0.02414	0.02414	0.02414
0.02830	0.02726	0.02726	0.02622	0.02518	0.02518	0.02414	0.02414
0.02726	0.02622	0.02622	0.02518	0.02622	0.02518	0.02518	0.02414
0.02726	0.02726	0.02622	0.02622	0.02622	0.02518	0.02414	0.02414
0.02726	0.02726	0.02622	0.02622	0.02622	0.02518	0.02414	0.02414
0.02830	0.02726	0.02622	0.02622	0.02518	0.02414	0.02414	0.02311
0.02830	0.02726	0.02622	0.02622	0.02414	0.02518	0.02414	0.02311
0.02726	0.02726	0.02518	0.02622	0.02414	0.02414	0.02414	0.02311
0.02726	0.02726	0.02622	0.02622	0.02518	0.02518	0.02518	0.02311
0.02830	0.02830	0.02622	0.02518	0.02518	0.02414	0.02518	0.02311
0.02726	0.02726	0.02726	0.02518	0.02414	0.02518	0.02414	0.02414
0.02726	0.02726	0.02622	0.02518	0.02414	0.02518	0.02311	0.02414
0.02726	0.02726	0.02622	0.02622	0.02518	0.02518	0.02414	0.02311
0.02726	0.02726	0.02622	0.02622	0.02518	0.02518	0.02414	0.02518
0.02726	0.02726	0.02622	0.02622	0.02518	0.02518	0.02414	0.02414
0.02726	0.02622	0.02518	0.02622	0.02622	0.02518	0.02311	0.02414
0.02726	0.02726	0.02518	0.02622	0.02518	0.02518	0.02414	0.02414
0.02830	0.02622	0.02622	0.02518	0.02518	0.02518	0.02414	0.02414
0.02830	0.02622	0.02622	0.02518	0.02414	0.02414	0.02414	0.02414
0.02726	0.02622	0.02622	0.02622	0.02518	0.02518	0.02518	0.02518
0.02726	0.02726	0.02518	0.02622	0.02518	0.02518	0.02414	0.02414
0.02726	0.02726	0.02622	0.02622	0.02518	0.02518	0.02311	0.02414
0.02726	0.02726	0.02518	0.02622	0.02414	0.02518	0.02414	0.02518

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.02414	0.02208	0.02208	0.02311	0.02208	0.02208	0.02105	0.02105
0.02414	0.02414	0.02208	0.02208	0.02208	0.02208	0.02105	0.02105
0.02414	0.02311	0.02311	0.02208	0.02105	0.02208	0.02003	0.02105
0.02414	0.02311	0.02311	0.02208	0.02208	0.02208	0.02105	0.02105
0.02311	0.02311	0.02311	0.02208	0.02208	0.02105	0.02105	0.02105
0.02311	0.02311	0.02414	0.02208	0.02208	0.02208	0.02105	0.02105
0.02311	0.02208	0.02311	0.02208	0.02105	0.02105	0.02003	0.02208
0.02414	0.02311	0.02311	0.02208	0.02311	0.02208	0.02105	0.02105
0.02311	0.02208	0.02311	0.02105	0.02105	0.02105	0.02003	0.02105
0.02414	0.02208	0.02311	0.02208	0.02208	0.02208	0.02105	0.02105
0.02311	0.02208	0.02311	0.02208	0.02105	0.02208	0.02003	0.02105
0.02311	0.02208	0.02311	0.02208	0.02105	0.02208	0.02105	0.02208
0.02414	0.02311	0.02208	0.02208	0.02105	0.02208	0.02003	0.02105
0.02414	0.02311	0.02311	0.02208	0.02208	0.02105	0.02105	0.02105
0.02311	0.02208	0.02208	0.02208	0.02208	0.02105	0.02105	0.02105
0.02414	0.02208	0.02208	0.02208	0.02208	0.02208	0.02003	0.02105
0.02311	0.02208	0.02105	0.02208	0.02105	0.02208	0.02105	0.02003
0.02414	0.02311	0.02208	0.02208	0.02208	0.02105	0.02105	0.02105
0.02311	0.02311	0.02414	0.02208	0.02208	0.02105	0.02208	0.02105
0.02311	0.02105	0.02311	0.02208	0.02208	0.02208	0.02105	0.02105
0.02311	0.02311	0.02311	0.02208	0.02208	0.02208	0.02003	0.02105
0.02414	0.02208	0.02414	0.02105	0.02311	0.02208	0.02105	0.02208
0.02311	0.02208	0.02208	0.02208	0.02105	0.02105	0.02105	0.02105
0.02311	0.02208	0.02311	0.02105	0.02311	0.02105	0.02105	0.02208
0.02311	0.02311	0.02208	0.02208	0.02208	0.02105	0.02105	0.02105
0.02311	0.02208	0.02208	0.02105	0.02311	0.02105	0.02105	0.02105
0.02208	0.02311	0.02311	0.02208	0.02208	0.02208	0.02105	0.02003
0.02311	0.02208	0.02208	0.02208	0.02208	0.02105	0.02105	0.02105
0.02311	0.02311	0.02208	0.02208	0.02208	0.02105	0.02208	0.02105
0.02311	0.02311	0.02414	0.02208	0.02208	0.02105	0.02105	0.02105
0.02311	0.02311	0.02311	0.02208	0.02105	0.02105	0.02003	0.02105
0.02311	0.02208	0.02311	0.02208	0.02208	0.02105	0.02105	0.02003
0.02208	0.02414	0.02311	0.02105	0.02208	0.02105	0.02105	0.02105
0.02311	0.02208	0.02208	0.02105	0.02105	0.02105	0.02105	0.02003
0.02414	0.02208	0.02208	0.02208	0.02105	0.02105	0.02208	0.02105
0.02311	0.02208	0.02208	0.02208	0.02208	0.02105	0.02105	0.02105
0.02414	0.02414	0.02208	0.02208	0.02208	0.02105	0.02105	0.02003
0.02414	0.02311	0.02208	0.02105	0.02208	0.02105	0.02105	0.02003
0.02208	0.02208	0.02208	0.02208	0.02208	0.02105	0.02105	
0.02208	0.02208	0.02208	0.02208	0.02208	0.02105	0.02208	
0.02311	0.02208	0.02208	0.02105	0.02105	0.02003	0.02105	
0.02311	0.02311	0.02208	0.02105	0.02105	0.02105	0.02105	
0.02311	0.02208	0.02208	0.02105	0.02105	0.02208	0.02208	

Date - concentrații egale și egale cu  $10 \cdot 10^{-3}$  M, extincții în unități de curent (mA)

0.009	0.016	0.021	0.028	0.039	0.046	0.062	0.087	0.108	0.136
0.014	0.016	0.023	0.028	0.041	0.049	0.065	0.096	0.117	0.142
0.011	0.016	0.026	0.031	0.044	0.051	0.068	0.102	0.126	0.149
0.011	0.018	0.026	0.036	0.041	0.054	0.076	0.105	0.129	0.155

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.159	0.401	0.515	0.628	0.609	0.590	0.555	0.564	0.572	0.572
0.155	0.401	0.507	0.628	0.599	0.572	0.564	0.572	0.581	0.581
0.165	0.407	0.523	0.609	0.609	0.572	0.564	0.581	0.590	0.564
0.172	0.407	0.531	0.609	0.618	0.572	0.564	0.581	0.590	0.564
0.183	0.419	0.539	0.618	0.609	0.572	0.564	0.581	0.590	0.564
0.183	0.413	0.539	0.628	0.609	0.581	0.564	0.581	0.590	0.564
0.194	0.419	0.539	0.628	0.599	0.572	0.564	0.590	0.581	0.564
0.194	0.419	0.547	0.609	0.599	0.564	0.564	0.590	0.572	0.564
0.197	0.425	0.555	0.628	0.599	0.572	0.564	0.581	0.581	0.555
0.205	0.425	0.555	0.618	0.599	0.572	0.564	0.581	0.590	0.564
0.213	0.425	0.555	0.609	0.581	0.581	0.564	0.590	0.572	0.564
0.216	0.431	0.564	0.618	0.590	0.555	0.564	0.581	0.581	0.564
0.224	0.425	0.572	0.618	0.590	0.572	0.564	0.590	0.572	0.572
0.224	0.431	0.581	0.609	0.590	0.572	0.555	0.590	0.572	0.564
0.228	0.438	0.581	0.618	0.590	0.572	0.555	0.581	0.572	0.564
0.236	0.438	0.581	0.618	0.581	0.581	0.564	0.581	0.581	0.564
0.240	0.438	0.590	0.609	0.590	0.581	0.555	0.581	0.572	0.572
0.248	0.438	0.590	0.618	0.599	0.581	0.555	0.572	0.572	0.572
0.257	0.431	0.599	0.609	0.599	0.581	0.564	0.590	0.564	0.564
0.261	0.438	0.609	0.609	0.609	0.590	0.572	0.581	0.564	0.564
0.265	0.438	0.609	0.609	0.609	0.572	0.564	0.581	0.572	0.564
0.274	0.444	0.599	0.609	0.599	0.581	0.572	0.572	0.555	0.564
0.278	0.444	0.609	0.609	0.599	0.572	0.572	0.581	0.572	0.564
0.287	0.444	0.609	0.599	0.599	0.590	0.572	0.581	0.572	0.572
0.292	0.444	0.599	0.609	0.590	0.564	0.581	0.572	0.564	0.572
0.297	0.451	0.609	0.599	0.599	0.564	0.581	0.572	0.572	0.572
0.297	0.451	0.609	0.599	0.599	0.555	0.572	0.572	0.572	0.564
0.301	0.451	0.609	0.599	0.590	0.564	0.564	0.572	0.572	0.572
0.306	0.451	0.609	0.609	0.599	0.555	0.572	0.572	0.572	0.564
0.311	0.451	0.609	0.599	0.590	0.564	0.581	0.572	0.572	0.564
0.320	0.451	0.609	0.609	0.590	0.564	0.572	0.564	0.564	0.564
0.330	0.451	0.609	0.609	0.581	0.564	0.572	0.555	0.572	0.555
0.330	0.464	0.609	0.590	0.581	0.564	0.572	0.572	0.555	0.572
0.340	0.464	0.618	0.599	0.590	0.555	0.572	0.572	0.564	0.572
0.335	0.464	0.609	0.599	0.590	0.564	0.572	0.572	0.555	0.572
0.335	0.471	0.609	0.590	0.590	0.564	0.572	0.581	0.564	0.564
0.346	0.464	0.628	0.590	0.590	0.564	0.581	0.564	0.564	0.564
0.346	0.471	0.628	0.599	0.581	0.572	0.572	0.564	0.572	0.564
0.356	0.478	0.618	0.581	0.581	0.572	0.572	0.564	0.572	0.564
0.361	0.471	0.628	0.599	0.581	0.555	0.572	0.564	0.572	0.555
0.367	0.478	0.618	0.599	0.581	0.564	0.564	0.572	0.572	0.564
0.372	0.485	0.618	0.599	0.590	0.564	0.564	0.572	0.581	0.564
0.384	0.492	0.628	0.599	0.590	0.564	0.572	0.581	0.581	0.564
0.389	0.485	0.609	0.599	0.581	0.564	0.581	0.581	0.590	0.564
0.389	0.485	0.618	0.590	0.572	0.555	0.581	0.590	0.581	0.564
0.395	0.500	0.628	0.599	0.581	0.555	0.572	0.581	0.581	0.555
0.395	0.507	0.618	0.599	0.581	0.547	0.572	0.590	0.572	0.555
0.407	0.500	0.618	0.590	0.581	0.555	0.572	0.581	0.572	0.547

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.547	0.547	0.515	0.500	0.478	0.438	0.425	0.401	0.340	0.205
0.547	0.539	0.507	0.507	0.471	0.438	0.425	0.401	0.335	0.197
0.555	0.539	0.515	0.500	0.471	0.438	0.425	0.407	0.335	0.197
0.555	0.539	0.515	0.485	0.471	0.438	0.425	0.401	0.325	0.197
0.555	0.547	0.515	0.485	0.471	0.438	0.425	0.407	0.330	0.194
0.555	0.539	0.507	0.500	0.471	0.438	0.419	0.407	0.325	0.194
0.547	0.539	0.507	0.492	0.471	0.438	0.419	0.395	0.320	0.190
0.547	0.539	0.515	0.507	0.471	0.431	0.425	0.401	0.325	0.187
0.555	0.539	0.515	0.507	0.471	0.431	0.425	0.401	0.316	0.187
0.547	0.539	0.515	0.500	0.464	0.431	0.425	0.401	0.311	0.183
0.555	0.539	0.507	0.500	0.464	0.431	0.425	0.401	0.311	0.179
0.555	0.531	0.507	0.500	0.464	0.431	0.425	0.395	0.311	0.176
0.547	0.531	0.507	0.492	0.464	0.431	0.419	0.395	0.301	0.176
0.555	0.531	0.515	0.492	0.458	0.431	0.419	0.395	0.301	0.176
0.564	0.531	0.515	0.492	0.458	0.431	0.419	0.395	0.297	0.172
0.555	0.531	0.515	0.485	0.458	0.425	0.419	0.395	0.292	0.169
0.564	0.531	0.515	0.500	0.458	0.425	0.425	0.395	0.287	0.169
0.555	0.539	0.515	0.492	0.464	0.425	0.425	0.389	0.287	0.169
0.572	0.539	0.515	0.492	0.464	0.425	0.419	0.389	0.287	0.165
0.572	0.547	0.523	0.500	0.464	0.425	0.419	0.389	0.283	0.162
0.572	0.531	0.515	0.492	0.458	0.425	0.419	0.384	0.274	0.162
0.564	0.531	0.515	0.492	0.464	0.425	0.419	0.389	0.270	0.155
0.564	0.539	0.523	0.471	0.451	0.419	0.419	0.384	0.270	0.159
0.564	0.531	0.515	0.485	0.464	0.419	0.413	0.384	0.265	0.152
0.572	0.531	0.515	0.478	0.458	0.419	0.419	0.384	0.265	0.155
0.572	0.531	0.515	0.478	0.464	0.419	0.413	0.384	0.261	0.152
0.572	0.523	0.515	0.485	0.464	0.419	0.407	0.384	0.253	0.149
0.555	0.523	0.500	0.478	0.458	0.419	0.407	0.389	0.253	0.152
0.564	0.523	0.515	0.478	0.458	0.419	0.407	0.384	0.244	0.149
0.555	0.515	0.515	0.485	0.458	0.419	0.413	0.384	0.248	0.149
0.555	0.515	0.515	0.485	0.451	0.419	0.407	0.378	0.240	0.145
0.555	0.523	0.507	0.492	0.451	0.419	0.407	0.378	0.240	0.145
0.555	0.515	0.500	0.485	0.451	0.419	0.407	0.372	0.236	0.145
0.547	0.523	0.500	0.492	0.451	0.413	0.413	0.372	0.236	0.142
0.547	0.523	0.500	0.485	0.451	0.413	0.407	0.372	0.232	0.142
0.547	0.523	0.492	0.492	0.451	0.419	0.407	0.372	0.232	0.142
0.547	0.515	0.492	0.485	0.444	0.413	0.407	0.367	0.232	0.139
0.539	0.523	0.492	0.478	0.451	0.419	0.407	0.367	0.224	0.139
0.539	0.523	0.492	0.478	0.444	0.419	0.413	0.361	0.220	0.132
0.531	0.531	0.485	0.478	0.444	0.419	0.413	0.367	0.224	0.139
0.539	0.523	0.492	0.485	0.451	0.425	0.407	0.361	0.216	0.136
0.539	0.531	0.500	0.478	0.444	0.425	0.407	0.367	0.213	0.136
0.539	0.523	0.492	0.492	0.444	0.425	0.407	0.356	0.213	0.132
0.539	0.515	0.492	0.485	0.444	0.425	0.407	0.356	0.213	0.132
0.539	0.523	0.492	0.485	0.444	0.425	0.407	0.351	0.209	0.129
0.539	0.515	0.500	0.492	0.438	0.425	0.401	0.346	0.205	0.129
0.547	0.515	0.492	0.478	0.438	0.425	0.395	0.346	0.205	0.126
0.547	0.515	0.507	0.478	0.438	0.431	0.401	0.340	0.205	0.129

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.126	0.099	0.084	0.076	0.068	0.059	0.057	0.054	0.051	0.049
0.129	0.096	0.084	0.073	0.068	0.062	0.059	0.054	0.051	0.049
0.126	0.099	0.082	0.076	0.068	0.059	0.059	0.054	0.049	0.049
0.123	0.096	0.084	0.079	0.065	0.059	0.057	0.054	0.051	0.051
0.123	0.099	0.082	0.076	0.068	0.059	0.057	0.054	0.051	0.046
0.126	0.096	0.084	0.076	0.068	0.059	0.054	0.054	0.049	0.049
0.120	0.096	0.084	0.079	0.068	0.062	0.059	0.054	0.049	0.049
0.123	0.096	0.082	0.076	0.065	0.059	0.057	0.054	0.051	0.049
0.123	0.093	0.084	0.076	0.068	0.059	0.057	0.054	0.051	0.049
0.120	0.096	0.084	0.076	0.065	0.062	0.054	0.054	0.051	0.049
0.123	0.096	0.084	0.073	0.065	0.059	0.057	0.054	0.049	0.049
0.120	0.093	0.082	0.076	0.065	0.059	0.057	0.054	0.049	0.049
0.117	0.096	0.082	0.073	0.065	0.059	0.054	0.054	0.051	0.049
0.120	0.093	0.082	0.073	0.065	0.057	0.057	0.054	0.051	0.049
0.120	0.093	0.082	0.073	0.065	0.062	0.057	0.054	0.049	0.049
0.117	0.096	0.082	0.073	0.068	0.062	0.057	0.054	0.051	0.049
0.114	0.093	0.082	0.073	0.065	0.059	0.054	0.054	0.049	0.049
0.114	0.093	0.082	0.073	0.065	0.059	0.057	0.054	0.049	0.049
0.114	0.093	0.082	0.070	0.065	0.059	0.057	0.054	0.049	0.049
0.114	0.093	0.082	0.073	0.065	0.059	0.054	0.054	0.051	0.049
0.114	0.090	0.082	0.073	0.065	0.059	0.057	0.054	0.049	0.049
0.114	0.093	0.079	0.073	0.065	0.059	0.057	0.054	0.051	0.049
0.114	0.090	0.082	0.070	0.065	0.059	0.057	0.051	0.049	0.049
0.111	0.093	0.079	0.073	0.065	0.059	0.054	0.054	0.049	0.046
0.114	0.093	0.079	0.070	0.062	0.059	0.057	0.051	0.049	0.049
0.108	0.093	0.082	0.070	0.065	0.059	0.057	0.054	0.049	0.049
0.108	0.090	0.079	0.070	0.065	0.059	0.054	0.054	0.049	0.049
0.108	0.090	0.079	0.070	0.065	0.057	0.057	0.054	0.049	0.049
0.105	0.090	0.082	0.070	0.065	0.059	0.057	0.054	0.051	0.049
0.108	0.087	0.082	0.073	0.065	0.059	0.057	0.051	0.046	0.049
0.111	0.090	0.079	0.070	0.062	0.057	0.054	0.051	0.049	0.049
0.105	0.090	0.082	0.070	0.062	0.057	0.057	0.051	0.049	0.049
0.105	0.087	0.079	0.070	0.065	0.059	0.054	0.054	0.051	0.046
0.108	0.090	0.079	0.070	0.065	0.057	0.054	0.054	0.049	0.049
0.105	0.087	0.079	0.068	0.062	0.057	0.054	0.051	0.049	0.046
0.105	0.090	0.079	0.068	0.065	0.059	0.054	0.054	0.049	0.046
0.105	0.090	0.079	0.070	0.059	0.057	0.054	0.051	0.049	0.046
0.105	0.090	0.079	0.068	0.062	0.059	0.054	0.051	0.049	0.046
0.102	0.087	0.076	0.068	0.062	0.057	0.054	0.049	0.051	0.049
0.105	0.087	0.079	0.068	0.062	0.059	0.054	0.051	0.049	0.049
0.105	0.087	0.076	0.068	0.062	0.059	0.057	0.054	0.049	0.049
0.102	0.084	0.079	0.073	0.062	0.059	0.054	0.051	0.049	0.049
0.102	0.087	0.079	0.070	0.062	0.057	0.057	0.051	0.049	0.046
0.102	0.084	0.079	0.068	0.062	0.057	0.054	0.054	0.049	0.046
0.099	0.084	0.076	0.068	0.062	0.057	0.054	0.054	0.049	0.049
0.099	0.084	0.076	0.068	0.059	0.057	0.054	0.051	0.049	0.046
0.102	0.084	0.076	0.068	0.059	0.057	0.054	0.049	0.051	0.046
0.099	0.084	0.076	0.068	0.059	0.057	0.054	0.051	0.049	0.046

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.049	0.044	0.046	0.044	0.041	0.041	0.039	0.039	0.036	0.036
0.046	0.044	0.044	0.044	0.041	0.039	0.039	0.039	0.039	0.036
0.046	0.046	0.046	0.041	0.041	0.039	0.039	0.039	0.039	0.036
0.049	0.046	0.044	0.044	0.041	0.041	0.039	0.039	0.039	0.036
0.046	0.046	0.044	0.044	0.041	0.039	0.036	0.039	0.039	0.033
0.049	0.046	0.044	0.041	0.041	0.039	0.039	0.036	0.036	0.036
0.049	0.044	0.044	0.046	0.041	0.039	0.036	0.039	0.036	0.033
0.049	0.044	0.044	0.044	0.044	0.041	0.041	0.036	0.039	0.036
0.046	0.046	0.046	0.044	0.041	0.041	0.041	0.039	0.036	0.033
0.046	0.044	0.044	0.041	0.041	0.041	0.039	0.039	0.039	0.036
0.046	0.046	0.041	0.041	0.039	0.044	0.039	0.039	0.039	0.036
0.046	0.046	0.044	0.041	0.041	0.039	0.039	0.039	0.036	0.036
0.046	0.046	0.044	0.041	0.041	0.039	0.039	0.036	0.036	0.039
0.046	0.046	0.041	0.044	0.041	0.041	0.039	0.039	0.036	0.036
0.046	0.046	0.046	0.041	0.041	0.039	0.041	0.039	0.036	0.036
0.049	0.046	0.044	0.041	0.041	0.041	0.039	0.039	0.039	0.036
0.049	0.046	0.041	0.039	0.041	0.039	0.039	0.036	0.036	0.036
0.049	0.046	0.044	0.044	0.039	0.041	0.039	0.039	0.036	0.036
0.046	0.046	0.044	0.041	0.041	0.039	0.039	0.039	0.036	0.033
0.046	0.046	0.041	0.044	0.041	0.041	0.039	0.039	0.039	0.036
0.046	0.046	0.046	0.041	0.041	0.039	0.041	0.039	0.036	0.039
0.046	0.046	0.041	0.041	0.039	0.039	0.041	0.041	0.036	0.036
0.046	0.046	0.044	0.041	0.041	0.039	0.039	0.036	0.036	0.036
0.049	0.046	0.044	0.044	0.039	0.041	0.036	0.039	0.036	0.036
0.049	0.046	0.041	0.041	0.041	0.041	0.039	0.039	0.039	0.039
0.046	0.046	0.044	0.041	0.041	0.041	0.039	0.036	0.036	0.036
0.046	0.044	0.044	0.044	0.039	0.039	0.039	0.039	0.036	0.036
0.046	0.041	0.041	0.044	0.041	0.039	0.039	0.039	0.039	0.039
0.046	0.046	0.044	0.041	0.041	0.041	0.039	0.039	0.036	0.036
0.046	0.044	0.044	0.041	0.041	0.041	0.036	0.039	0.036	0.036
0.046	0.044	0.044	0.039	0.041	0.041	0.036	0.039	0.036	0.033
0.049	0.046	0.041	0.044	0.041	0.039	0.039	0.039	0.036	0.036
0.046	0.046	0.044	0.041	0.041	0.039	0.036	0.039	0.036	0.036
0.046	0.046	0.041	0.041	0.039	0.039	0.039	0.039	0.036	0.036
0.046	0.044	0.044	0.041	0.041	0.039	0.036	0.036	0.036	0.036
0.046	0.044	0.041	0.044	0.041	0.039	0.039	0.039	0.036	0.033
0.044	0.044	0.044	0.041	0.041	0.039	0.039	0.041	0.036	0.036
0.046	0.046	0.044	0.041	0.041	0.039	0.039	0.036	0.036	0.036
0.046	0.046	0.046	0.041	0.041	0.041	0.039	0.036	0.033	0.036
0.046	0.044	0.044	0.041	0.041	0.039	0.036	0.036	0.036	0.036
0.046	0.044	0.044	0.044	0.041	0.039	0.039	0.039	0.036	0.036
0.046	0.046	0.046	0.044	0.041	0.039	0.039	0.036	0.039	0.036
0.046	0.046	0.044	0.041	0.039	0.039	0.039	0.036	0.039	0.036
0.046	0.044	0.044	0.041	0.041	0.041	0.036	0.036	0.036	0.036
0.046	0.044	0.041	0.041	0.039	0.039	0.036	0.039	0.033	0.036
0.046	0.044	0.041	0.041	0.039	0.041	0.036	0.039	0.036	0.036
0.044	0.046	0.046	0.041	0.039	0.039	0.039	0.036	0.036	0.036
0.046	0.044	0.041	0.044	0.041	0.039	0.039	0.036	0.036	0.036

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.033	0.036	0.036	0.033	0.033	0.033	0.031	0.031	0.031	0.028
0.036	0.036	0.033	0.033	0.033	0.031	0.033	0.028	0.033	0.031
0.036	0.033	0.036	0.033	0.033	0.028	0.031	0.031	0.031	0.028
0.039	0.036	0.033	0.033	0.033	0.031	0.028	0.033	0.031	0.031
0.036	0.033	0.036	0.033	0.033	0.033	0.031	0.031	0.033	0.031
0.036	0.036	0.036	0.033	0.033	0.031	0.033	0.033	0.031	0.031
0.036	0.033	0.036	0.031	0.033	0.031	0.033	0.031	0.031	0.028
0.036	0.036	0.036	0.033	0.031	0.031	0.031	0.031	0.028	0.031
0.036	0.033	0.031	0.033	0.031	0.031	0.031	0.033	0.028	0.031
0.039	0.033	0.033	0.031	0.036	0.031	0.031	0.028	0.031	0.028
0.036	0.036	0.036	0.033	0.033	0.031	0.031	0.031	0.031	0.028
0.036	0.033	0.031	0.036	0.033	0.031	0.031	0.031	0.031	0.031
0.033	0.033	0.033	0.031	0.031	0.033	0.033	0.031	0.031	0.028
0.036	0.033	0.036	0.033	0.031	0.031	0.033	0.033	0.031	0.031
0.036	0.036	0.036	0.036	0.031	0.031	0.033	0.031	0.031	0.031
0.033	0.033	0.033	0.033	0.031	0.033	0.033	0.028	0.031	0.031
0.036	0.033	0.036	0.031	0.031	0.033	0.031	0.033	0.028	0.028
0.036	0.036	0.033	0.033	0.033	0.031	0.033	0.028	0.031	0.028
0.036	0.033	0.033	0.033	0.033	0.031	0.031	0.031	0.031	0.028
0.036	0.036	0.033	0.031	0.031	0.031	0.028	0.031	0.033	0.028
0.036	0.036	0.033	0.031	0.031	0.031	0.031	0.028	0.033	0.028
0.036	0.033	0.033	0.033	0.033	0.028	0.031	0.031	0.031	0.028
0.036	0.036	0.033	0.033	0.031	0.031	0.031	0.033	0.031	0.031
0.036	0.033	0.033	0.033	0.031	0.031	0.033	0.033	0.031	0.031
0.036	0.036	0.033	0.033	0.033	0.033	0.033	0.028	0.031	0.028
0.036	0.036	0.033	0.033	0.033	0.031	0.033	0.028	0.028	0.031
0.036	0.036	0.036	0.036	0.033	0.031	0.031	0.031	0.031	0.031
0.036	0.033	0.033	0.033	0.031	0.031	0.031	0.031	0.031	0.028
0.033	0.033	0.033	0.031	0.031	0.031	0.033	0.031	0.031	0.033
0.036	0.036	0.031	0.033	0.031	0.031	0.028	0.031	0.031	0.028
0.036	0.036	0.033	0.031	0.033	0.031	0.031	0.031	0.028	0.028
0.033	0.036	0.033	0.033	0.031	0.028	0.031	0.031	0.028	0.028
0.036	0.033	0.033	0.033	0.031	0.031	0.033	0.028	0.031	0.028
0.036	0.033	0.033	0.033	0.031	0.033	0.031	0.031	0.031	0.028
0.036	0.033	0.033	0.033	0.031	0.031	0.028	0.031	0.031	0.028
0.033	0.036	0.036	0.033	0.033	0.031	0.031	0.031	0.033	0.031
0.036	0.033	0.031	0.031	0.033	0.033	0.028	0.031	0.028	0.031
0.033	0.036	0.033	0.031	0.033	0.033	0.031	0.031	0.031	0.031
0.033	0.033	0.036	0.033	0.031	0.033	0.033	0.031	0.031	0.031
0.033	0.033	0.033	0.031	0.031	0.031	0.031	0.031	0.031	0.031
0.031	0.036	0.036	0.033	0.031	0.033	0.031	0.031	0.031	0.028
0.036	0.033	0.033	0.031	0.033	0.031	0.031	0.031	0.028	0.028
0.036	0.033	0.031	0.033	0.031	0.033	0.033	0.033	0.031	0.028
0.033	0.033	0.033	0.033	0.033	0.033	0.031	0.031	0.028	0.028
0.036	0.033	0.036	0.033	0.028	0.031	0.033	0.031	0.031	0.028
0.036	0.033	0.033	0.033	0.033	0.033	0.031	0.031	0.028	0.028
0.036	0.033	0.033	0.031	0.031	0.031	0.028	0.028	0.031	0.031
0.036	0.033	0.033	0.031	0.033	0.033	0.031	0.031	0.028	0.031

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

0.028	0.033	0.031	0.028	0.028	0.028	0.028	0.028	0.028	0.028
0.028	0.028	0.031	0.028	0.031	0.028	0.028	0.028	0.026	0.028
0.031	0.028	0.028	0.028	0.028	0.028	0.028	0.028	0.026	0.026
0.028	0.028	0.031	0.028	0.028	0.031	0.028	0.028	0.028	0.028
0.028	0.031	0.028	0.028	0.026	0.028	0.028	0.026	0.028	0.028
0.028	0.031	0.028	0.028	0.028	0.028	0.028	0.028	0.028	0.028
0.031	0.031	0.028	0.028	0.028	0.028	0.028	0.028	0.028	0.028
0.031	0.028	0.028	0.028	0.028	0.031	0.028	0.028	0.028	0.026
0.031	0.031	0.031	0.031	0.031	0.031	0.028	0.028	0.028	0.026
0.028	0.028	0.028	0.031	0.028	0.028	0.028	0.026	0.028	0.026
0.031	0.031	0.031	0.028	0.028	0.031	0.026	0.028	0.028	0.026
0.031	0.028	0.028	0.028	0.028	0.028	0.031	0.026	0.028	0.026
0.031	0.028	0.031	0.028	0.028	0.028	0.028	0.028	0.028	0.028
0.028	0.028	0.031	0.031	0.028	0.031	0.028	0.028	0.028	0.028
0.028	0.028	0.026	0.028	0.028	0.028	0.028	0.028	0.026	0.028
0.028	0.028	0.028	0.031	0.028	0.028	0.028	0.028	0.026	0.031
0.028	0.031	0.028	0.028	0.028	0.028	0.026	0.028	0.028	0.028
0.028	0.028	0.028	0.028	0.031	0.028	0.028	0.028	0.028	0.028
0.031	0.031	0.028	0.028	0.028	0.028	0.028	0.028	0.028	
0.028	0.031	0.031	0.028	0.031	0.028	0.028	0.028	0.028	
0.031	0.028	0.026	0.031	0.031	0.028	0.031	0.028	0.028	
0.028	0.028	0.028	0.028	0.031	0.031	0.028	0.026	0.026	

Rezultate - Primul set de date de test

It	k <sub>0</sub>	k <sub>1</sub>	k <sub>2</sub>	y <sub>0</sub>	y <sub>1</sub>	y <sub>2</sub>	y <sub>3</sub>	ε
0	1.00E+10	1.40E+03	1.20E-01	4.00E+03	1.00E+00	1.00E+00	1.00E+00	2.00E+00
1	6.86E-02	1.41E+03	1.21E-01	4.04E+03	9.90E-01	9.90E-01	9.90E-01	1.98E+00
2	6.48E-02	1.43E+03	1.22E-01	4.08E+03	9.80E-01	9.80E-01	9.80E-01	1.96E+00
3	6.07E-02	1.44E+03	1.24E-01	4.12E+03	9.70E-01	9.70E-01	9.70E-01	1.94E+00
4	5.63E-02	1.46E+03	1.25E-01	4.16E+03	9.61E-01	9.61E-01	9.61E-01	1.92E+00
5	5.17E-02	1.47E+03	1.26E-01	4.20E+03	9.51E-01	9.51E-01	9.51E-01	1.90E+00
6	4.69E-02	1.49E+03	1.27E-01	4.25E+03	9.41E-01	9.41E-01	9.41E-01	1.88E+00
7	4.20E-02	1.50E+03	1.29E-01	4.29E+03	9.32E-01	9.32E-01	9.32E-01	1.86E+00
8	3.71E-02	1.52E+03	1.30E-01	4.33E+03	9.23E-01	9.23E-01	9.23E-01	1.85E+00
9	3.22E-02	1.53E+03	1.31E-01	4.37E+03	9.14E-01	9.14E-01	9.14E-01	1.83E+00
10	2.75E-02	1.55E+03	1.33E-01	4.42E+03	9.04E-01	9.04E-01	9.04E-01	1.81E+00
11	2.30E-02	1.56E+03	1.34E-01	4.46E+03	8.95E-01	8.95E-01	8.95E-01	1.79E+00
12	1.89E-02	1.58E+03	1.35E-01	4.51E+03	8.86E-01	8.86E-01	8.86E-01	1.77E+00
13	1.52E-02	1.59E+03	1.37E-01	4.55E+03	8.78E-01	8.78E-01	8.78E-01	1.76E+00
14	1.20E-02	1.61E+03	1.38E-01	4.60E+03	8.69E-01	8.69E-01	8.69E-01	1.74E+00
15	9.49E-03	1.63E+03	1.39E-01	4.64E+03	8.60E-01	8.60E-01	8.60E-01	1.72E+00
16	7.68E-03	1.64E+03	1.38E-01	4.69E+03	8.51E-01	8.51E-01	8.69E-01	1.70E+00
17	6.67E-03	1.66E+03	1.37E-01	4.74E+03	8.43E-01	8.43E-01	8.77E-01	1.69E+00
18	6.48E-03	1.67E+03	1.35E-01	4.74E+03	8.35E-01	8.35E-01	8.86E-01	1.69E+00
19	6.46E-03	1.66E+03	1.34E-01	4.69E+03	8.26E-01	8.35E-01	8.95E-01	1.69E+00
20	6.45E-03	1.66E+03	1.32E-01	4.64E+03	8.18E-01	8.26E-01	9.04E-01	1.70E+00
21	6.44E-03	1.64E+03	1.31E-01	4.60E+03	8.10E-01	8.26E-01	9.13E-01	1.70E+00

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

22	6.43E-03	1.62E+03	1.30E-01	4.55E+03	8.18E-01	8.18E-01	9.22E-01	1.70E+00
23	6.42E-03	1.61E+03	1.29E-01	4.51E+03	8.10E-01	8.18E-01	9.31E-01	1.70E+00
24	6.41E-03	1.59E+03	1.27E-01	4.46E+03	8.18E-01	8.10E-01	9.41E-01	1.70E+00
25	6.41E-03	1.59E+03	1.26E-01	4.42E+03	8.10E-01	8.18E-01	9.50E-01	1.70E+00
26	6.40E-03	1.58E+03	1.25E-01	4.37E+03	8.10E-01	8.26E-01	9.60E-01	1.69E+00
27	6.39E-03	1.56E+03	1.23E-01	4.33E+03	8.18E-01	8.18E-01	9.69E-01	1.69E+00
28	6.39E-03	1.55E+03	1.22E-01	4.28E+03	8.09E-01	8.18E-01	9.79E-01	1.69E+00
29	6.37E-03	1.53E+03	1.21E-01	4.24E+03	8.18E-01	8.10E-01	9.89E-01	1.69E+00
30	6.37E-03	1.53E+03	1.20E-01	4.20E+03	8.09E-01	8.18E-01	9.99E-01	1.69E+00
31	6.36E-03	1.51E+03	1.19E-01	4.16E+03	8.01E-01	8.18E-01	1.01E+00	1.69E+00
32	6.35E-03	1.50E+03	1.17E-01	4.12E+03	8.09E-01	8.09E-01	1.02E+00	1.69E+00
33	6.35E-03	1.48E+03	1.16E-01	4.07E+03	8.01E-01	8.09E-01	1.03E+00	1.69E+00
34	6.34E-03	1.47E+03	1.15E-01	4.03E+03	8.09E-01	8.01E-01	1.04E+00	1.69E+00
35	6.33E-03	1.47E+03	1.14E-01	3.99E+03	8.01E-01	8.09E-01	1.05E+00	1.69E+00
36	6.32E-03	1.45E+03	1.13E-01	3.95E+03	8.01E-01	8.17E-01	1.06E+00	1.67E+00
37	6.32E-03	1.44E+03	1.12E-01	3.91E+03	8.09E-01	8.09E-01	1.07E+00	1.67E+00
38	6.31E-03	1.43E+03	1.11E-01	3.87E+03	8.01E-01	8.09E-01	1.08E+00	1.67E+00
39	6.30E-03	1.41E+03	1.09E-01	3.84E+03	8.09E-01	8.01E-01	1.09E+00	1.67E+00
40	6.29E-03	1.40E+03	1.08E-01	3.80E+03	8.09E-01	7.93E-01	1.10E+00	1.67E+00
41	6.28E-03	1.38E+03	1.07E-01	3.76E+03	8.01E-01	8.01E-01	1.11E+00	1.67E+00
42	6.28E-03	1.38E+03	1.06E-01	3.72E+03	8.09E-01	7.93E-01	1.13E+00	1.67E+00
43	6.27E-03	1.37E+03	1.05E-01	3.68E+03	8.09E-01	7.85E-01	1.14E+00	1.67E+00
44	6.26E-03	1.36E+03	1.04E-01	3.65E+03	8.01E-01	7.93E-01	1.15E+00	1.67E+00
45	6.26E-03	1.34E+03	1.03E-01	3.61E+03	8.01E-01	7.85E-01	1.16E+00	1.67E+00
46	6.24E-03	1.33E+03	1.02E-01	3.58E+03	7.93E-01	7.93E-01	1.17E+00	1.67E+00
47	6.24E-03	1.32E+03	1.01E-01	3.54E+03	7.93E-01	8.01E-01	1.18E+00	1.65E+00
48	6.23E-03	1.30E+03	1.00E-01	3.50E+03	8.01E-01	7.93E-01	1.19E+00	1.65E+00
49	6.22E-03	1.30E+03	9.90E-02	3.47E+03	7.93E-01	8.01E-01	1.21E+00	1.65E+00
50	6.21E-03	1.29E+03	9.80E-02	3.43E+03	7.85E-01	8.01E-01	1.22E+00	1.65E+00
51	6.21E-03	1.28E+03	9.70E-02	3.40E+03	7.93E-01	7.93E-01	1.23E+00	1.65E+00
52	6.20E-03	1.26E+03	9.61E-02	3.37E+03	7.85E-01	7.93E-01	1.24E+00	1.65E+00
53	6.19E-03	1.25E+03	9.51E-02	3.33E+03	7.93E-01	7.85E-01	1.26E+00	1.65E+00
54	6.18E-03	1.24E+03	9.41E-02	3.30E+03	7.93E-01	7.77E-01	1.27E+00	1.65E+00
55	6.17E-03	1.23E+03	9.32E-02	3.27E+03	7.85E-01	7.85E-01	1.28E+00	1.65E+00
56	6.17E-03	1.23E+03	9.23E-02	3.23E+03	7.93E-01	7.77E-01	1.29E+00	1.65E+00
57	6.16E-03	1.21E+03	9.13E-02	3.20E+03	8.01E-01	7.77E-01	1.31E+00	1.64E+00
58	6.15E-03	1.20E+03	9.04E-02	3.17E+03	7.93E-01	7.85E-01	1.32E+00	1.64E+00
59	6.14E-03	1.19E+03	8.95E-02	3.14E+03	7.93E-01	7.77E-01	1.33E+00	1.64E+00
60	6.13E-03	1.18E+03	8.86E-02	3.11E+03	7.85E-01	7.85E-01	1.35E+00	1.64E+00
61	6.13E-03	1.17E+03	8.77E-02	3.08E+03	7.77E-01	7.85E-01	1.36E+00	1.64E+00
62	6.12E-03	1.15E+03	8.69E-02	3.04E+03	7.85E-01	7.77E-01	1.37E+00	1.64E+00
63	6.11E-03	1.14E+03	8.60E-02	3.01E+03	7.85E-01	7.69E-01	1.39E+00	1.64E+00
64	6.10E-03	1.13E+03	8.51E-02	2.98E+03	7.77E-01	7.77E-01	1.40E+00	1.64E+00
65	6.10E-03	1.13E+03	8.43E-02	2.95E+03	7.84E-01	7.69E-01	1.41E+00	1.64E+00
66	6.09E-03	1.12E+03	8.34E-02	2.92E+03	7.92E-01	7.69E-01	1.43E+00	1.62E+00

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

67	6.08E-03	1.11E+03	8.26E-02	2.90E+03	7.84E-01	7.77E-01	1.44E+00	1.62E+00
68	6.07E-03	1.10E+03	8.18E-02	2.87E+03	7.84E-01	7.69E-01	1.46E+00	1.62E+00
69	6.06E-03	1.09E+03	8.10E-02	2.84E+03	7.77E-01	7.77E-01	1.47E+00	1.62E+00
70	6.06E-03	1.08E+03	8.02E-02	2.81E+03	7.69E-01	7.77E-01	1.49E+00	1.62E+00
71	6.05E-03	1.07E+03	7.94E-02	2.78E+03	7.76E-01	7.69E-01	1.50E+00	1.62E+00
72	6.04E-03	1.05E+03	7.86E-02	2.75E+03	7.76E-01	7.61E-01	1.52E+00	1.62E+00
73	6.03E-03	1.04E+03	7.78E-02	2.73E+03	7.69E-01	7.69E-01	1.53E+00	1.62E+00
74	6.03E-03	1.03E+03	7.70E-02	2.70E+03	7.61E-01	7.69E-01	1.55E+00	1.62E+00
75	6.01E-03	1.02E+03	7.62E-02	2.67E+03	7.69E-01	7.61E-01	1.56E+00	1.62E+00
76	6.01E-03	1.02E+03	7.55E-02	2.64E+03	7.76E-01	7.69E-01	1.58E+00	1.60E+00
77	6.00E-03	1.01E+03	7.47E-02	2.62E+03	7.76E-01	7.61E-01	1.59E+00	1.60E+00
78	5.99E-03	1.00E+03	7.40E-02	2.59E+03	7.69E-01	7.69E-01	1.61E+00	1.60E+00
79	5.99E-03	9.93E+02	7.32E-02	2.57E+03	7.61E-01	7.69E-01	1.63E+00	1.60E+00
80	5.98E-03	9.83E+02	7.25E-02	2.54E+03	7.68E-01	7.61E-01	1.64E+00	1.60E+00
81	5.97E-03	9.73E+02	7.18E-02	2.52E+03	7.68E-01	7.53E-01	1.66E+00	1.60E+00
82	5.96E-03	9.63E+02	7.10E-02	2.49E+03	7.61E-01	7.61E-01	1.68E+00	1.60E+00
83	5.95E-03	9.54E+02	7.03E-02	2.47E+03	7.53E-01	7.61E-01	1.69E+00	1.60E+00
84	5.94E-03	9.44E+02	6.96E-02	2.44E+03	7.61E-01	7.53E-01	1.71E+00	1.60E+00
85	5.94E-03	9.35E+02	6.89E-02	2.42E+03	7.61E-01	7.46E-01	1.73E+00	1.60E+00
86	5.93E-03	9.26E+02	6.82E-02	2.39E+03	7.68E-01	7.53E-01	1.74E+00	1.59E+00
87	5.92E-03	9.16E+02	6.76E-02	2.37E+03	7.68E-01	7.46E-01	1.76E+00	1.59E+00
88	5.91E-03	9.07E+02	6.69E-02	2.34E+03	7.61E-01	7.53E-01	1.78E+00	1.59E+00
89	5.90E-03	8.98E+02	6.62E-02	2.32E+03	7.61E-01	7.46E-01	1.80E+00	1.59E+00
90	5.89E-03	8.89E+02	6.56E-02	2.30E+03	7.53E-01	7.53E-01	1.81E+00	1.59E+00
91	5.89E-03	8.80E+02	6.49E-02	2.27E+03	7.53E-01	7.45E-01	1.83E+00	1.59E+00
92	5.88E-03	8.71E+02	6.43E-02	2.25E+03	7.45E-01	7.53E-01	1.85E+00	1.59E+00
93	5.87E-03	8.63E+02	6.36E-02	2.23E+03	7.38E-01	7.53E-01	1.87E+00	1.59E+00
94	5.86E-03	8.54E+02	6.30E-02	2.21E+03	7.45E-01	7.45E-01	1.89E+00	1.59E+00
95	5.86E-03	8.45E+02	6.23E-02	2.19E+03	7.45E-01	7.38E-01	1.91E+00	1.59E+00
96	5.84E-03	8.37E+02	6.17E-02	2.16E+03	7.53E-01	7.45E-01	1.93E+00	1.57E+00
97	5.84E-03	8.37E+02	6.11E-02	2.14E+03	7.45E-01	7.53E-01	1.94E+00	1.57E+00
98	5.83E-03	8.29E+02	6.05E-02	2.12E+03	7.38E-01	7.53E-01	1.96E+00	1.57E+00
99	5.82E-03	8.20E+02	5.99E-02	2.10E+03	7.45E-01	7.45E-01	1.98E+00	1.57E+00

**Rezultate - Al doilea set de date de test**

It	$k_0$	$k_1$	$k_2$	$y_0$	$y_1$	$y_2$	$y_3$	$\varepsilon$
0	1.00E+10	1.40E+03	1.20E-01	4.00E+03	1.00E+00	1.00E+00	1.00E+00	2.00E+00
1	6.86E-02	1.41E+03	1.21E-01	4.04E+03	9.90E-01	9.90E-01	9.90E-01	1.98E+00
2	6.48E-02	1.43E+03	1.22E-01	4.08E+03	9.80E-01	9.80E-01	9.80E-01	1.96E+00
3	6.07E-02	1.44E+03	1.24E-01	4.12E+03	9.70E-01	9.70E-01	9.70E-01	1.94E+00
4	5.63E-02	1.46E+03	1.25E-01	4.16E+03	9.61E-01	9.61E-01	9.61E-01	1.92E+00
5	5.17E-02	1.47E+03	1.26E-01	4.20E+03	9.51E-01	9.51E-01	9.51E-01	1.90E+00
6	4.69E-02	1.49E+03	1.27E-01	4.25E+03	9.41E-01	9.41E-01	9.41E-01	1.88E+00
7	4.20E-02	1.50E+03	1.29E-01	4.29E+03	9.32E-01	9.32E-01	9.32E-01	1.86E+00
8	3.71E-02	1.52E+03	1.30E-01	4.33E+03	9.23E-01	9.23E-01	9.23E-01	1.85E+00
9	3.22E-02	1.53E+03	1.31E-01	4.37E+03	9.14E-01	9.14E-01	9.14E-01	1.83E+00

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

10	2.75E-02	1.55E+03	1.33E-01	4.42E+03	9.04E-01	9.04E-01	9.04E-01	1.81E+00
11	2.30E-02	1.56E+03	1.34E-01	4.46E+03	8.95E-01	8.95E-01	8.95E-01	1.79E+00
12	1.89E-02	1.58E+03	1.35E-01	4.51E+03	8.86E-01	8.86E-01	8.86E-01	1.77E+00
13	1.52E-02	1.59E+03	1.37E-01	4.55E+03	8.78E-01	8.78E-01	8.78E-01	1.76E+00
14	1.20E-02	1.61E+03	1.38E-01	4.60E+03	8.69E-01	8.69E-01	8.69E-01	1.74E+00
15	9.49E-03	1.63E+03	1.39E-01	4.64E+03	8.60E-01	8.60E-01	8.60E-01	1.72E+00
16	7.68E-03	1.64E+03	1.38E-01	4.69E+03	8.51E-01	8.51E-01	8.69E-01	1.70E+00
17	6.67E-03	1.66E+03	1.37E-01	4.74E+03	8.43E-01	8.43E-01	8.77E-01	1.69E+00
18	6.48E-03	1.67E+03	1.35E-01	4.74E+03	8.35E-01	8.35E-01	8.86E-01	1.69E+00
19	6.46E-03	1.66E+03	1.34E-01	4.69E+03	8.26E-01	8.35E-01	8.95E-01	1.69E+00
20	6.45E-03	1.66E+03	1.32E-01	4.64E+03	8.18E-01	8.26E-01	9.04E-01	1.70E+00
21	6.44E-03	1.64E+03	1.31E-01	4.60E+03	8.10E-01	8.26E-01	9.13E-01	1.70E+00
22	6.43E-03	1.62E+03	1.30E-01	4.55E+03	8.18E-01	8.18E-01	9.22E-01	1.70E+00
23	6.42E-03	1.61E+03	1.29E-01	4.51E+03	8.10E-01	8.18E-01	9.31E-01	1.70E+00
24	6.41E-03	1.59E+03	1.27E-01	4.46E+03	8.18E-01	8.10E-01	9.41E-01	1.70E+00
25	6.41E-03	1.59E+03	1.26E-01	4.42E+03	8.10E-01	8.18E-01	9.50E-01	1.70E+00
26	6.40E-03	1.58E+03	1.25E-01	4.37E+03	8.10E-01	8.26E-01	9.60E-01	1.69E+00
27	6.39E-03	1.56E+03	1.23E-01	4.33E+03	8.18E-01	8.18E-01	9.69E-01	1.69E+00
28	6.39E-03	1.55E+03	1.22E-01	4.28E+03	8.09E-01	8.18E-01	9.79E-01	1.69E+00
29	6.37E-03	1.53E+03	1.21E-01	4.24E+03	8.18E-01	8.10E-01	9.89E-01	1.69E+00
30	6.37E-03	1.53E+03	1.20E-01	4.20E+03	8.09E-01	8.18E-01	9.99E-01	1.69E+00
31	6.36E-03	1.51E+03	1.19E-01	4.16E+03	8.01E-01	8.18E-01	1.01E+00	1.69E+00
32	6.35E-03	1.50E+03	1.17E-01	4.12E+03	8.09E-01	8.09E-01	1.02E+00	1.69E+00
33	6.35E-03	1.48E+03	1.16E-01	4.07E+03	8.01E-01	8.09E-01	1.03E+00	1.69E+00
34	6.34E-03	1.47E+03	1.15E-01	4.03E+03	8.09E-01	8.01E-01	1.04E+00	1.69E+00
35	6.33E-03	1.47E+03	1.14E-01	3.99E+03	8.01E-01	8.09E-01	1.05E+00	1.69E+00
36	6.32E-03	1.45E+03	1.13E-01	3.95E+03	8.01E-01	8.17E-01	1.06E+00	1.67E+00
37	6.32E-03	1.44E+03	1.12E-01	3.91E+03	8.09E-01	8.09E-01	1.07E+00	1.67E+00
38	6.31E-03	1.43E+03	1.11E-01	3.87E+03	8.01E-01	8.09E-01	1.08E+00	1.67E+00
39	6.30E-03	1.41E+03	1.09E-01	3.84E+03	8.09E-01	8.01E-01	1.09E+00	1.67E+00
40	6.29E-03	1.40E+03	1.08E-01	3.80E+03	8.09E-01	7.93E-01	1.10E+00	1.67E+00
41	6.28E-03	1.38E+03	1.07E-01	3.76E+03	8.01E-01	8.01E-01	1.11E+00	1.67E+00
42	6.28E-03	1.38E+03	1.06E-01	3.72E+03	8.09E-01	7.93E-01	1.13E+00	1.67E+00
43	6.27E-03	1.37E+03	1.05E-01	3.68E+03	8.09E-01	7.85E-01	1.14E+00	1.67E+00
44	6.26E-03	1.36E+03	1.04E-01	3.65E+03	8.01E-01	7.93E-01	1.15E+00	1.67E+00
45	6.26E-03	1.34E+03	1.03E-01	3.61E+03	8.01E-01	7.85E-01	1.16E+00	1.67E+00
46	6.24E-03	1.33E+03	1.02E-01	3.58E+03	7.93E-01	7.93E-01	1.17E+00	1.67E+00
47	6.24E-03	1.32E+03	1.01E-01	3.54E+03	7.93E-01	8.01E-01	1.18E+00	1.65E+00
48	6.23E-03	1.30E+03	1.00E-01	3.50E+03	8.01E-01	7.93E-01	1.19E+00	1.65E+00
49	6.22E-03	1.30E+03	9.90E-02	3.47E+03	7.93E-01	8.01E-01	1.21E+00	1.65E+00
50	6.21E-03	1.29E+03	9.80E-02	3.43E+03	7.85E-01	8.01E-01	1.22E+00	1.65E+00
51	6.21E-03	1.28E+03	9.70E-02	3.40E+03	7.93E-01	7.93E-01	1.23E+00	1.65E+00
52	6.20E-03	1.26E+03	9.61E-02	3.37E+03	7.85E-01	7.93E-01	1.24E+00	1.65E+00
53	6.19E-03	1.25E+03	9.51E-02	3.33E+03	7.93E-01	7.85E-01	1.26E+00	1.65E+00
54	6.18E-03	1.24E+03	9.41E-02	3.30E+03	7.93E-01	7.77E-01	1.27E+00	1.65E+00

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

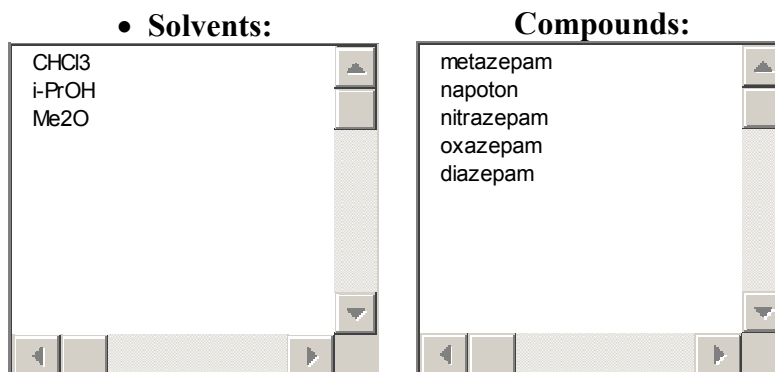
55	6.17E-03	1.23E+03	9.32E-02	3.27E+03	7.85E-01	7.85E-01	1.28E+00	1.65E+00
56	6.17E-03	1.23E+03	9.23E-02	3.23E+03	7.93E-01	7.77E-01	1.29E+00	1.65E+00
57	6.16E-03	1.21E+03	9.13E-02	3.20E+03	8.01E-01	7.77E-01	1.31E+00	1.64E+00
58	6.15E-03	1.20E+03	9.04E-02	3.17E+03	7.93E-01	7.85E-01	1.32E+00	1.64E+00
59	6.14E-03	1.19E+03	8.95E-02	3.14E+03	7.93E-01	7.77E-01	1.33E+00	1.64E+00
60	6.13E-03	1.18E+03	8.86E-02	3.11E+03	7.85E-01	7.85E-01	1.35E+00	1.64E+00
61	6.13E-03	1.17E+03	8.77E-02	3.08E+03	7.77E-01	7.85E-01	1.36E+00	1.64E+00
62	6.12E-03	1.15E+03	8.69E-02	3.04E+03	7.85E-01	7.77E-01	1.37E+00	1.64E+00
63	6.11E-03	1.14E+03	8.60E-02	3.01E+03	7.85E-01	7.69E-01	1.39E+00	1.64E+00
64	6.10E-03	1.13E+03	8.51E-02	2.98E+03	7.77E-01	7.77E-01	1.40E+00	1.64E+00
65	6.10E-03	1.13E+03	8.43E-02	2.95E+03	7.84E-01	7.69E-01	1.41E+00	1.64E+00
66	6.09E-03	1.12E+03	8.34E-02	2.92E+03	7.92E-01	7.69E-01	1.43E+00	1.62E+00
67	6.08E-03	1.11E+03	8.26E-02	2.90E+03	7.84E-01	7.77E-01	1.44E+00	1.62E+00
68	6.07E-03	1.10E+03	8.18E-02	2.87E+03	7.84E-01	7.69E-01	1.46E+00	1.62E+00
69	6.06E-03	1.09E+03	8.10E-02	2.84E+03	7.77E-01	7.77E-01	1.47E+00	1.62E+00
70	6.06E-03	1.08E+03	8.02E-02	2.81E+03	7.69E-01	7.77E-01	1.49E+00	1.62E+00
71	6.05E-03	1.07E+03	7.94E-02	2.78E+03	7.76E-01	7.69E-01	1.50E+00	1.62E+00
72	6.04E-03	1.05E+03	7.86E-02	2.75E+03	7.76E-01	7.61E-01	1.52E+00	1.62E+00
73	6.03E-03	1.04E+03	7.78E-02	2.73E+03	7.69E-01	7.69E-01	1.53E+00	1.62E+00
74	6.03E-03	1.03E+03	7.70E-02	2.70E+03	7.61E-01	7.69E-01	1.55E+00	1.62E+00
75	6.01E-03	1.02E+03	7.62E-02	2.67E+03	7.69E-01	7.61E-01	1.56E+00	1.62E+00
76	6.01E-03	1.02E+03	7.55E-02	2.64E+03	7.76E-01	7.69E-01	1.58E+00	1.60E+00
77	6.00E-03	1.01E+03	7.47E-02	2.62E+03	7.76E-01	7.61E-01	1.59E+00	1.60E+00
78	5.99E-03	1.00E+03	7.40E-02	2.59E+03	7.69E-01	7.69E-01	1.61E+00	1.60E+00
79	5.99E-03	9.93E+02	7.32E-02	2.57E+03	7.61E-01	7.69E-01	1.63E+00	1.60E+00
80	5.98E-03	9.83E+02	7.25E-02	2.54E+03	7.68E-01	7.61E-01	1.64E+00	1.60E+00
81	5.97E-03	9.73E+02	7.18E-02	2.52E+03	7.68E-01	7.53E-01	1.66E+00	1.60E+00
82	5.96E-03	9.63E+02	7.10E-02	2.49E+03	7.61E-01	7.61E-01	1.68E+00	1.60E+00
83	5.95E-03	9.54E+02	7.03E-02	2.47E+03	7.53E-01	7.61E-01	1.69E+00	1.60E+00
84	5.94E-03	9.44E+02	6.96E-02	2.44E+03	7.61E-01	7.53E-01	1.71E+00	1.60E+00
85	5.94E-03	9.35E+02	6.89E-02	2.42E+03	7.61E-01	7.46E-01	1.73E+00	1.60E+00
86	5.93E-03	9.26E+02	6.82E-02	2.39E+03	7.68E-01	7.53E-01	1.74E+00	1.59E+00
87	5.92E-03	9.16E+02	6.76E-02	2.37E+03	7.68E-01	7.46E-01	1.76E+00	1.59E+00
88	5.91E-03	9.07E+02	6.69E-02	2.34E+03	7.61E-01	7.53E-01	1.78E+00	1.59E+00
89	5.90E-03	8.98E+02	6.62E-02	2.32E+03	7.61E-01	7.46E-01	1.80E+00	1.59E+00
90	5.89E-03	8.89E+02	6.56E-02	2.30E+03	7.53E-01	7.53E-01	1.81E+00	1.59E+00
91	5.89E-03	8.80E+02	6.49E-02	2.27E+03	7.53E-01	7.45E-01	1.83E+00	1.59E+00
92	5.88E-03	8.71E+02	6.43E-02	2.25E+03	7.45E-01	7.53E-01	1.85E+00	1.59E+00
93	5.87E-03	8.63E+02	6.36E-02	2.23E+03	7.38E-01	7.53E-01	1.87E+00	1.59E+00
94	5.86E-03	8.54E+02	6.30E-02	2.21E+03	7.45E-01	7.45E-01	1.89E+00	1.59E+00
95	5.86E-03	8.45E+02	6.23E-02	2.19E+03	7.45E-01	7.38E-01	1.91E+00	1.59E+00
96	5.84E-03	8.37E+02	6.17E-02	2.16E+03	7.53E-01	7.45E-01	1.93E+00	1.57E+00
97	5.84E-03	8.37E+02	6.11E-02	2.14E+03	7.45E-01	7.53E-01	1.94E+00	1.57E+00
98	5.83E-03	8.29E+02	6.05E-02	2.12E+03	7.38E-01	7.53E-01	1.96E+00	1.57E+00
99	5.82E-03	8.20E+02	5.99E-02	2.10E+03	7.45E-01	7.45E-01	1.98E+00	1.57E+00

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

Au fost testate modulele aplicației de optimizare a fazei mobile.

Următorul este un exemplu de date de test:

÷ Faza 1. Alegerea solventilor și compușilor de interes:



÷ Faza 2. Selectarea modelului de experimentare (designului experimental):

**Experiments:**

Experiment	Include	CHCl3	i-PrOH	Me2O
0	<input checked="" type="checkbox"/>	33.3%	33.3%	33.3%
1	<input checked="" type="checkbox"/>	10%	10%	80%
2	<input checked="" type="checkbox"/>	10%	80%	10%
3	<input checked="" type="checkbox"/>	80%	10%	10%
4	<input checked="" type="checkbox"/>	50%	0%	50%
5	<input checked="" type="checkbox"/>	50%	50%	0%
6	<input checked="" type="checkbox"/>	0%	50%	50%
7	<input checked="" type="checkbox"/>	100%	0%	0%
8	<input checked="" type="checkbox"/>	0%	0%	100%
9	<input checked="" type="checkbox"/>	0%	100%	0%

÷ Faza 3. Completarea cu valori experimentale a modelului experimental:

Compound	Experiments results for solvents = ( CHCl3, i-PrOH, Me2O )									
	33.3, 33.3, pos, width	10, 10, 8 pos, width	10, 80, 1 pos, width	80, 10, 1 pos, width	50, 0, 50 pos, width	50, 50, 0 pos, width	0, 50, 50 pos, width	100, 0, 0 pos, width	0, 0, 100 pos, width	0, 100, 0 pos, width
metazepam	5.62, 0.39	4.92, 0.37	5.90, 0.39	3.38, 0.41	2.91, 0.43	6.07, 0.44	5.91, 0.51	0.56, 0.28	6.05, 0.44	8.23, 0.43
napoton	5.95, 0.38	5.42, 0.37	5.35, 0.49	3.84, 0.37	4.52, 0.47	6.30, 0.42	6.47, 0.42	0.55, 0.30	7.14, 0.40	9.31, 0.23
nitrazepam	6.12, 0.25	5.99, 0.39	6.00, 0.28	4.67, 0.22	5.60, 0.40	6.79, 0.38	6.64, 0.32	1.42, 0.25	9.03, 0.27	9.50, 0.25
oxazepam	6.32, 0.30	5.56, 0.49	5.91, 0.32	5.49, 0.28	5.97, 0.42	6.87, 0.33	6.99, 0.36	2.52, 0.24	8.25, 0.28	9.28, 0.22
diazepam	6.46, 0.32	5.99, 0.32	6.15, 0.35	5.77, 0.28	6.35, 0.36	7.03, 0.29	7.06, 0.47	2.72, 0.21	8.77, 0.30	9.39, 0.24
eluent	6.88	6.88	6.99	6.97	7.72	7.39	7.64	10.0	10.0	10.0

÷ Faza 4. Selectarea modelelor

Model Equation:	
<input checked="" type="checkbox"/>	$Y = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3$
<input checked="" type="checkbox"/>	$Y = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3$
Dependent Variable:	Graph:
<input checked="" type="checkbox"/> FO	<input type="checkbox"/> Red (best) - Green (worst)
<input checked="" type="checkbox"/> RS	<input checked="" type="checkbox"/> Green gradient only
<input checked="" type="checkbox"/> RF	

÷ Faza 5. Calcularea datelor auxiliare

solvents	CHCl3	i-PrOH	Me2O							
experiment	0	1	2	3	4	5	6	7	8	9
compound_pair										
	(metazepam, napoton)									
	(metazepam, nitrazepam)									
	(metazepam, oxazepam)									
	(metazepam, diazepam)									
	(napoton, nitrazepam)									
	(napoton, oxazepam)									
	(napoton, diazepam)									
	(nitrazepam, oxazepam)									
	(nitrazepam, diazepam)									
	(oxazepam, diazepam)									
resolutions_pair	(0, 1)	(1, 2)	(2, 3)	(3, 4)						
length	6.88	6.88	6.99	6.97	7.72	7.39	7.64	10.0	10.0	10.0
mixtures	CHCl3	i-PrOH	Me2O							
0	33.3000	33.3000	33.3000							
1	10.0000	10.0000	80.0000							
2	10.0000	80.0000	10.0000							
3	80.0000	10.0000	10.0000							
4	50.0000	0.0000	50.0000							
5	50.0000	50.0000	0.0000							
6	0.0000	50.0000	50.0000							
7	100.0000	0.0000	0.0000							
8	0.0000	0.0000	100.0000							
9	0.0000	100.0000	0.0000							

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

data	0	1	2	3	4	5	6	7	8	9
metazepam	5.62:0.39	4.92:0.37	5.90:0.39	3.38:0.41	2.91:0.43	6.07:0.44	5.91:0.51	0.56:0.28	6.05:0.44	8.23:0.43
napoton	5.95:0.38	5.42:0.37	5.35:0.49	3.84:0.37	4.52:0.47	6.30:0.42	6.47:0.42	0.55:0.30	7.14:0.40	9.31:0.23
nitrazepam	6.12:0.25	5.99:0.39	6.00:0.28	4.67:0.22	5.60:0.40	6.79:0.38	6.64:0.32	1.42:0.25	9.03:0.27	9.50:0.25
oxazepam	6.32:0.30	5.56:0.49	5.91:0.32	5.49:0.28	5.97:0.42	6.87:0.33	6.99:0.36	2.52:0.24	8.25:0.28	9.28:0.22
diazepam	6.46:0.32	5.99:0.32	6.15:0.35	5.77:0.28	6.35:0.36	7.03:0.29	7.06:0.47	2.72:0.21	8.77:0.30	9.39:0.24

retention_factor	0	1	2	3	4	5	6	7	8	9
metazepam	0.8169	0.7151	0.8441	0.4849	0.3769	0.8214	0.7736	0.0560	0.6050	0.8230
napoton	0.8648	0.7878	0.7654	0.5509	0.5855	0.8525	0.8469	0.0550	0.7140	0.9310
nitrazepam	0.8895	0.8706	0.8584	0.6700	0.7254	0.9188	0.8691	0.1420	0.9030	0.9500
oxazepam	0.9186	0.8081	0.8455	0.7877	0.7733	0.9296	0.9149	0.2520	0.8250	0.9280
diazepam	0.9390	0.8706	0.8798	0.8278	0.8225	0.9513	0.9241	0.2720	0.8770	0.9390

resolutions_all	0	1	2	3	4	5	6	7	8	9
(metazepam, napoton)	0.8571	1.3514	1.2500	1.1795	3.5778	0.5349	1.2043	0.0345	2.5952	3.2727
(metazepam, nitrazepam)	1.5625	2.8158	0.2985	4.0952	6.4819	1.7561	1.7590	3.2453	8.3944	3.7353
(metazepam, oxazepam)	2.0290	1.4884	0.0282	6.1159	7.2000	2.0779	2.4828	7.5385	6.1111	3.2308
(metazepam, diazepam)	2.3662	3.1014	0.6757	6.9275	8.7089	2.6301	2.3469	8.8163	7.3514	3.4627
(napoton, nitrazepam)	0.5397	1.5000	1.6883	2.8136	2.4828	1.2250	0.4595	3.1636	5.6418	0.7917
(napoton, oxazepam)	1.0882	0.3256	1.3827	5.0769	3.2584	1.5200	1.3333	7.2963	3.2647	0.1333
(napoton, diazepam)	1.4571	1.6522	1.9048	5.9385	4.4096	2.0563	1.3258	8.5098	4.6571	0.3404
(nitrazepam, oxazepam)	0.7273	0.9773	0.3000	3.2800	0.9024	0.2254	1.0294	4.4898	2.8364	0.9362
(nitrazepam, diazepam)	1.1930	0.0000	0.4762	4.4000	1.9737	0.7164	1.0633	5.6522	0.9123	0.4490
(oxazepam, diazepam)	0.4516	1.0617	0.7164	1.0000	0.9744	0.5161	0.1687	0.8889	1.7931	0.4783

resolutions	0	1	2	3	4	5	6	7	8	9
(0, 1)	0.8571	1.3514	1.2500	1.1795	3.5778	0.5349	1.2043	0.0345	2.5952	3.2308
(1, 2)	0.5397	0.3256	0.0282	2.8136	2.4828	1.2250	0.4595	3.2453	3.2647	0.1333
(2, 3)	0.7273	0.9773	0.3000	3.2800	0.9024	0.2254	1.0294	4.4898	1.7931	0.3404
(3, 4)	0.4516	0.0000	0.4762	1.0000	0.9744	0.5161	0.1687	0.8889	0.9123	0.4490

resolutions_sort	0	1	2	3	4	5	6	7	8	9
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**ET108/2006 – Et. Finală/2007 – Lucrare in extenso**

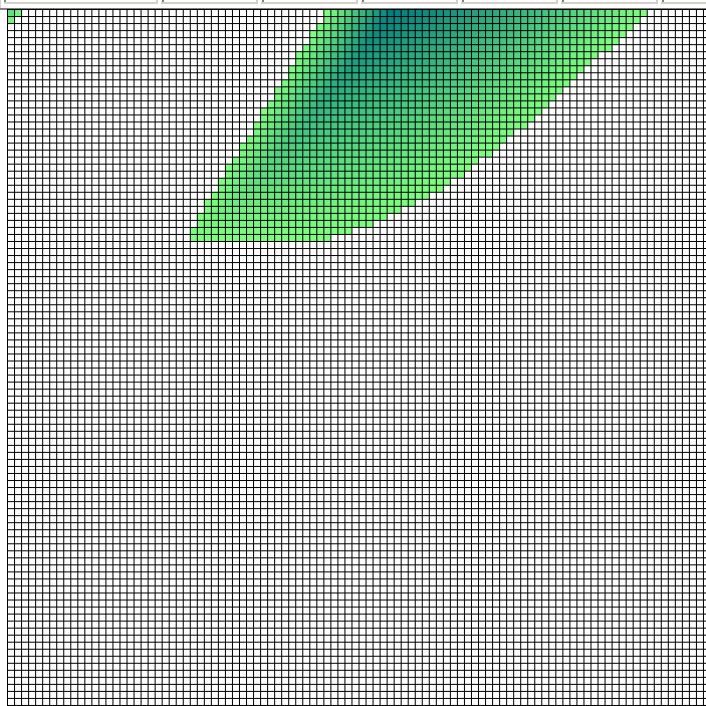
(0, 1)	0.4516	0.0000	0.0282	1.0000	0.9024	0.2254	0.1687	0.0345	0.9123	0.1333
(1, 2)	0.5397	0.3256	0.3000	1.1795	0.9744	0.5161	0.4595	0.8889	1.7931	0.3404
(2, 3)	0.7273	0.9773	0.4762	2.8136	2.4828	0.5349	1.0294	3.2453	2.5952	0.4490
(3, 4)	0.8571	1.3514	1.2500	3.2800	3.5778	1.2250	1.2043	4.4898	3.2647	3.2308

÷ Faza 6. Obținere rezultate pe fiecare funcție obiectiv:

$$\Delta rf = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3$$

retention_factor	0	1	2	3	4	5	6	7	8	9
metazepam	0.8169	0.7151	0.8441	0.4849	0.3769	0.8214	0.7736	0.0560	0.6050	0.8230
napoton	0.8648	0.7878	0.7654	0.5509	0.5855	0.8525	0.8469	0.0550	0.7140	0.9310
nitrazepam	0.8895	0.8706	0.8584	0.6700	0.7254	0.9188	0.8691	0.1420	0.9030	0.9500
oxazepam	0.9186	0.8081	0.8455	0.7877	0.7733	0.9296	0.9149	0.2520	0.8250	0.9280
diazepam	0.9390	0.8706	0.8798	0.8278	0.8225	0.9513	0.9241	0.2720	0.8770	0.9390

6 calc	0	1	2	3	4	5	6	7	8	9
metazepam	0.7716	0.6613	0.8747	0.3852	0.4449	0.8657	0.8050	0.0970	0.6203	0.7910
napoton	0.8392	0.7697	0.9044	0.4390	0.6329	0.8559	0.8240	0.1156	0.7220	0.8510
nitrazepam	0.8986	0.8866	0.9409	0.5339	0.7565	0.9313	0.8390	0.2162	0.8921	0.9018
oxazepam	0.9349	0.8568	0.9402	0.6235	0.7993	0.9427	0.8684	0.3441	0.7979	0.8751
diazepam	0.9656	0.9043	0.9577	0.6543	0.8523	0.9687	0.8835	0.3671	0.8561	0.8934



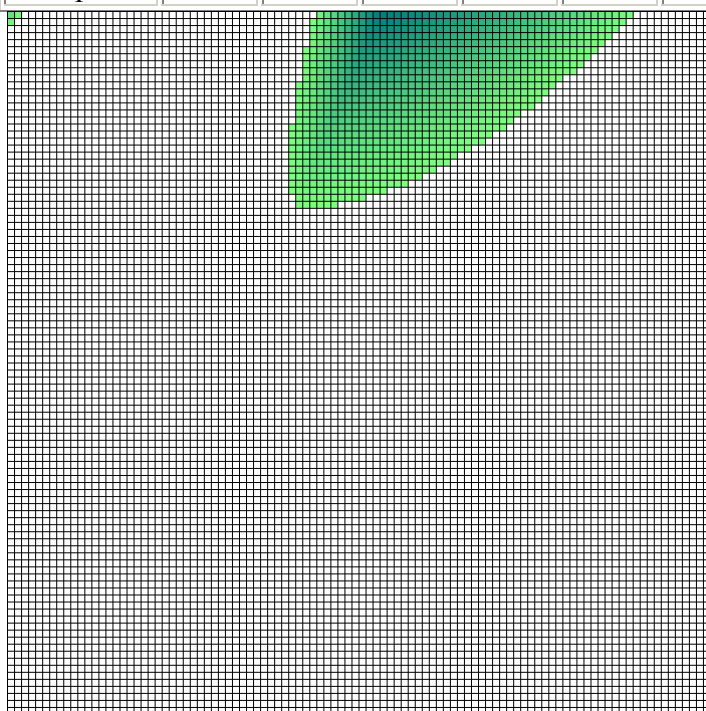
$$\Delta rf = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3$$

retention_factor	0	1	2	3	4	5	6	7	8	9
metazepam	0.8169	0.7151	0.8441	0.4849	0.3769	0.8214	0.7736	0.0560	0.6050	0.8230

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

napoton	0.8648	0.7878	0.7654	0.5509	0.5855	0.8525	0.8469	0.0550	0.7140	0.9310
nitrazepam	0.8895	0.8706	0.8584	0.6700	0.7254	0.9188	0.8691	0.1420	0.9030	0.9500
oxazepam	0.9186	0.8081	0.8455	0.7877	0.7733	0.9296	0.9149	0.2520	0.8250	0.9280
diazepam	0.9390	0.8706	0.8798	0.8278	0.8225	0.9513	0.9241	0.2720	0.8770	0.9390

7 calc	0	1	2	3	4	5	6	7	8	9
metazepam	0.8407	0.6656	0.8790	0.3895	0.4114	0.8321	0.7715	0.1033	0.6266	0.7973
napoton	0.8620	0.7711	0.9058	0.4404	0.6218	0.8449	0.8130	0.1176	0.7241	0.8531
nitrazepam	0.8977	0.8865	0.9409	0.5339	0.7569	0.9317	0.8394	0.2161	0.8920	0.9017
oxazepam	0.9236	0.8561	0.9395	0.6228	0.8048	0.9482	0.8739	0.3430	0.7969	0.8741
diazepam	0.9529	0.9035	0.9570	0.6536	0.8585	0.9749	0.8897	0.3660	0.8550	0.8922

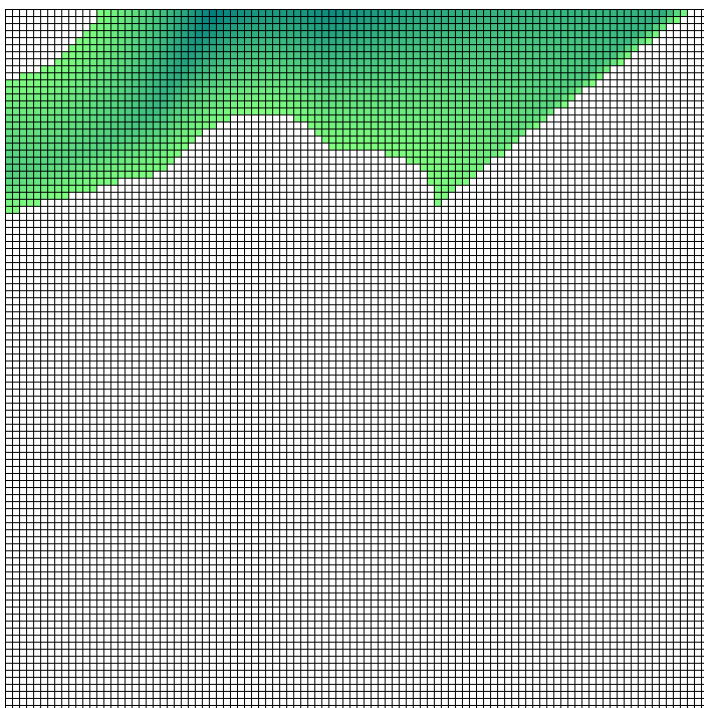


$$\text{all\_rs} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3$$

resolutions_all	0	1	2	3	4	5	6	7	8	9
(metazepam, napoton)	0.8571	1.3514	1.2500	1.1795	3.5778	0.5349	1.2043	0.0345	2.5952	3.2727
(metazepam, nitrazepam)	1.5625	2.8158	0.2985	4.0952	6.4819	1.7561	1.7590	3.2453	8.3944	3.7353
(metazepam, oxazepam)	2.0290	1.4884	0.0282	6.1159	7.2000	2.0779	2.4828	7.5385	6.1111	3.2308
(metazepam, diazepam)	2.3662	3.1014	0.6757	6.9275	8.7089	2.6301	2.3469	8.8163	7.3514	3.4627
(napoton, nitrazepam)	0.5397	1.5000	1.6883	2.8136	2.4828	1.2250	0.4595	3.1636	5.6418	0.7917

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

(napoton, oxazepam)	1.0882	0.3256	1.3827	5.0769	3.2584	1.5200	1.3333	7.2963	3.2647	0.1333
(napoton, diazepam)	1.4571	1.6522	1.9048	5.9385	4.4096	2.0563	1.3258	8.5098	4.6571	0.3404
(nitrazepam, oxazepam)	0.7273	0.9773	0.3000	3.2800	0.9024	0.2254	1.0294	4.4898	2.8364	0.9362
(nitrazepam, diazepam)	1.1930	0.0000	0.4762	4.4000	1.9737	0.7164	1.0633	5.6522	0.9123	0.4490
(oxazepam, diazepam)	0.4516	1.0617	0.7164	1.0000	0.9744	0.5161	0.1687	0.8889	1.7931	0.4783
6 calc	0	1	2	3	4	5	6	7	8	9
(metazepam, napoton)	1.2297	2.0911	1.7231	0.8779	3.2534	0.2852	0.6630	0.3175	2.2950	3.1219
(metazepam, nitrazepam)	1.8341	5.0659	1.5321	3.3541	5.8293	1.3881	0.5535	3.9097	7.3837	3.2939
(metazepam, oxazepam)	2.2571	4.0018	1.4016	5.7978	6.3414	1.5385	1.1505	8.0274	5.0143	2.7724
(metazepam, diazepam)	2.8378	5.1104	1.6402	6.8342	7.8481	2.0618	1.1900	9.1511	6.5089	3.2051
(napoton, nitrazepam)	0.7169	2.8245	0.6734	2.3515	2.1688	1.5661	0.3003	3.4298	4.9074	1.3674
(napoton, oxazepam)	1.2931	1.8339	0.5222	4.8314	2.7979	1.7228	1.0450	7.4886	2.4749	0.6701
(napoton, diazepam)	1.7820	2.8816	0.7427	5.7855	3.9676	2.2839	1.1663	8.6245	3.9977	1.0202
(nitrazepam, oxazepam)	0.3195	1.4732	0.3818	2.6251	1.1309	0.5698	1.0516	4.8053	2.5074	0.8391
(nitrazepam, diazepam)	0.9985	0.7179	0.4127	3.7940	2.0267	0.9882	0.9644	5.9739	0.4926	0.4669
(oxazepam, diazepam)	0.4809	1.1282	0.4099	0.8170	1.0109	0.6572	0.2398	0.9608	1.7252	0.6193

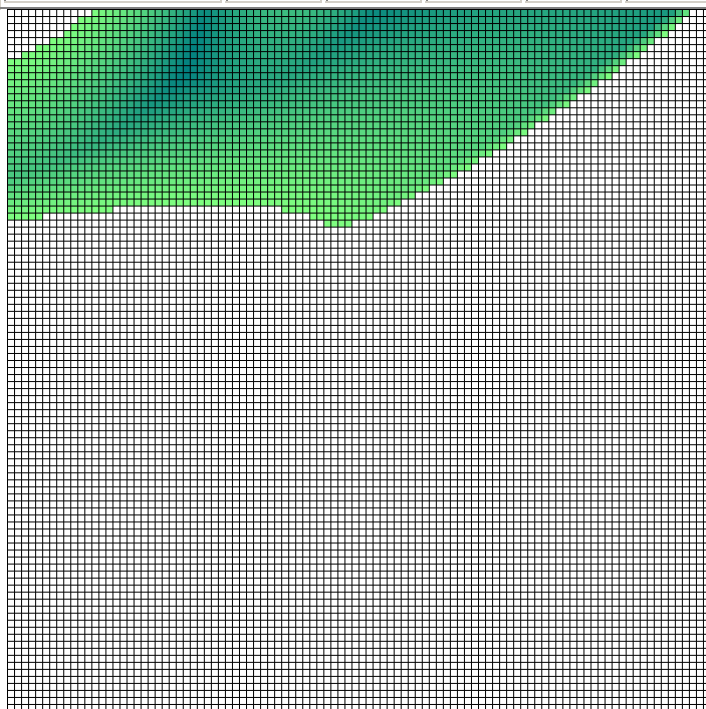


$$\text{all\_rs} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3$$

resolutions_all	0	1	2	3	4	5	6	7	8	9
(metazepam, napoton)	0.8571	1.3514	1.2500	1.1795	3.5778	0.5349	1.2043	0.0345	2.5952	3.2727
(metazepam, nitrazepam)	1.5625	2.8158	0.2985	4.0952	6.4819	1.7561	1.7590	3.2453	8.3944	3.7353
(metazepam, oxazepam)	2.0290	1.4884	0.0282	6.1159	7.2000	2.0779	2.4828	7.5385	6.1111	3.2308
(metazepam, diazepam)	2.3662	3.1014	0.6757	6.9275	8.7089	2.6301	2.3469	8.8163	7.3514	3.4627
(napoton, nitrazepam)	0.5397	1.5000	1.6883	2.8136	2.4828	1.2250	0.4595	3.1636	5.6418	0.7917
(napoton, oxazepam)	1.0882	0.3256	1.3827	5.0769	3.2584	1.5200	1.3333	7.2963	3.2647	0.1333
(napoton, diazepam)	1.4571	1.6522	1.9048	5.9385	4.4096	2.0563	1.3258	8.5098	4.6571	0.3404
(nitrazepam, oxazepam)	0.7273	0.9773	0.3000	3.2800	0.9024	0.2254	1.0294	4.4898	2.8364	0.9362
(nitrazepam, diazepam)	1.1930	0.0000	0.4762	4.4000	1.9737	0.7164	1.0633	5.6522	0.9123	0.4490
(oxazepam, diazepam)	0.4516	1.0617	0.7164	1.0000	0.9744	0.5161	0.1687	0.8889	1.7931	0.4783
7 calc	0	1	2	3	4	5	6	7	8	9
(metazepam,	0.6818	2.0572	1.6891	0.8439	3.5195	0.5513	0.9291	0.2678	2.2453	3.0722

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

napoton)										
(metazepam, nitrazepam)	1.0018	5.0143	1.4805	3.3026	6.2335	1.7923	0.9577	3.8342	7.3082	3.2184
(metazepam, oxazepam)	1.2946	3.9422	1.3419	5.7381	6.8089	2.0060	1.6180	7.9400	4.9270	2.6851
(metazepam, diazepam)	1.7846	5.0452	1.5749	6.7690	8.3596	2.5733	1.7015	9.0556	6.4133	3.1096
(napoton, nitrazepam)	0.5783	2.8159	0.6648	2.3429	2.2361	1.6334	0.3676	3.4172	4.8949	1.3549
(napoton, oxazepam)	1.0124	1.8165	0.5048	4.8140	2.9342	1.8591	1.1813	7.4632	2.4494	0.6446
(napoton, diazepam)	1.4876	2.8633	0.7245	5.7672	4.1106	2.4269	1.3093	8.5978	3.9710	0.9935
(nitrazepam, oxazepam)	0.7276	1.4985	0.4071	2.6504	0.9327	0.3716	0.8534	4.8423	2.5444	0.8761
(nitrazepam, diazepam)	1.1754	0.7288	0.4236	3.8050	1.9408	0.9023	0.8785	5.9899	0.5087	0.4830
(oxazepam, diazepam)	0.5409	1.1320	0.4136	0.8207	0.9818	0.6280	0.2107	0.9662	1.7307	0.6248

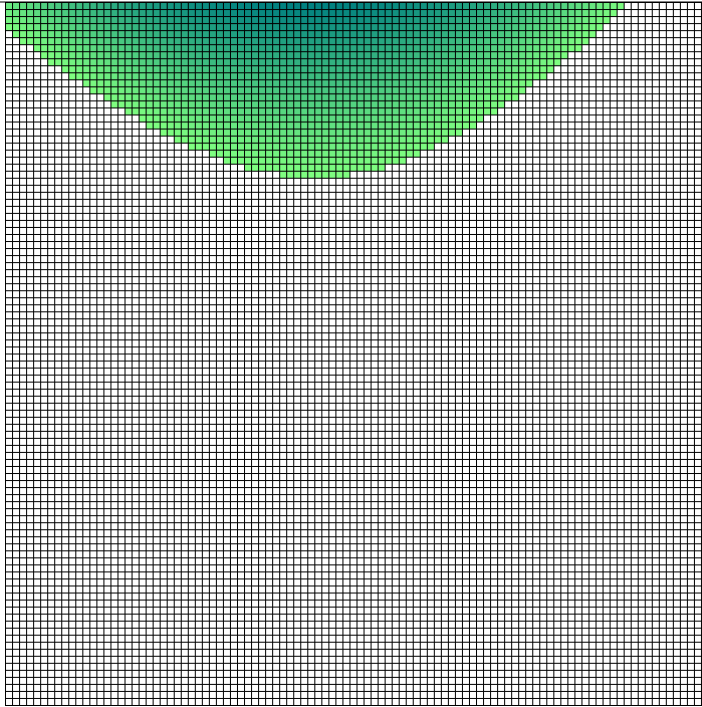


$$\text{sort\_rs} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3$$

resolutions_sort	0	1	2	3	4	5	6	7	8	9
(0, 1)	0.4516	0.0000	0.0282	1.0000	0.9024	0.2254	0.1687	0.0345	0.9123	0.1333
(1, 2)	0.5397	0.3256	0.3000	1.1795	0.9744	0.5161	0.4595	0.8889	1.7931	0.3404
(2, 3)	0.7273	0.9773	0.4762	2.8136	2.4828	0.5349	1.0294	3.2453	2.5952	0.4490

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

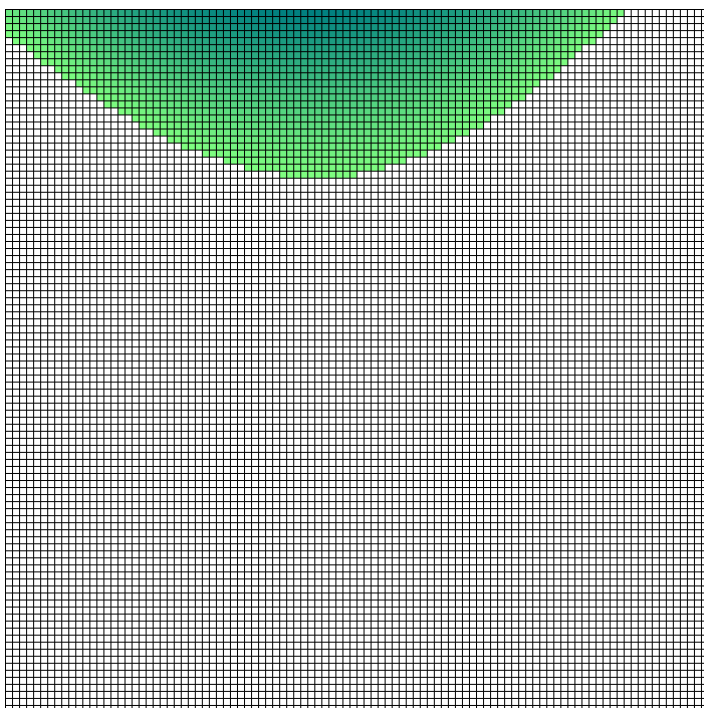
(3, 4)	0.8571	1.3514	1.2500	3.2800	3.5778	1.2250	1.2043	4.4898	3.2647	3.2308
6 calc	0	1	2	3	4	5	6	7	8	9
(0, 1)	0.4316	0.5558	0.1142	0.4957	0.8914	0.3459	0.0000	0.3257	0.6098	0.0940
(1, 2)	0.4780	0.9814	0.2976	0.8695	0.8912	0.6172	0.2901	1.0831	1.4465	0.3624
(2, 3)	0.9203	1.7346	0.3382	2.4137	2.2883	0.5911	0.7616	3.5081	2.2101	0.5651
(3, 4)	1.0586	2.1174	1.6019	3.1575	3.2684	1.0316	0.7621	4.6603	2.9376	3.1356



$$\text{sort\_rs} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3$$

resolutions_sort	0	1	2	3	4	5	6	7	8	9
(0, 1)	0.4516	0.0000	0.0282	1.0000	0.9024	0.2254	0.1687	0.0345	0.9123	0.1333
(1, 2)	0.5397	0.3256	0.3000	1.1795	0.9744	0.5161	0.4595	0.8889	1.7931	0.3404
(2, 3)	0.7273	0.9773	0.4762	2.8136	2.4828	0.5349	1.0294	3.2453	2.5952	0.4490
(3, 4)	0.8571	1.3514	1.2500	3.2800	3.5778	1.2250	1.2043	4.4898	3.2647	3.2308

7 calc	0	1	2	3	4	5	6	7	8	9
(0, 1)	0.4222	0.5552	0.1136	0.4951	0.8960	0.3504	0.0000	0.3248	0.6090	0.0931
(1, 2)	0.4658	0.9806	0.2968	0.8687	0.8971	0.6232	0.2961	1.0820	1.4454	0.3613
(2, 3)	0.6890	1.7202	0.3239	2.3994	2.4006	0.7034	0.8739	3.4871	2.1891	0.5442
(3, 4)	0.6576	2.0926	1.5771	3.1327	3.4631	1.2263	0.9568	4.6239	2.9013	3.0992



Funcții obiectiv

f_sm	0	1	2	3	4	5	6	7	8	9
f_sm	8.0234	7.7855	8.1567	6.1249	5.6269	7.9791	7.8057	7.3348	6.5468	8.1183
f_rsa	0	1	2	3	4	5	6	7	8	9
f_rsa	0.6439	0.6636	0.5136	2.0683	1.9843	0.6253	0.7155	2.1646	2.1413	1.0384
f_rrp	0	1	2	3	4	5	6	7	8	9
f_rrp	0.2359	0.0000	0.0098	5.2628	3.9361	0.1219	0.1343	0.2063	6.4725	0.0634
f_inf	0	1	2	3	4	5	6	7	8	9
f_inf	1.3710	1.5219	0.7219	1.9219	1.9219	1.9219	1.5219	1.9219	2.3219	1.3710
f_ob1	0	1	2	3	4	5	6	7	8	9
f_ob1	1.4956	1.6504	0.8445	2.0852	2.0996	2.0473	1.6500	2.0583	2.4747	1.4941
f_ob2	0	1	2	3	4	5	6	7	8	9
f_ob2	0.3177	0.3311	0.2138	0.8174	0.7574	0.3837	0.3415	0.5469	0.9572	0.3346
f_ob3	0	1	2	3	4	5	6	7	8	9
f_ob3	3.1479	3.0200	4.6768	1.2235	1.3203	2.6062	2.9286	1.8286	1.0448	2.9884
f_ob4	0	1	2	3	4	5	6	7	8	9
f_ob4	122.737	34.161	2117.983	20.156	21.155	193.932	181.678	114.281	17.966	344.884
f_ob5	0	1	2	3	4	5	6	7	8	9
f_ob5	2.3152	2.3523	1.5229	7.4805	6.7021	2.7383	2.4696	4.2967	8.8616	2.4602

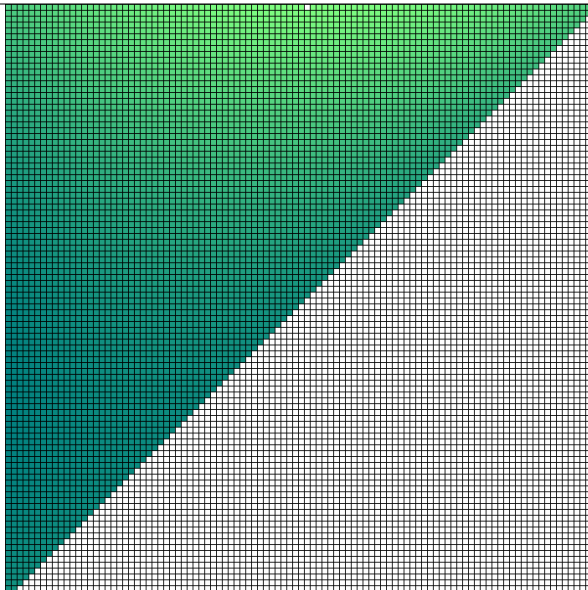
Codul sursă al funcțiilor obiectiv este redat în continuare:

```

function f_ob1($sm,$rsa,$rrp,$inf){
    for($i=0;$i<count($sm);$i++)
        $f_tot[$i]=1/$sm[$i]+$inf[$i];
    return $f_tot;
}
function f_ob2($sm,$rsa,$rrp,$inf){
    for($i=0;$i<count($sm);$i++)
        $f_tot[$i]=1/$sm[$i]+$inf[$i]/10+$inf[$i]*$rsa[$i]/20+$rrp[$i]/20;
    return $f_tot;
}
function f_ob3($sm,$rsa,$rrp,$inf){
    for($i=0;$i<count($sm);$i++)
        $f_tot[$i]=1/(1/$sm[$i]+$inf[$i]/10+$inf[$i]*$rsa[$i]/20+$rrp[$i]/20);
    return $f_tot;
}
function f_ob4($sm,$rsa,$rrp,$inf){
    for($i=0;$i<count($sm);$i++){
        $f_tot[$i]=$sm[$i];
        if($inf[$i])
            $f_tot[$i]+=10/$inf[$i];
        if(($inf[$i])&&($rsa[$i]))
            $f_tot[$i]+=20/$inf[$i]/$rsa[$i];
        if($rrp[$i])
            $f_tot[$i]+=20/$rrp[$i];
    }
    return $f_tot;
}
function f_ob5($sm,$rsa,$rrp,$inf){
    $sm=div_row($sm,array_sum($sm)/count($sm));
    $rsa=div_row($rsa,array_sum($rsa)/count($rsa));
    $rrp=div_row($rrp,array_sum($rrp)/count($rrp));
    $inf=div_row($inf,array_sum($inf)/count($inf));
    for($i=0;$i<count($sm);$i++)
        $f_tot[$i]=1/$sm[$i]+$inf[$i]+$inf[$i]*$rsa[$i]+$rrp[$i];
    return $f_tot;
}
function Worst_OF($f_oo){
    return $f_oo[0];
}
    
```

$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3$$

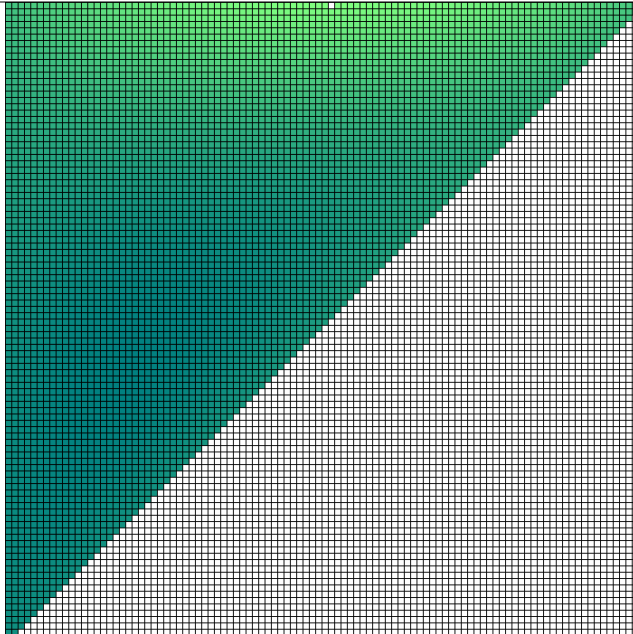
f_sm	0	1	2	3	4	5	6	7	8	9
o	8.0234	7.7855	8.1567	6.1249	5.6269	7.9791	7.8057	7.3348	6.5468	8.1183
6 calc	0	1	2	3	4	5	6	7	8	9
o	7.4340	6.9918	8.2016	6.8760	5.9002	8.0176	8.2767	6.8492	6.9263	8.0281



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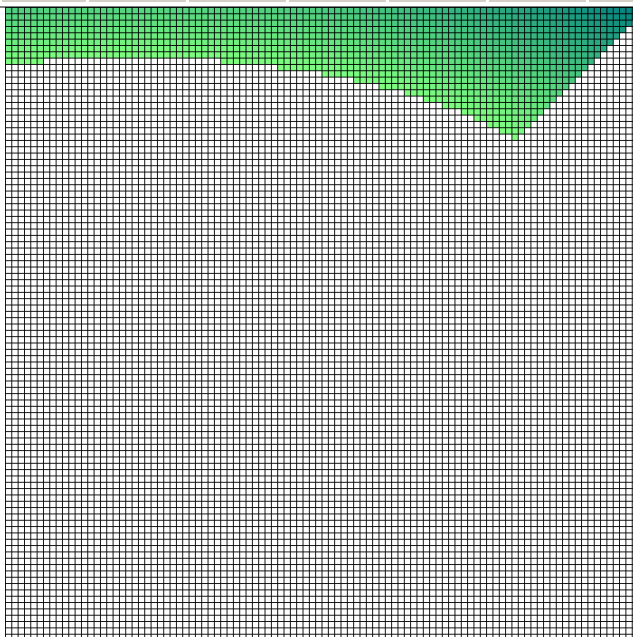
$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3$$

f_sm	0	1	2	3	4	5	6	7	8	9
o	8.0234	7.7855	8.1567	6.1249	5.6269	7.9791	7.8057	7.3348	6.5468	8.1183
7 calc	0	1	2	3	4	5	6	7	8	9
o	8.0001	7.0268	8.2367	6.9111	5.6252	7.7426	8.0018	6.9005	6.9777	8.0795



$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3$$

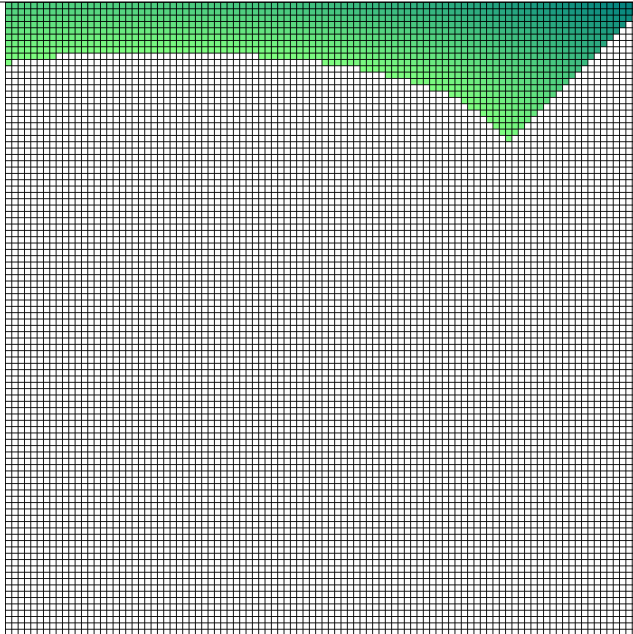
f_rsa	0	1	2	3	4	5	6	7	8	9
o	0.6439	0.6636	0.5136	2.0683	1.9843	0.6253	0.7155	2.1646	2.1413	1.0384
6 calc	0	1	2	3	4	5	6	7	8	9
o	0.7221	1.3473	0.5880	1.7341	1.8348	0.6464	0.4515	2.3943	1.8010	1.0393



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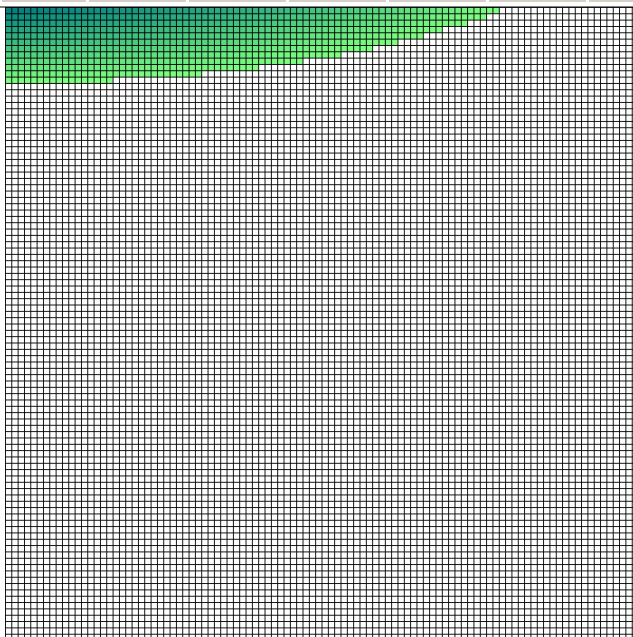
$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3$$

f_rsa	0	1	2	3	4	5	6	7	8	9
o	0.6439	0.6636	0.5136	2.0683	1.9843	0.6253	0.7155	2.1646	2.1413	1.0384
7 calc	0	1	2	3	4	5	6	7	8	9
o	0.5587	1.3372	0.5778	1.7240	1.9142	0.7258	0.5309	2.3795	1.7862	1.0245



$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3$$

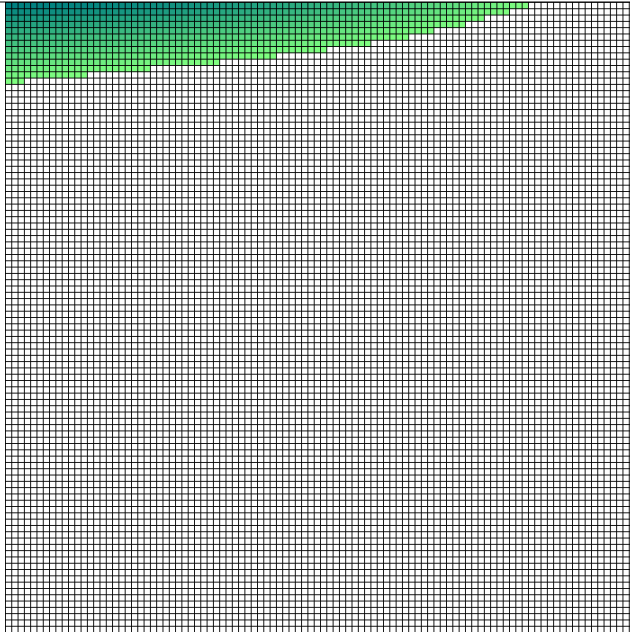
f_rrp	0	1	2	3	4	5	6	7	8	9
o	0.2359	0.0000	0.0098	5.2628	3.9361	0.1219	0.1343	0.2063	6.4725	0.0634
6 calc	0	1	2	3	4	5	6	7	8	9
o	0.8551	3.0573	0.0000	2.0160	3.7340	0.8585	0.0000	2.0542	4.7901	0.2585



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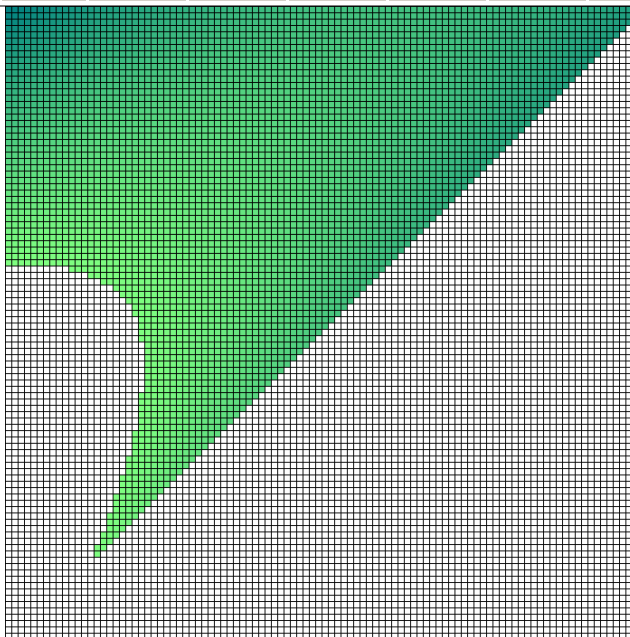
$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3$$

f_rrp	0	1	2	3	4	5	6	7	8	9
o	0.2359	0.0000	0.0098	5.2628	3.9361	0.1219	0.1343	0.2063	6.4725	0.0634
7 calc	0	1	2	3	4	5	6	7	8	9
o	0.3609	3.0267	0.0000	1.9853	3.9740	1.0985	0.0000	2.0094	4.7452	0.2136



$$f_{inf} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3$$

f_inf	0	1	2	3	4	5	6	7	8	9
o	1.3710	1.5219	0.7219	1.9219	1.9219	1.9219	1.5219	1.9219	2.3219	1.3710
6 calc	0	1	2	3	4	5	6	7	8	9
o	1.4854	1.8336	1.2258	1.8658	1.7692	1.7154	1.2125	2.0268	2.2208	1.1622

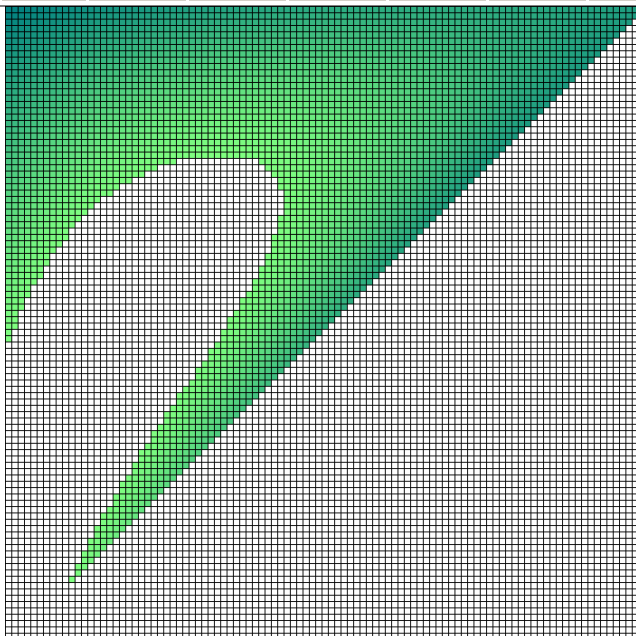


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$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3$$

f_inf	0	1	2	3	4	5	6	7	8	9
o	1.3710	1.5219	0.7219	1.9219	1.9219	1.9219	1.5219	1.9219	2.3219	1.3710

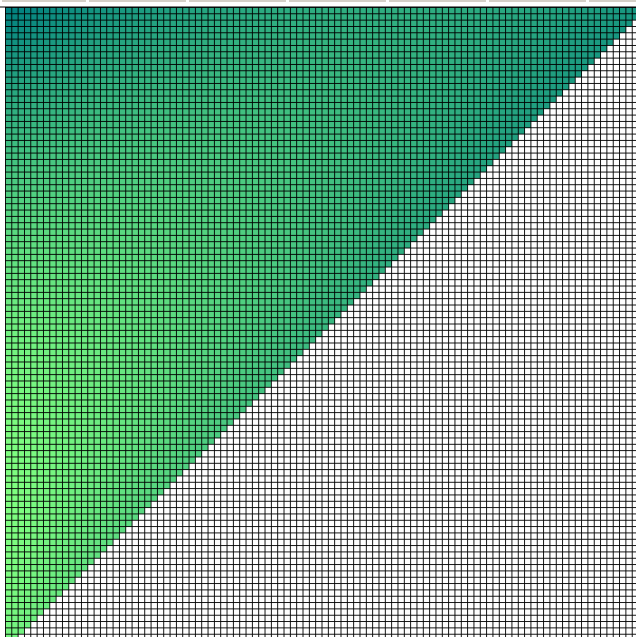
7 calc	0	1	2	3	4	5	6	7	8	9
o	1.2172	1.8170	1.2091	1.8492	1.8995	1.8457	1.3427	2.0024	2.1965	1.1379



$$f_{ob1} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3$$

f_ob1	0	1	2	3	4	5	6	7	8	9
o	1.4956	1.6504	0.8445	2.0852	2.0996	2.0473	1.6500	2.0583	2.4747	1.4941

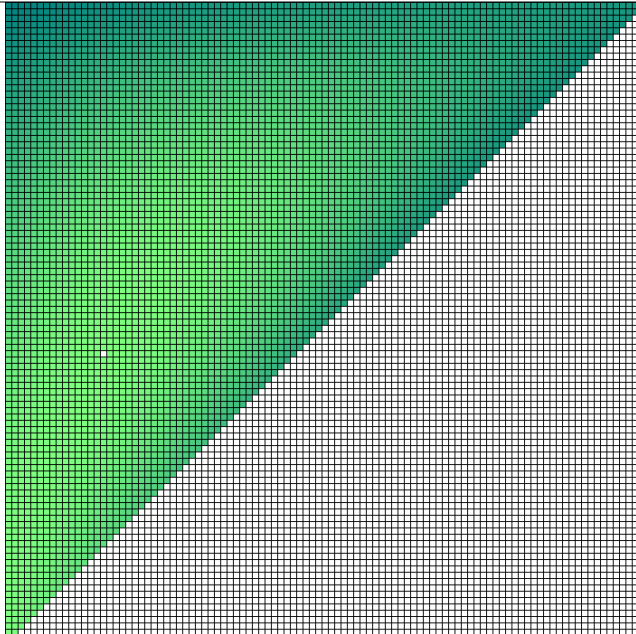
6 calc	0	1	2	3	4	5	6	7	8	9
o	1.6229	1.9790	1.3470	2.0138	1.9408	1.8397	1.3305	2.1731	2.3655	1.2876



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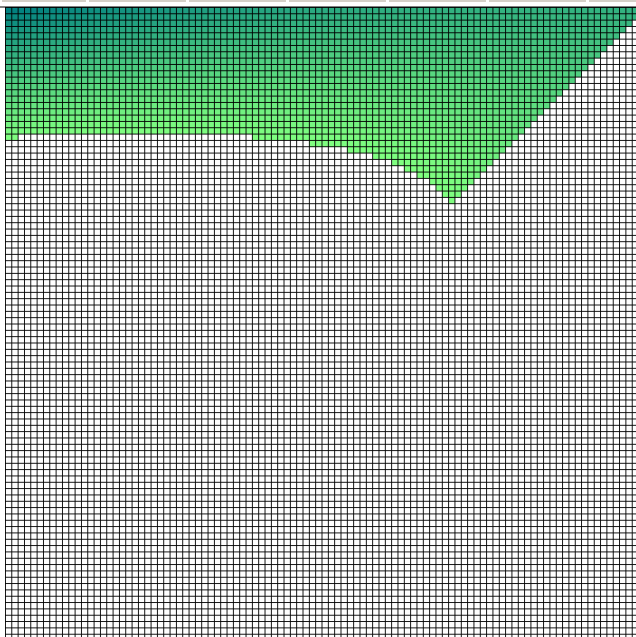
$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3$$

f_ob1	0	1	2	3	4	5	6	7	8	9
o	1.4956	1.6504	0.8445	2.0852	2.0996	2.0473	1.6500	2.0583	2.4747	1.4941
7 calc	0	1	2	3	4	5	6	7	8	9
o	1.3423	1.9616	1.3297	1.9964	2.0771	1.9760	1.4668	2.1476	2.3400	1.2621



$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3$$

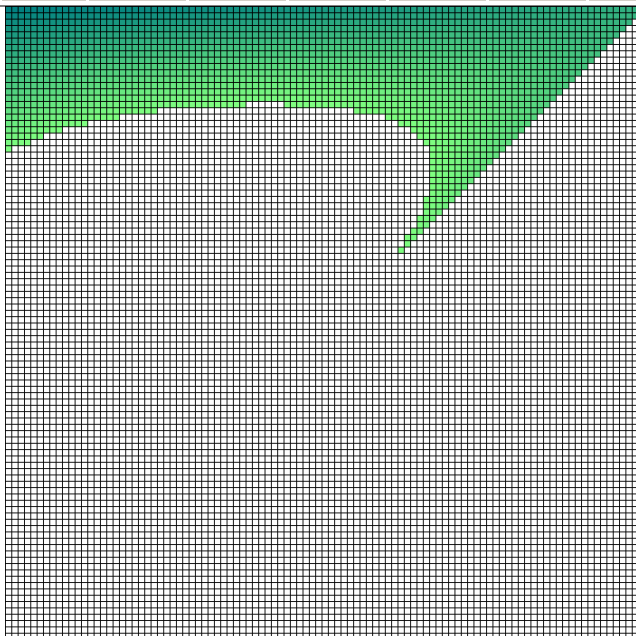
f_ob2	0	1	2	3	4	5	6	7	8	9
o	0.3177	0.3311	0.2138	0.8174	0.7574	0.3837	0.3415	0.5469	0.9572	0.3346
6 calc	0	1	2	3	4	5	6	7	8	9
o	0.3826	0.6190	0.2604	0.5994	0.7044	0.3982	0.2143	0.6854	0.8124	0.3250



*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

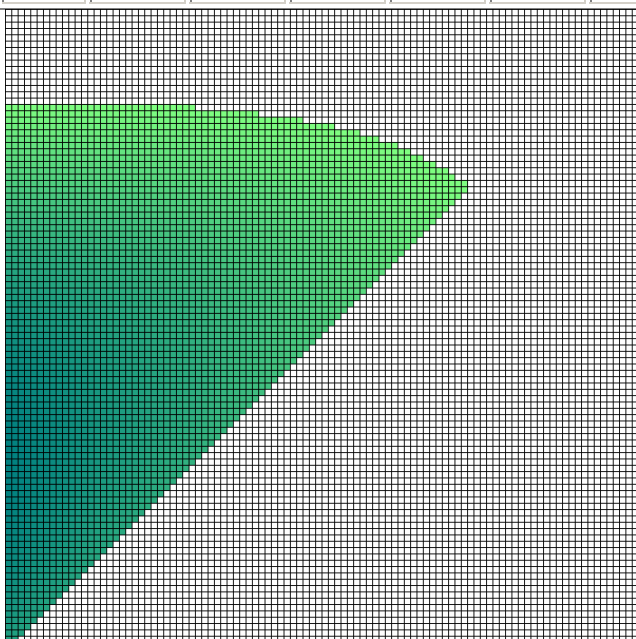
$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3$$

f_ob2	0	1	2	3	4	5	6	7	8	9
o	0.3177	0.3311	0.2138	0.8174	0.7574	0.3837	0.3415	0.5469	0.9572	0.3346
7 calc	0	1	2	3	4	5	6	7	8	9
o	0.2959	0.6137	0.2550	0.5940	0.7465	0.4403	0.2564	0.6775	0.8046	0.3172



$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3$$

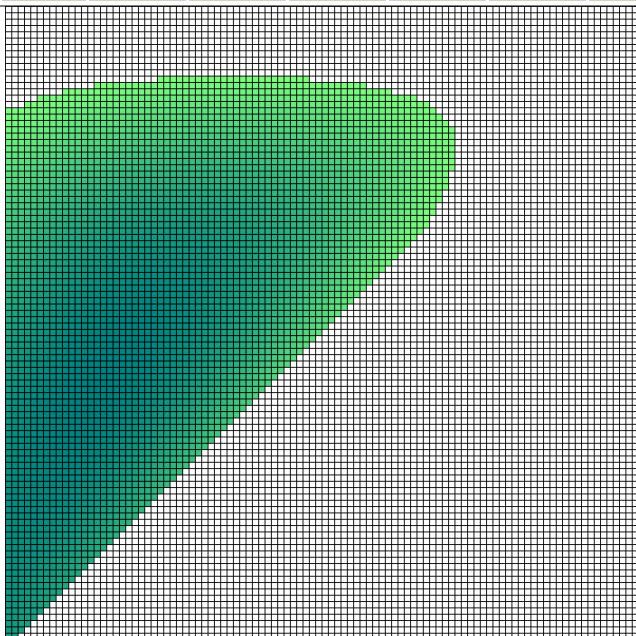
f_ob3	0	1	2	3	4	5	6	7	8	9
o	3.1479	3.0200	4.6768	1.2235	1.3203	2.6062	2.9286	1.8286	1.0448	2.9884
6 calc	0	1	2	3	4	5	6	7	8	9
o	2.9132	2.0885	3.5956	1.8330	1.5707	2.8984	3.6524	1.3491	1.4282	3.4557



*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

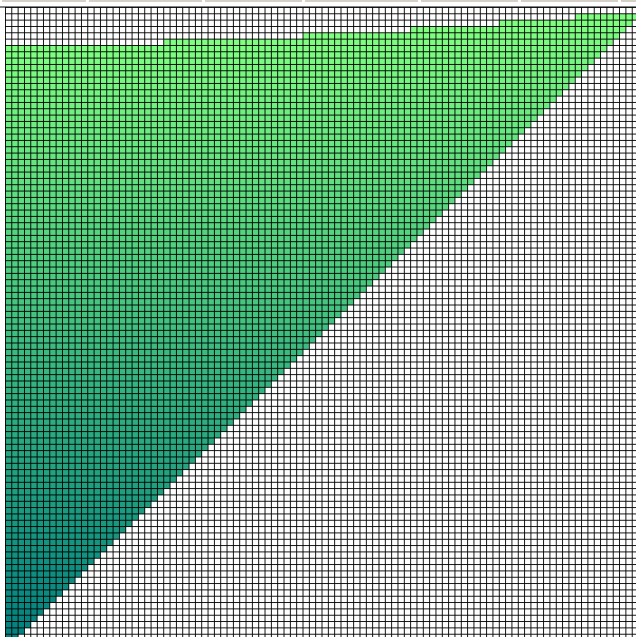
$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3$$

f_ob3	0	1	2	3	4	5	6	7	8	9
o	3.1479	3.0200	4.6768	1.2235	1.3203	2.6062	2.9286	1.8286	1.0448	2.9884
7 calc	0	1	2	3	4	5	6	7	8	9
o	3.4311	2.1205	3.6277	1.8651	1.3192	2.6469	3.4009	1.3960	1.4752	3.5027



$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3$$

f_ob4	0	1	2	3	4	5	6	7	8	9
o	122.737	34.161	2117.983	20.159	21.155	193.932	181.678	114.281	17.966	344.884
6 calc	0	1	2	3	4	5	6	7	8	9
o	322.752	53.868	806.964	91.138	0.0000	501.239	503.341	0.0000	0.0000	1003.540

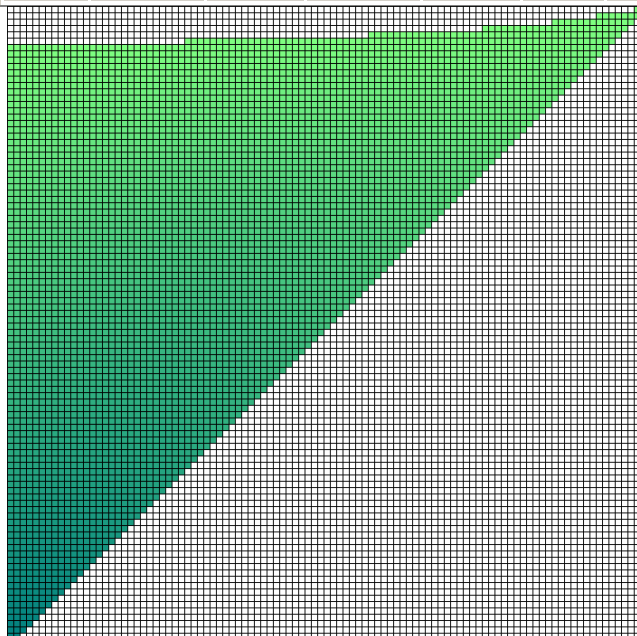


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$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3$$

f_ob4	0	1	2	3	4	5	6	7	8	9
o	122.737	34.161	2117.983	20.159	21.155	193.932	181.678	114.281	17.966	344.884

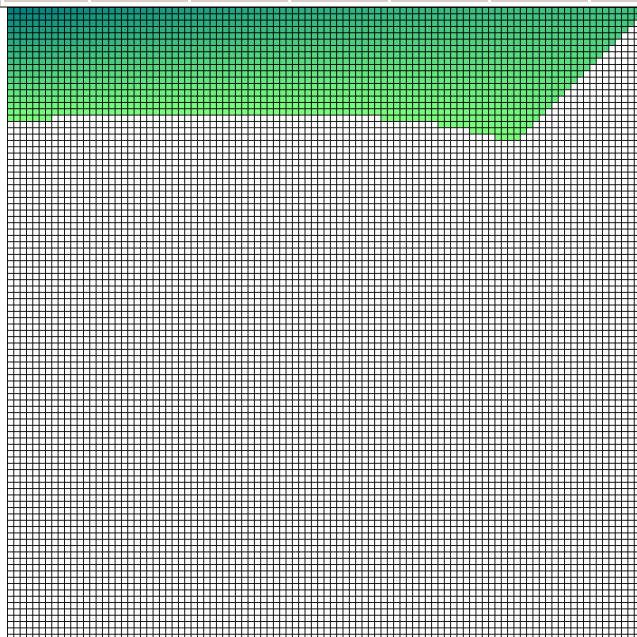
7 calc	0	1	2	3	4	5	6	7	8	9
o	384.629	57.702	810.798	94.971	0.000	471.186	473.288	4.633	0.000	1009.154



$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3$$

f_ob5	0	1	2	3	4	5	6	7	8	9
o	2.3152	2.3523	1.5229	7.4805	6.7021	2.7383	2.4696	4.2967	8.8616	2.4602

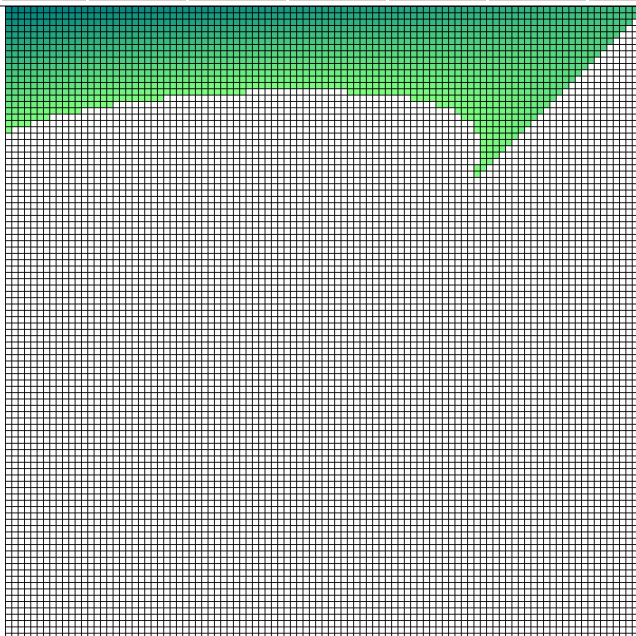
6 calc	0	1	2	3	4	5	6	7	8	9
o	2.9487	5.3632	1.7570	5.0249	6.2341	3.0477	1.2485	5.8051	7.3088	2.4623



**ET108/2006 – Et. Finală/2007 – Lucrare in extenso**

$$f_{of} = a_1x_1 + a_2x_2 + a_3x_3 + a_4x_1x_2 + a_5x_1x_3 + a_6x_2x_3 + a_7x_1x_2x_3$$

f_ob5	0	1	2	3	4	5	6	7	8	9
o	2.3152	2.3523	1.5229	7.4805	6.7021	2.7383	2.4696	4.2967	8.8616	2.4602
7 calc	0	1	2	3	4	5	6	7	8	9
o	2.1753	5.3152	1.7090	4.9769	6.6097	3.4234	1.6241	5.7349	7.2386	2.3922



**Etapa 3, Activitatea 2. Corelarea cu experimentele, alegerea funcțiilor obiectiv optime**

÷ Așa cum a rezultat din analiza rezultatelor experimentale (parte din ele prezentate mai sus) funcția obiectiv optimă pentru modelarea cinetică a reacțiilor chimice este:

```

procedure s_CC(var x,y:x_array; n_e:longint; o_o_s: extended; var s_sum: extended);
var
  i : longint; i_n : longint; n_s : longint; s1,s2,p1,p2 : extended;
begin
  n_s := 6*n_e div 14;
  s1 := 0.0; s2 := 0.0; p1 := 0.0; p2 := 0.0; i_n := 0;
  for i:= 1 to n_s do if(y[i]<o_o_s) then begin
    s1 := s1 + y[i]/x[i]; s2 := s2 + x[i]/y[i];
    i_n := i_n + 1;
  end;
  s1 := s1/i_n; s2 := s2/i_n;
  for i:= 1 to n_s do if(y[i]<o_o_s) then begin
    p1 := p1 + power(abs(y[i]/x[i]-s1),4.0);
    p2 := p2 + power(abs(x[i]/y[i]-s2),4.0);
  end;
  s_sum := power(p1*p2,0.5);
end;
    
```

funcție care penalizează după formula:

$$\min \leftarrow \sqrt{\left( \sum_{i=0}^N \left( \frac{X_i}{t_i} - \frac{\bar{X}}{\bar{t}} \right)^4 \right) \left( \sum_{i=0}^N \left( \frac{t_i}{X_i} - \frac{\bar{t}}{\bar{X}} \right)^4 \right)}$$

÷ În cazul optimizării fazei mobile a amestecurilor de solvenți pentru cromatografie, o serie de funcții obiectiv au dovedit abilitate predictivă. Lista acestor funcții împreună cu predicția realizată este redată în tabelul de mai jos:

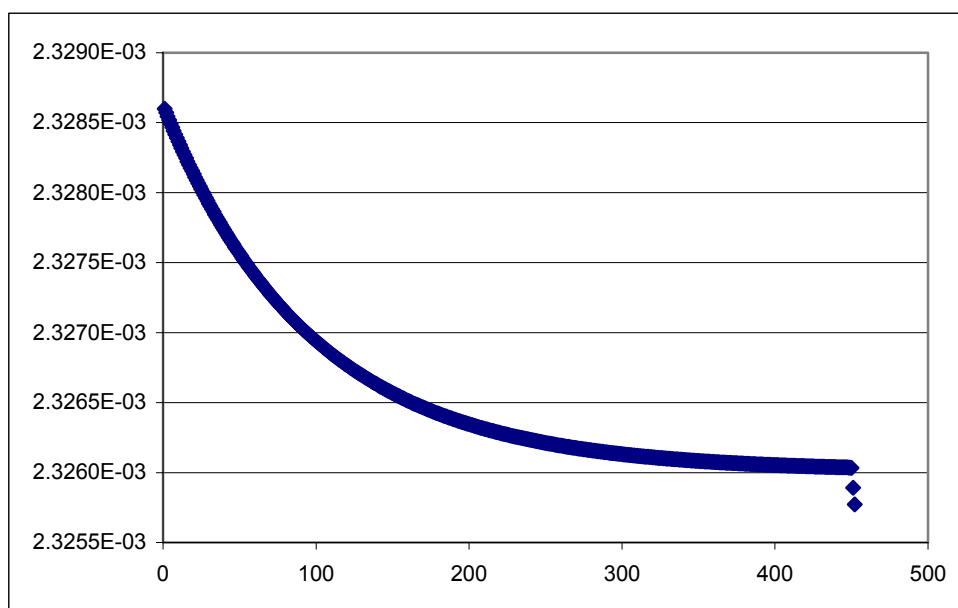
Funcție	Punct de optim (CHCl <sub>3</sub> :i-PrOH:Me <sub>2</sub> O)		
Δrf-M6	54	0	46
Δrf-M7	53	0	47
sort_rs-M6	42	0	58
sort_rs-M7	42	0	58
f_sm-M6	51	0	49
f_sm-M7	51	0	49
f_ob4-M7	57	4	39

Ultima dintre aceste funcții (f\_ob4) s-a dovedit a fi cel mai aproape de cazul ideal experimental, când pentru optimizarea amestecului propus s-a observat prin analiza factorială completă (variind întâi din 20 în 20 unități fiecare concentrație de solvent - un număr total de 20 de experimente, apoi pe domeniul cel mai potrivit variind din 5 în 5 unități - un număr total de 12 experimente, apoi variind din 1 în 1 - un număr total de 20 experimente), a rezultat concentrația optimă a fazei mobile ca fiind CHCl<sub>3</sub>:i-PrOH:Me<sub>2</sub>O = 55:5:40.

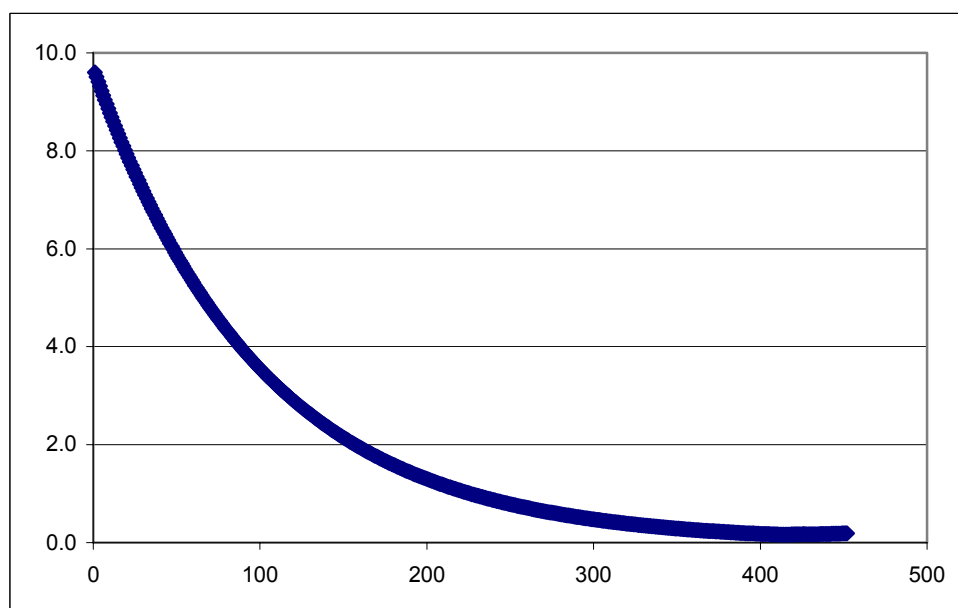
**Etapa 3, Activitatea 3. Calcularea parametrilor de model prin optimizare, și a parametrilor de experiment prin formule de calcul**

Modul de calcul al parametrilor de model prin optimizare și a parametrilor de experiment prin formule de calcul s-a ilustrat în expunerea rezultatelor de la etapele anterioare.

În continuare se redau grafic rezultatele obținute prin iterarea până la iterația 452 a coeficientului de extincție (constantă necunoscută) de model cinetic pentru cea mai bogată sursă de date, experimentul pentru concentrații ale reactanților de  $10^{-2}M$ , precum și variația sumei reziduurilor:

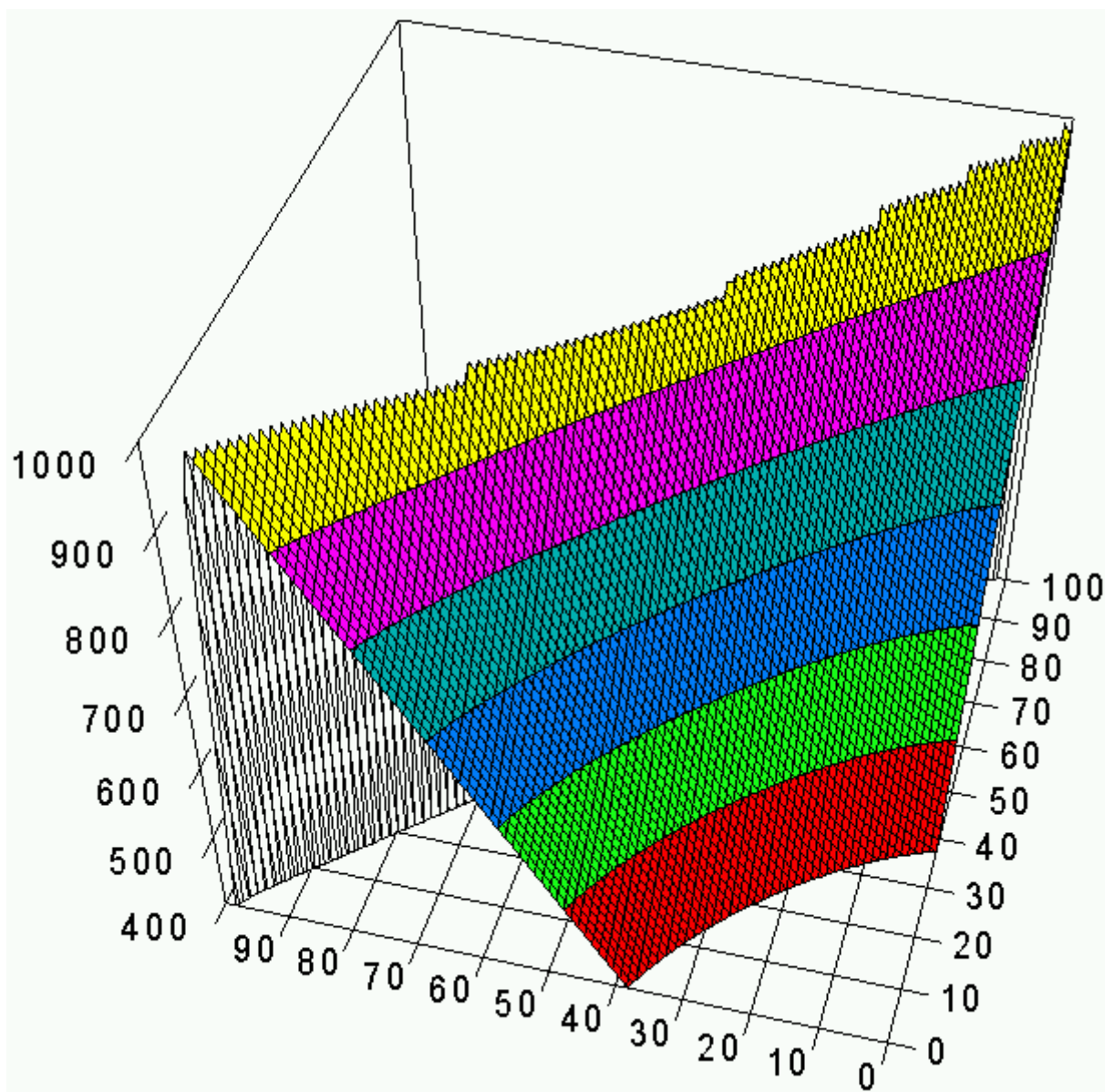


Valori ale coeficientului de extincție,  $\epsilon$

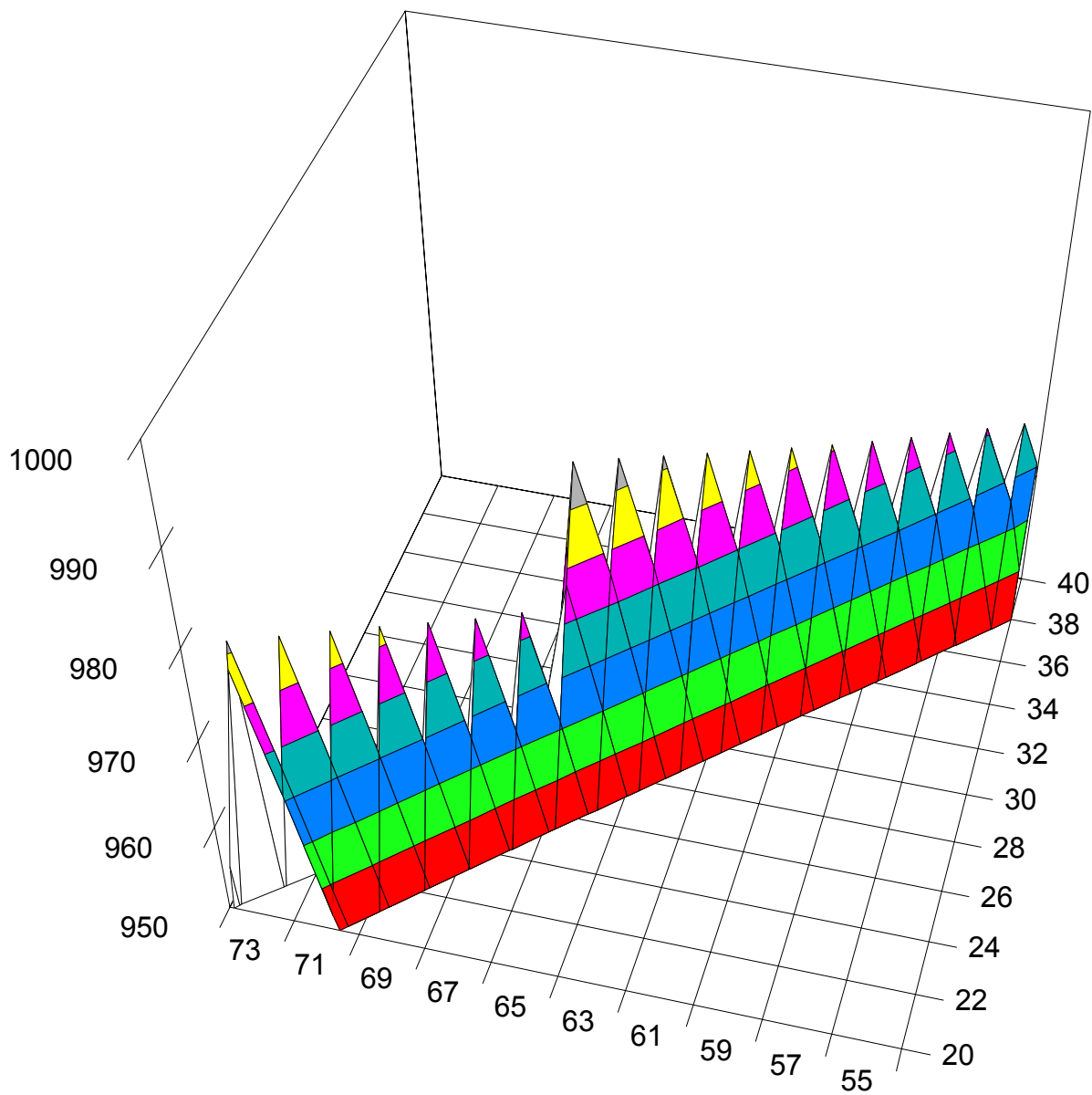


Valori ale funcției de penalitate (suma reziduurilor), S

Parametrii de model și parametrii de experiment au fost calculați și pentru compoziția optimă a fazei mobile folosind funcția obiectiv  $f_{ob4}$  și modelul cu 7 termeni (M7). Cu ajutorul lor s-a reprezentat suprafața de variație a funcției obiectiv în funcție de concentrațiile  $CHCl_3$  și  $Me_2O$ , grafic care este redat în continuare.



Graficul detaliat în regiunea de interes este reprezentat în următoarea figură:



*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

**Etapa 1, Activitatea 4, Etapa 2, Activitatea 2, și Etapa 3, Activitatea 4. Participări la manifestări științifice și dobândirea de competențe complementare**


S-a participat la manifestări științifice pentru dobândirea de competențe complementare în fiecare etapă.

Astfel în etapa 1 s-a participat cu lucrări științifice la 2 conferințe internaționale:


	Lorentz JÄNTSCHI, Sorana Daniela BOLBOACĂ, Processes Kinetics Modeling: A Numerical Study, Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences [ <a href="http://sizemat.igic.bas.bg">http://sizemat.igic.bas.bg</a> ], FP6: EC-INCO-CT-2005-016414 Specific Support Action, Plovdiv, Bulgaria, April 19-21, 2007.
	Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI, Data Mining on Structure-Activity/Property Relationships Models, The 11th Electronic Computational Chemistry Conference, online, Monmouth University, New Jersey, USA, <a href="http://www.Internet">www, Internet</a> , paper #29, ECCC11, April 2-30, 2007.

În etapa 2 s-a participat cu lucrări științifice la 2 conferințe internaționale:


	Carmen E. STOENOIU, Lorentz JÄNTSCHI, Ioan ABRUDAN, Sorana D. BOLBOACĂ, Romanian Higher Education: Modelling Evolution Tendencies, The International Management Education Conference 2007 Proceedings, Faculty of Business and Economics, University Pendidikan Sultan Idris, ISBN 978-983-3759-19-4, Penang, Malaysia, paper #10§02 (6 pages), 2007. Lorentz JÄNTSCHI, Carmen E. STOENOIU, Sorana D. BOLBOACĂ, Research Policy via Funding Allocation Analysis, The International Management Education Conference 2007 Proceedings, Faculty of Business and Economics,
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	<p>University Pendidikan Sultan Idris, ISBN 978-983-3759-19-4, Penang, Malaysia, paper #10§03 (7 pages), 2007.</p>
	<p>Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI, Modelling the Inhibitory Activity on Carbonic Anhydrase I of Some Substituted Thiadiazole- and Thiadiazoline-Disulfonamides: Integration of Structure Information, ESCAPE17 - 17th European Symposium on Computer Aided Process Engineering, CAPE Working Party of the European Federation of Chemical Engineering then Elsevier Netherlands &amp; UK, ISBN 978-0-444-53157-5 &amp; eISBN 0-444-53158-2, Bucharest, Romania then Amsterdam, Netherlands, T4-212 (oral presentation), May 27-30 then p. 965-970, 2007.</p>

În etapa 3 s-a participat cu lucrări științifice la 2 conferințe internaționale:

 <p>Fourth International Conference of Applied Mathematics and Computing August 12 - 18, 2007 Plovdiv, Bulgaria</p>	<p>Sorana-Daniela BOLBOACĂ, Lorentz JÄNTSCHI, Structure-Property Based Model Estimation of Alkanes Boiling Points, Fourth International Conference of Applied Mathematics and Computing, August 12-18, 2007, University of Chemical Technology and Metallurgy Sofia &amp; Technical University of Plovdiv, Invited lecture, presented on August 13, from 18.30 to 19.00, Plovdiv, Bulgaria, p. 48, 2007.</p> <p>Carmen Elena STOENOIU, Sorana-Daniela BOLBOACĂ, Lorentz JÄNTSCHI, Model Formulation and Interpretation for Chemical Reactions Mechanisms - From Experiment to Theory, Fourth International Conference of Applied Mathematics and Computing, August 12-</p>
--	--

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

	<p>18, 2007, University of Chemical Technology and Metallurgy Sofia &amp; Technical University of Plovdiv, Invited lecture, presented on August 15, from 11.30 to 12.10, Plovdiv, Bulgaria, p. 511, 2007.</p>
 <p>19-23 September, 2007 Sunny Beach, Bulgaria</p>	<p>Lorentz JÄNTSCHI, Sorana D. BOLBOACĂ, Molecular Descriptors Family on Chromatography, BBCAC-4 4th Black Sea Basin Conference on Analytical Chemistry, "St. Kliment Ohridski" University of Sofia, Poster P128, Sunny Beach, Bulgaria, September 19-23, 2007.</p> <p>Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI, Solvent Mixtures Tool for Separation of Biological Active Compounds, BBCAC-4 4th Black Sea Basin Conference on Analytical Chemistry, "St. Kliment Ohridski" University of Sofia, Poster P127, Sunny Beach, Bulgaria, September 19-23, 2007.</p>

### Publicații

Următoarele publicații valorifică rezultatele obținute ca urmare a cercetării derulate prin prezentul grant în anul 2007:

Nr	Tip	Publicație
1	Articol indexat în baze de date internaționale	<b>Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI</b> , <i>Amino Acids Sequences Analysis on Collagen</i> , Bulletin of University of Agricultural Sciences and Veterinary Medicine - Animal Sciences and Biotechnologies, AcademicPres, ISSN 1843-5262, eISSN 1843-536X, Cluj-Napoca, Romania, 63-64, p. 311-316, <b>2007</b> .
2	Conferință internațională	<b>Lorentz JÄNTSCHI, Sorana D. BOLBOACĂ</b> , <i>Molecular Descriptors Family on Chromatography</i> , BBCAC-4 4 <sup>th</sup> Black Sea Basin Conference on Analytical Chemistry, “St. Kliment Ohridski” University of Sofia, Poster P128, Sunny Beach, Bulgaria, September 19-23, <b>2007</b> .
3	Conferință internațională	<b>Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI</b> , <i>Solvent Mixtures Tool for Separation of Biological Active Compounds</i> , BBCAC-4 4 <sup>th</sup> Black Sea Basin Conference on Analytical Chemistry, “St. Kliment Ohridski” University of Sofia, Poster P127, Sunny Beach, Bulgaria, September 19-23, <b>2007</b> .
4	Conferință internațională, articol indexat IEEE	<b>Lorentz JÄNTSCHI, Mugur BĂLAN, Margareta Emilia PODAR, Sorana Daniela BOLBOACĂ</b> , <i>Thermal Energy Efficiency Analysis for Residential Buildings</i> , Eurocon 2007 Conference, IEEE Region 8, Poster 143, Warsaw, Poland, September 9-12, <b>2007</b> , <i>IEEE Region 8 Eurocon 2007: The International Conference on Computer as a Tool - Proceedings (ISBN: 1-4244-0813-X, IEEE: 07EX1617C, LoC: 2006937182)</i> , 2009-2014, <b>2007</b>
5	Articol indexat Thompson ISI	<b>Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI</b> , <i>Data Mining on Structure-Activity/Property Relationships Models</i> , World Applied Sciences Journal, IDOSI Publications, ISSN 1818-4952, www, Internet & Faisalabad, Pakistan, 2(4), p. 323-332,

		<b>2007.</b>
6	Conferință internațională, viitor articol indexat în baze de date internaționale	<b>Sorana-Daniela BOLBOACĂ, Lorentz JÄNTSCHI,</b> <i>Structure-Property Based Model Estimation of Alkanes Boiling Points</i> , Fourth International Conference of Applied Mathematics and Computing, August 12-18, 2007, University of Chemical Technology and Metallurgy Sofia & Technical University of Plovdiv, Invited lecture, presented on August 13, from 18.30 to 19.00, Plovdiv, Bulgaria, p. 48, <b>2007,</b> <b><i>International Journal of Pure and Applied Mathematics, 40(3), p. XX-YY, 2007.</i></b>
7	Conferință internațională, viitor articol indexat în baze de date internaționale	<b>Carmen Elena STOENOIU, Sorana-Daniela BOLBOACĂ, Lorentz JÄNTSCHI,</b> <i>Model Formulation and Interpretation for Chemical Reactions Mechanisms - From Experiment to Theory</i> , Fourth International Conference of Applied Mathematics and Computing, August 12-18, 2007, University of Chemical Technology and Metallurgy Sofia & Technical University of Plovdiv, Invited lecture, presented on August 15, from 11.30 to 12.10, Plovdiv, Bulgaria, p. 511, <b>2007,</b> <b><i>International Journal of Pure and Applied Mathematics, 40(3), p. XX-YY, 2007.</i></b>
8	Lucrare în revistă indexată CNCSIS tip B	<b>Lorentz JÄNTSCHI, Sorana D. BOLBOACĂ,</b> <i>Antiallergic Activity of Substituted Benzamides: Characterization, Estimation and Prediction</i> , Clujul Medical, Editura Iuliu Hatieganu, ISSN 1222-2119, Cluj-Napoca, Romania, LXXX(1), p. 125-132, <b>2007.</b>
9	Articol indexat Thompson ISI SCI Expanded	<b>Lorentz JÄNTSCHI, Sorin HODIȘAN, Claudia CIMPOIU, Anamaria HOSU, Eugen DARVASI, Teodor HODIȘAN,</b> <i>Modeling of thin-layer chromatographic separation of androstane isomers</i> , JPC - Journal of Planar Chromatography - Modern TLC, Akadémiai Kiadó, ISSN 0933-4173, Budapest, Hungary, 20(2), p. 91-94, <b>2007.</b>
10	Conferință	<b>Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI,</b> <i>Modelling the</i>

	<p>internațională, articol indexat în baze de date internaționale</p>	<p><i>Inhibitory Activity on Carbonic Anhydrase I of Some Substituted Thiadiazole- and Thiadiazoline-Disulfonamides: Integration of Structure Information</i>, ESCAPE17 - 17th European Symposium on Computer Aided Process Engineering, CAPE Working Party of the European Federation of Chemical Engineering then Elsevier Netherlands &amp; UK, ISBN 978-0-444-53157-5 &amp; eISBN 0-444-53158-2, Bucharest, Romania then Amsterdam, Netherlands, T4-212 (oral presentation), May 27-30 then p. 965-970, <b>2007</b>, Computer-Aided Chemical Engineering, Elsevier Netherlands &amp; UK, eISSN 1570-7946, Amsterdam, Netherlands, 24(2007), p. 965-970, <b>2007</b>.</p>
11	<p>Carte în lb. engleză</p>	<p><b>Lorentz JÄNTSCHI</b>, <i>Characteristic and Counting Polynomials of Nonane Isomers</i>, AcademicDirect, ISBN 973-86211-3-5 &amp; ISBN 980-973-86211-3-8, www, Internet, p. 101, <b>2007</b>.</p>
12	<p>Articol indexat în baze de date internaționale</p>	<p><b>Lorentz JÄNTSCHI, Sorana D. BOLBOACĂ</b>, <i>The Jungle of Linear Regression Revisited</i>, Leonardo Electronic Journal of Practices and Technologies, AcademicDirect, ISSN 1583-1078, www, Internet, 6(10), p. 169-187, <b>2007</b>.</p>
13	<p>Articol indexat Thompson ISI SCI Expanded</p>	<p><b>Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI</b>, <i>How Good the Characteristic Polynomial Can Be for Correlations?</i>, International Journal of Molecular Sciences, <a href="#">Molecular Diversity Preservation International</a>, ISSN 1422-0067, www &amp; Basel, Internet &amp; Switzerland, 8(4), p. 335-345, <b>2007</b>.</p>
14	<p>Conferință internațională și articol indexat Thompson ISI SCI Expanded</p>	<p><b>Lorentz JÄNTSCHI, Sorana-Daniela BOLBOACĂ</b>, <i>Modeling the Octanol-Water Partition Coefficient of Substituted Phenols by the Use of Structure Information</i>, International Journal of Quantum Chemistry, Wiley InterScience, ISSN 0020-7608, eISSN 1097-461X, New York, NY, USA, Volume 107, Issue 8 (Special Issue: Proceedings from the 3rd Humboldt Conference on Computational Chemistry . Issue Edited by Georgi N. Vayssilov, Tzonka Mineva), p. 1736-1744, <b>2007</b>.</p>

15	Conferință internațională	<b>Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI</b> , <i>Data Mining on Structure-Activity/Property Relationships Models</i> , ECC11-The 11th <a href="#">Electronic Computational Chemistry Conference</a> , online, Monmouth University, New Jersey, USA, N/A, www, Internet, paper #29, April 2-30, <b>2007</b> .
16	Conferință internațională	<b>Lorentz JÄNTSCHI, Sorana Daniela BOLBOACĂ</b> , <i>Processes Kinetics Modeling: A Numerical Study</i> , Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences [http://sizemat.igic.bas.bg], FP6: EC-INCO-CT-2005-016414 Specific Support Action, Plovdiv, Bulgaria, p. 72-73, April 19-21, <b>2007</b> .
17	Conferință internațională și viitor articol indexat Thompson ISI SCI Expanded	<b>Sorana Daniela BOLBOACĂ, Lorentz JÄNTSCHI</b> , <i>Modeling the Property of Compounds from Structure: Statistical Methods for Models Validation</i> , Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences [http://sizemat.igic.bas.bg], FP6: EC-INCO-CT-2005-016414 Specific Support Action, Plovdiv, Bulgaria, p. 71, April 19-21, <b>2007</b> , <i>Environmental Chemistry Letters</i> , <a href="https://doi.org/10.1007/s10311-007-0119-9">DOI 10.1007/s10311-007-0119-9</a>
18	Conferință internațională	<b>Carmen Elena STOENOIU, Sorana Daniela BOLBOACĂ, Lorentz JÄNTSCHI</b> , <i>Characterization of Marine Sediments Toxicity based on Structural Information</i> , Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences [http://sizemat.igic.bas.bg], FP6: EC-INCO-CT-2005-016414 Specific Support Action, Plovdiv, Bulgaria, p. 54, April 19-21, <b>2007</b> .
19	Articol indexat Thompson ISI SCI Expanded	<b>Lorentz JÄNTSCHI, Sorana BOLBOACĂ</b> , <i>Results from the Use of Molecular Descriptors Family on Structure Property/Activity Relationships</i> , International Journal of Molecular Sciences, <a href="#">Molecular Diversity Preservation International</a> , ISSN 1422-0067, www & Basel, Internet & Switzerland, <a href="#">8(3), p. 189-203</a> , <b>2007</b> .

**Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI**, *Amino Acids Sequences Analysis on Collagen*,  
Bulletin of University of Agricultural Sciences and Veterinary Medicine - Animal Sciences  
and Biotechnologies, AcademicPres, ISSN 1843-5262, eISSN 1843-536X, Cluj-Napoca,  
Romania, 63-64, p. 311-316, **2007**.

- [id] => 158
- [recorddate] => 2007:10:06:17:47:01
- [lastupdate] => 2007:10:06:17:47:01
- [type] => article
- [place] => Cluj-Napoca, Romania
- [subject] => engineering - agriculture; medicine - evidence based; medicine - informatics
- [relatedworks] =>
  - 4 (some):
    - National Trends on Agricultural Crops Production: Cluster Analysis, [?id=155](#)
    - The Control of the Infrastructure of the Rural Water Wells in the Plain Area, [?id=156](#)
- [file] => [?f=158](#)
- [mime] => application/pdf
- [size] => 421293
- [pubname] => Bulletin of University of Agricultural Sciences and Veterinary Medicine - Animal Sciences and Biotechnologies
- [pubinfo] => AcademicPres
- [pubkey] => ISSN 1843-5262, eISSN 1843-536X
- [workinfo] => 63-64, p. 311-316
- [year] => 2007
- [title] => Amino Acids Sequences Analysis on Collagen
- [authors] => Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI
- [abstract] =>

Starting from available information about amino acids properties and sequences on collagen type I chains, the aims of the study were to identify the principal property component and to analyze the similarities within and between collagens on five species. The principal component analysis applied on twentyfour amino acids properties revealed that the hydrophobic or hydrophilic character measured by Wealling et al. is more stable comparing with the other investigated properties. Similarity analysis identified similar and dissimilar within and between studied species from the viewpoint of amino acids sequences on collagen type I alpha 1 and 2 chains.
- [keywords] => Amino Acids; Collagen Type I; Properties; Multivariate Analysis
- [acknowledgment] => The research was partly supported by CNCSIS Romania through project AT93/2007 and UEFISCSU Romania through project ET108/2006.

*Lorentz JÄNTSCHI, Sorana D. BOLBOACĂ, Molecular Descriptors Family on Chromatography, BBCAC-4 4<sup>th</sup> Black Sea Basin Conference on Analytical Chemistry, “St. Kliment Ohridski” University of Sofia, Poster P128, Sunny Beach, Bulgaria, September 19-23, 2007.*

- [id] => 154
- [recorddate] => 2007:10:06:17:03:37
- [lastupdate] => 2007:10:06:17:03:37
- [type] => conference
- [place] => Sunny Beach, Bulgaria
- [subject] => chemistry - analytical; chemistry - organic; informatics - models implementation; informatics - web programming
- [relatedworks] =>
  - 2 (average):
    - Solvent Mixtures Tool for Separation of Biological Active Compounds, [?id=153](#)
  - 3 (low):
    - Information Theory and Others for Steroids Separation, [?id=100](#)
  - 4 (some):
    - QSPR on Estimating of Polychlorinated Biphenyls Relative Response Factor using Molecular Descriptors Family, [?id=40](#)
- [pubname] => BBCAC-4 4th Black Sea Basin Conference on Analytical Chemistry
- [pubinfo] => "St. Kliment Ohridski" University of Sofia
- [pubkey] => Poster P128
- [workinfo] => September 19-23
- [year] => 2007
- [title] => Molecular Descriptors Family on Chromatography
- [authors] => Lorentz JÄNTSCHI, Sorana D. BOLBOACĂ
- [abstract] =>

A new method on Structure-Activity Relationships methodology was been recently defined. It is uses so called Molecular Descriptors Family, a set of molecular descriptors obtained purely from molecular structure, by using tools of molecular topology and 3D geometry.

The experiments made on three sets of compounds on which retention time was measured in same experimental conditions on every set shown a good ability of the method to predict the retention time.

The method can serve as a tool for unknown samples on which a given compound is suspected to be present. The method can provide the expected retention time, and the confidence band where this compound is expected to be found, if it is present. Note that the method can produce reliable results only when experimental conditions of known compounds determinations are the same with the conditions for unknown compounds, such as are in same sample.
- [keywords] => Structure-retention relationships
- [acknowledgment] => Thanks for financial support from UEFISCSU Romania, through Grant no. 108/2006.

**Sorana D. BOLBOACĂ, Lorentz JĂNTSCHI**, *Solvent Mixtures Tool for Separation of Biological Active Compounds*, BBCAC-4 4<sup>th</sup> Black Sea Basin Conference on Analytical Chemistry, “St. Kliment Ohridski” University of Sofia, Poster P127, Sunny Beach, Bulgaria, September 19-23, 2007.

- [id] => 153
- [recorddate] => 2007:10:06:17:02:35
- [lastupdate] => 2007:10:06:17:02:35
- [type] => conference
- [place] => Sunny Beach, Bulgaria
- [subject] => chemistry - analytical; informatics - models implementation; informatics - web programming
- [relatedworks] =>
  - 2 (average):
    - Molecular Descriptors Family on Chromatography, [?id=154](#)
  - 3 (low):
    - Free Software Development. 3. Numerical Description of Soft Acid with Soft Base Titration, [?id=14](#)
- [pubname] => BBCAC-4 4th Black Sea Basin Conference on Analytical Chemistry
- [pubinfo] => "St. Kliment Ohridski" University of Sofia
- [pubkey] => Poster P127
- [workinfo] => September 19-23
- [year] => 2007
- [title] => Solvent Mixtures Tool for Separation of Biological Active Compounds
- [authors] => Sorana D. BOLBOACĂ, Lorentz JĂNTSCHI
- [abstract] =>

Chromatographic mobile phase mixtures offer a great opportunity for better analytical separation in both qualitative TLC and quantitative HPLC methods. The chromatographic mobile phase preparation involves a numeric taxonomy procedure for mixture constituents selecting, based on solvent strengths, and a optimization of its composition based on a series of factorial analysis designed experiments [1,2]. A set of samples containing compounds with same biological activity were investigated using the previous described procedures. A mathematical model was build in order to apply the factorial analysis on given set of experiments. Following classes were subject of the investigations: steroids, androstane isomers, hydrophilic vitamins, N-alkyl phenothiazine sulfones, and benzodiazepines. Features of the developed application are underlined, such as choosing of the mathematical model type (with six of seven unknown parameters), choosing of the desired chromatographic parameter (retention time, resolution, information energy, etc.), choosing of behavior of the objective function (minimizing of, or maximizing of), and choosing the plot characteristics (colors, domain of interest, etc.). The application is available online and it is freely to be use:  
[http://l.academicdirect.org/Engineering/hptlc/mobile\\_phase\\_opt/](http://l.academicdirect.org/Engineering/hptlc/mobile_phase_opt/)  
The mobile phase optimization process proved to be able to provide accurate, precise and reproducible method on characterization and analysis of chromatographic parameters.
- [keywords] => Mobile phase optimization
- [acknowledgment] => Acknowledgment Thanks for financial support from UEFISCSU Romania, through Grant no. 108/2006.

**Lorentz JÄNTSCHI, Mugur BĂLAN, Margareta Emilia PODAR, Sorana Daniela BOLBOACĂ**, *Thermal Energy Efficiency Analysis for Residential Buildings*, Eurocon 2007 Conference, IEEE Region 8, Poster 143, Warsaw, Poland, September 9-12, **2007**, *IEEE Region 8 Eurocon 2007: The International Conference on Computer as a Tool - Proceedings (ISBN: 1-4244-0813-X, IEEE: 07EX1617C, LoC: 2006937182)*, 2009-2014, **2007**.

- [id] => 148
- [recorddate] => 2007:10:06:15:24:40
- [lastupdate] => 2007:10:06:15:24:40
- [type] => conference
- [place] => Warsaw, Poland
- [subject] => education - training; informatics - applied
- [relatedworks] =>
  - 4 (some):
    - Computer Aided System for Student's Knowledge Assessment, [?id=91](#)
- [file] => [?f=148](#)
- [mime] => application/pdf
- [size] => 358642
- [pubname] => Eurocon 2007 Conference
- [pubinfo] => IEEE Region 8
- [pubkey] => Poster 143
- [workinfo] => September 9-12
- [year] => 2007
- [title] => Thermal Energy Efficiency Analysis for Residential Buildings
- [authors] => Lorentz JÄNTSCHI, Mugur BĂLAN, Margareta Emilia PODAR, Sorana Daniela BOLBOACĂ
- [abstract] =>

The concern of energy conservation, the reduction of green house gases and sustainability was continuously growing in last years. The concept of green building has been introduced, and refers the practice of increasing the efficiency with which buildings and their sites use and harvest energy, water, and materials, and reducing building impacts on human health and on environment, through better design, construction, operation, maintenance, and removal. Starting from the national and international trends in development of environmental performance of new and existing home buildings, an interactive system for assisting the calculation of home energy efficiency has been created and validated, and its performances are presented.
- [keywords] => online application; energetics; civil constructions

**Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI**, *Data Mining on Structure-Activity/Property Relationships Models*, World Applied Sciences Journal, IDOSI Publications, ISSN 1818-4952, www, Internet & Faisalabad, Pakistan, 2(4), p. 323-332, **2007**.

- [id] => 147
- [recorddate] => 2007:08:20:19:17:54
- [lastupdate] => 2007:08:20:19:17:54
- [type] => article
- [place] => www, Internet & Faisalabad, Pakistan
- [subject] => chemistry - computational; informatics - applied; mathematics - statistics; research - evaluation
- [relatedworks] =>
  - 2 (average):
    - MDF - A New QSAR/QSPR Molecular Descriptors Family, [?id=33](#)
- [file] => [?f=147](#)
- [mime] => application/pdf
- [size] => 220742
- [pubname] => World Applied Sciences Journal
- [pubinfo] => IDOSI Publications
- [pubkey] => ISSN 1818-4952
- [workinfo] => 2(4), p. 323-332
- [year] => 2007
- [title] => Data Mining on Structure-Activity/Property Relationships Models
- [authors] => Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI
- [abstract] =>

Molecular descriptors family on structure-activity/property relationships studies were carried out in order to identify the link between compounds structure and their activity/property. A number of fifty-five classes of properties or activities of different compounds sets were investigated. Single and multi-varied linear regression models using molecular descriptors as variables were identified. The models with estimation and prediction abilities and associated characteristics were stored into a database. A data mining analysis using classification and clustering were applied on the obtained database for searching and extracting useful information. The methodology applied in searching and extracting for information and the obtained results are presented.
- [keywords] => Knowledge-Discovery in Database (KDD); cluster analysis; Structure-Activity/Property Relationships (SAR/SPR); Molecular Descriptors Family (MDF)

**Sorana-Daniela BOLBOACĂ, Lorentz JÄNTSCHI**, *Structure-Property Based Model Estimation of Alkanes Boiling Points*, Fourth International Conference of Applied Mathematics and Computing, August 12-18, 2007, University of Chemical Technology and Metallurgy Sofia & Technical University of Plovdiv, Invited lecture, presented on August 13, from 18.30 to 19.00, Plovdiv, Bulgaria, p. 48, **2007**, *International Journal of Pure and Applied Mathematics*, 40(3), p. XX-YY, 2007.

- [id] => 145
- [recorddate] => 2007:08:19:19:14:50
- [lastupdate] => 2007:08:19:19:14:50
- [type] => conference
- [place] => Plovdiv, Bulgaria
- [subject] => chemistry - computational; chemistry - organic; chemistry - physical; informatics - fundamentals; mathematics - applied; mathematics - modeling; mathematics - statistics
- [relatedworks] =>
  - 2 (average):
    - Characteristic and Counting Polynomials on Modeling Nonane Isomers Properties, [?id=144](#)
  - 4 (some):
    - Modeling the Octanol-Water Partition Coefficient of Substituted Phenols by the Use of Structure Information, [?id=127](#)
- [pubname] => Fourth International Conference of Applied Mathematics and Computing, August 12-18, 2007
- [pubinfo] => University of Chemical Technology and Metallurgy Sofia & Technical University of Plovdiv
- [pubkey] => Invited lecture, presented on August 13, from 18.30 to 19.00
- [workinfo] => p. 48
- [year] => 2007
- [title] => Structure-Property Based Model Estimation of Alkanes Boiling Points
- [authors] => Sorana-Daniela BOLBOACĂ, Lorentz JÄNTSCHI
- [abstract] =>

This study discusses a family of molecular descriptors on structure-property relationships (MDF SPR) to model the boiling points of alkanes based on their chemical structure.

The proposed approach uses the complex information obtained from the all alkanes from C3 to C9 structures in order to generate and calculate the molecular descriptors family. The structure-property relationship models were built based on the generated descriptors.

The obtained models (model with one and two descriptors, respectively) were validated through the assessment of the cross-validation leave-one-out score. The comparison between the uni-varied model and the model with two descriptors was performed using Steiger's Z test. The best performing MDF SPR model was validated, and its correlation coefficient was compared with a previously reported model.

The analysis of the statistical characteristics of the obtained models demonstrated that the model with two descriptors has greater abilities in estimation and prediction

***ET108/2006 – Et. Finală/2007 – Lucrare in extenso***

compared with the model with one descriptor. This observation was also sustained by the results of training versus test analysis.

The results of this study revealed that the MDF SPR approach is a useful method to model the boiling points of alkanes providing stable models.

- [keywords] => Molecular Descriptor Family on Structure-Property Relationships (MDF SPR); Models assessment; Boiling point; Alkanes
- [acknowledgment] => UEFISCSU Romania – ET36/2005 & ET108/2006; Fourth International Conference of Applied Mathematics and Computing Organizers - Professor Drumi BAINOV

*Carmen Elena STOENOIU, Sorana-Daniela BOLBOACĂ, Lorentz JÄNTSCHI, Model Formulation and Interpretation for Chemical Reactions Mechanisms - From Experiment to Theory, Fourth International Conference of Applied Mathematics and Computing, August 12-18, 2007, University of Chemical Technology and Metallurgy Sofia & Technical University of Plovdiv, Invited lecture, presented on August 15, from 11.30 to 12.10, Plovdiv, Bulgaria, p. 511, 2007, International Journal of Pure and Applied Mathematics, 40(3), p. XX-YY, 2007.*

- [id] => 142
- [recorddate] => 2007:08:19:18:58:43
- [lastupdate] => 2007:08:19:18:58:43
- [type] => conference
- [place] => Plovdiv, Bulgaria
- [subject] => chemistry - computational; chemistry - inorganic; chemistry - physical; mathematics - applied
- [relatedworks] => N/A
- [file] => [?f=142](#)
- [mime] => application/pdf
- [size] => 300862
- [pubname] => Fourth International Conference of Applied Mathematics and Computing, August 12-18, 2007
- [pubinfo] => University of Chemical Technology and Metallurgy Sofia & Technical University of Plovdiv
- [pubkey] => Invited lecture, presented on August 15, from 11.30 to 12.10
- [workinfo] => p. 511
- [year] => 2007
- [title] => Model Formulation and Interpretation for Chemical Reactions Mechanisms - From Experiment to Theory
- [authors] => Carmen Elena STOENOIU, Sorana-Daniela BOLBOACĂ, Lorentz JÄNTSCHI
- [abstract] =>

From kinetics study of a given pair of reactants different types of mechanisms were investigated. A mathematical model was formulated. Model parameters were evaluated and assessed. Obtained results from the optimization procedure opened an interesting discussion about the limits of parameters obtained from experiments data for imposed conditions, such as mechanism type and collecting procedure. By using of a least squares method, obtained models as best fits correlates with experimental measurements; the results shown an average of 96.6% for a sample size average of 2967 pairs of data.

Comparing the results obtained by different experiments, all obtained parameters, which were not related with the experimental conditions, were in same range of 95% confidence interval. These results validates experimental data and as well as data obtained by model.
- [keywords] => Mathematical modeling; Chemical reaction mechanism; Model assessment

**Lorentz JĂNTSCHI, Sorana D. BOLBOACĂ**, *Antiallergic Activity of Substituted Benzamides: Characterization, Estimation and Prediction*, Clujul Medical, Editura Iuliu Hatieganu, ISSN 1222-2119, Cluj-Napoca, Romania, LXXX(1), p. 125-132, 2007.

- [id] => 137
- [recorddate] => 2007:06:16:18:57:12
- [lastupdate] => 2007:06:16:18:57:12
- [type] => article
- [place] => Cluj-Napoca, Romania
- [subject] => chemistry - biochemistry; chemistry - computational; informatics - models implementation; mathematics - modeling; mathematics - statistics; medicine - immunology
- [relatedworks] =>
- 4 (some):
  - Modelling the Inhibitory Activity on Carbonic Anhydrase I of Some Substituted Thiadiazole- and Thiadiazoline-Disulfonamides: Integration of Structure Information, [?id=131](#)
  - Modelling the Inhibitory Activity on Carbonic Anhydrase I of Some Substituted Thiadiazole and Thiadiazoline-Disulfonamides: Integration of Structure Information, [?id=133](#)
- [pubname] => Clujul Medical
- [pubinfo] => Editura Iuliu Hatieganu
- [pubkey] => ISSN 1222-2119
- [workinfo] => LXXX(1), p. 125-132
- [year] => 2007
- [title] => Antiallergic Activity of Substituted Benzamides: Characterization, Estimation and Prediction
- [authors] => Lorentz JĂNTSCHI, Sorana D. BOLBOACĂ
- [abstract] =>

Antiallergic activity of twenty-three substituted N 4-methoxyphenyl benzamides was model by the use of an original methodology. After sketching out the compounds structure and creating the file with the observed activities, strictly based on compounds structure, the molecular descriptors family was generated and descriptors entered into a multiple linear regression analysis. The multi-varied model with four descriptors proved to render higher ability in estimation (squared correlation coefficient,  $r^2 = 0.9986$ ) as well as in prediction (cross-validation leave-one-out score,  $r^2_{cv-loo} = 0.9956$ ) of antiallergic activity of compounds, obtained significantly greater correlation coefficient compared with the previously reported model ( $p < 0.01$ ).

Characterization of antiallergic activity of substituted N 4-methoxyphenyl benzamides by integration of complex structure information provides a stable and efficient multivaried model with four descriptors. According with the multi-varied model with four descriptors the antiallergic activity of substituted N 4-methoxyphenyl benzamides is like to be of geometry nature, depending by the number of directly bonded hydrogen's, and the atomic relative mass, being in relation with the partial charge of compounds.
- [keywords] => Molecular Descriptors Family on Structure-Activity Relationships (MDF-SAR); Substituted N 4-methoxyphenyl benzamides; Antiallergic activity; Multiple linear regression (MLR)
- [acknowledgment] => Research was in partly supported by UEFISCSU Romania through project ET108/2006.

**Lorentz JÄNTSCHI, Sorin HODIȘAN, Claudia CIMPOIU, Anamaria HOSU, Eugen DARVASI, Teodor HODIȘAN**, *Modeling of thin-layer chromatographic separation of androstane isomers*, JPC - Journal of Planar Chromatography - Modern TLC, Akadémiai Kiadó, ISSN 0933-4173, Budapest, Hungary, 20(2), p. 91-94, 2007.

- [id] => 134
- [recorddate] => 2007:06:01:13:30:04
- [lastupdate] => 2007:06:01:13:30:04
- [type] => article
- [place] => Budapest, Hungary
- [subject] => chemistry - analytical; chemistry - biochemistry; informatics - applied; informatics - models implementation; informatics - numerical optimization; mathematics - modeling; mathematics - optimization
- [relatedworks] => N/A
- [file] => [?f=134](#)
- [size] => 65927
- [pubname] => JPC - Journal of Planar Chromatography - Modern TLC
- [pubinfo] => Akadémiai Kiadó
- [pubkey] => ISSN 0933-4173
- [workinfo] => 20(2), p. 91-94
- [year] => 2007
- [title] => Modeling of thin-layer chromatographic separation of androstane isomers
- [authors] => Lorentz JÄNTSCHI, Sorin HODIȘAN, Claudia CIMPOIU, Anamaria HOSU, Eugen DARVASI, Teodor HODIȘAN
- [abstract] =>  
Modeling of thin-layer chromatographic separation of androstane isomers to find the optimum mobile phase is described in this paper. The isomers of androstane are present in a variety of samples, so achieving their optimum thin-layer chromatographic separation is very important. A mathematical model was developed and tested. The model takes into account the interaction between solvents and uses a complex function for modeling, so it provides reliable results. The proposed mathematical model gives results similar to those obtained by use of other optimization models, for example the ‘Simplex’ and ‘Prisma’ methods.
- [keywords] => Androstane isomers; Separation modeling; Thin-layer chromatography; Mobile-phase optimization

**Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI**, *Modelling the Inhibitory Activity on Carbonic Anhydrase I of Some Substituted Thiadiazole- and Thiadiazoline-Disulfonamides: Integration of Structure Information*, ESCAPE17 - 17th European Symposium on Computer Aided Process Engineering, CAPE Working Party of the European Federation of Chemical Engineering then Elsevier Netherlands & UK, ISBN 978-0-444-53157-5 & eISBN 0-444-53158-2, Bucharest, Romania then Amsterdam, Netherlands, T4-212 (oral presentation), May 27-30 then p. 965-970, **2007**, Computer-Aided Chemical Engineering, Elsevier Netherlands & UK, eISSN 1570-7946, Amsterdam, Netherlands, 24(2007), p. 965-970, **2007**.

- [id] => 131
- [recorddate] => 2007:05:07:17:08:31
- [lastupdate] => 2007:05:30:13:24:00
- [type] => conference
- [place] => Bucharest, Romania then Amsterdam, Netherlands
- [subject] => chemistry - biochemistry; chemistry - computational; informatics - applied; informatics - models implementation; mathematics - modeling; mathematics - statistics; medicine - immunology; medicine - informatics
- [relatedworks] =>
  - 0 (highest):
    - Modelling the Inhibitory Activity on Carbonic Anhydrase I of Some Substituted Thiadiazoleand Thiadiazoline-Disulfonamides: Integration of Structure Information, [?id=133](#)
  - 4 (some):
    - Antiallergic Activity of Substituted Benzamides: Characterization, Estimation and Prediction, [?id=137](#)
- [file] => [?f=131](#)
- [mime] => application/pdf
- [size] => 1335735
- [pubname] => ESCAPE17 - 17th European Symposium on Computer Aided Process Engineering
- [pubinfo] => CAPE Working Party of the European Federation of Chemical Engineering then Elsevier Netherlands & UK
- [pubkey] => ISBN 978-0-444-53157-5 & eISBN 0-444-53158-2
- [workinfo] => T4-212 (oral presentation), May 27-30 then p. 965-970
- [year] => 2007
- [title] => Modelling the Inhibitory Activity on Carbonic Anhydrase I of Some Substituted Thiadiazole- and Thiadiazoline-Disulfonamides: Integration of Structure Information
- [authors] => Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI
- [abstract] =>

Aim: The paper presents the abilities in estimation and prediction of the inhibition on carbonic anhydrase I of some substituted 1,3,4-thiadiazole- and 1,3,4-thiadiazoline-disulfonamides through the integration of complex structures information by using of an original molecular descriptors family on the structure-activity relationships

approach.

**Material and Method:** The proposed approach uses the complex information obtained from substituted 1,3,4-thiadiazole- and 1,3,4-thiadiazoline-disulfonamides structure in order to generate and calculate the molecular descriptors family. The structure-activity relationship models were built based on the generated descriptors. The obtained multivariate models (the models with two, respectively four descriptors) were validated by computing the cross-validation leave-one-out score ( $r_{2cv-loo}$ ), and analyzed through assessment of the squared correlation coefficients ( $r^2$ ), and the models stability ( $r^2 - r_{2cv-loo}$ ). The prediction ability of the multivariate MDF-SAR model with four descriptors was analyzed in training versus test sets.

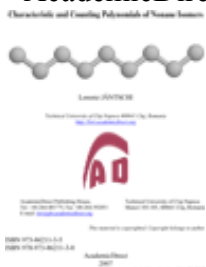
**Results:** The best performing MDF-SAR model proved to be the model with four descriptors ( $r^2 = 0.9175$ ). The MDF-SAR model with four descriptors shown that the inhibition on carbonic anhydrase I of substituted 1,3,4-thiadiazole- and 1,3,4-thiadiazoline-disulfonamides is likely to be of geometry and topology nature, being in relation with the partial charge and relative atomic mass of compounds. The estimation ability of this model is sustained by the multiple correlation coefficient ( $r = 0.9579$ , 95%CI = [0.9212, 0.9776]) and by the significance of the model ( $F = 97$ ,  $p < 0.001$ ). The prediction ability is sustained by the cross validation leave-one-out score ( $r_{2cv-loo} = 0.8911$ ), the model stability ( $r^2 - r_{2cv-loo} = 0.0264$ ), and by the results on training versus test analysis. The MDF-SAR model with four descriptors proved to render higher value of the correlation coefficient comparing with previously reported model ( $p < 0.01$ ).

**Conclusion:** Modelling the inhibition activity on carbonic anhydrase I of substituted 1,3,4-thiadiazole- and 1,3,4-thiadiazoline-disulfonamides by integration of complex structure information provide stable MDF-SAR models, revealing that there is a relationship between the compounds structure and their inhibition activity on carbonic anhydrase I.

- [keywords] => Molecular Descriptors Family on Structure-Activity Relationships (MDF-SAR); Substituted 1,3,4-Thiadiazole- and 1,3,4-Thiadiazoline-Disulfonamides; Carbonic Anhydrase I (CA I); Inhibition Activity
- [acknowledgment] => The research was partly supported by UEFISCSU Romania through project ET108/2006.

**Lorentz JÄNTSCHI**, *Characteristic and Counting Polynomials of Nonane Isomers*,  
AcademicDirect, ISBN 973-86211-3-5 & ISBN 980-973-86211-3-8, www, Internet, p. 101,  
**2007.**

- [id] => 132
- [recorddate] => 2007:05:28:17:05:32
- [lastupdate] => 2007:05:28:17:06:03
- [type] => book
- [place] => www, Internet
- [subject] => chemistry - computational; chemistry - organic; informatics - applied; mathematics - modeling
- [relatedworks] => N/A
- [file] => [?f=132](#)
- [size] => 5511299
- [pubname] => AcademicDirect



- [pubinfo] =>
- [pubkey] => ISBN 973-86211-3-5 & ISBN 980-973-86211-3-8
- [workinfo] => p. 101
- [year] => 2007
- [title] => Characteristic and Counting Polynomials of Nonane Isomers
- [authors] => Lorentz JÄNTSCHI
- [abstract] =>  
The characteristic and counting matrices and polynomials on nonane isomers were calculated.
- [keywords] => Henry law; Characteristic polynomial; Counting polynomials

**Lorentz JÄNTSCHI, Sorana D. BOLBOACĂ**, *The Jungle of Linear Regression Revisited*, Leonardo Electronic Journal of Practices and Technologies, AcademicDirect, ISSN 1583-1078, www, Internet, 6(10), p. 169-187, **2007**.

- [id] => 130
- [recorddate] => 2007:05:06:17:30:20
- [lastupdate] => 2007:05:20:17:30:20
- [type] => article
- [place] => www, Internet
- [subject] => mathematics - modeling; mathematics - statistics; research - evaluation; research - management
- [relatedworks] => N/A
- [file] => [?f=130](#)
- [mime] => application/pdf
- [size] => 166849
- [pubname] => Leonardo Electronic Journal of Practices and Technologies
- [pubinfo] => AcademicDirect
- [pubkey] => ISSN 1583-1078
- [workinfo] => 6(10), p. 169-187
- [year] => 2007
- [title] => The Jungle of Linear Regression Revisited
- [authors] => Lorentz JÄNTSCHI, Sorana D. BOLBOACĂ
- [abstract] =>  
Simple linear regression is reviewed. Some well known facts are analyzed from different approaches. Some new formulas and equations are posted and discussed.
- [keywords] => Simple Linear Regression; Least Squares Method; Independent and Dependent Variables

*Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI, How Good the Characteristic Polynomial Can Be for Correlations?*, International Journal of Molecular Sciences, [Molecular Diversity Preservation International](#), ISSN 1422-0067, www & Basel, Internet & Switzerland, 8(4), p. 335-345, 2007.

- [id] => 128
- [recorddate] => 2007:05:03:11:48:36
- [lastupdate] => 2007:05:03:11:49:36
- [type] => article
- [place] => www & Basel, Internet & Switzerland
- [subject] => chemistry - computational; chemistry - physical; informatics - applied; informatics - models implementation; mathematics - modeling; mathematics - statistics; research - methodology
- [relatedworks] => N/A
- [file] => [?f=128](#)
- [mime] => application/pdf
- [size] => 196540
- [pubname] => International Journal of Molecular Sciences
- [pubinfo] => [Molecular Diversity Preservation International](#)
- [pubkey] => ISSN 1422-0067
- [workinfo] => 8(4), p. 335-345
- [year] => 2007
- [title] => How Good the Characteristic Polynomial Can Be for Correlations?
- [authors] => Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI
- [abstract] =>  
The aim of this study was to investigate the characteristic polynomials resulting from the molecular graphs used as molecular descriptors in the characterization of the properties of chemical compounds. A formal calculus method is proposed in order to identify the value of the characteristic polynomial parameters for which the extremum values of the squared correlation coefficient are obtained in univariate regression models. The developed calculation algorithm was applied to a sample of nonane isomers. The obtained results revealed that the proposed method produced an accurate and unique solution for the best relationship between the characteristic polynomial as molecular descriptor and the property of interest.
- [keywords] => Characteristic polynomial; Graph theory; Structure-Property Relationships; Nonane isomers; Henry's law constant (solubility)
- [acknowledgment] => The research was partly supported by UEFISCSU Romania through project ET108/2006.

**Lorentz JÄNTSCHI, Sorana-Daniela BOLBOACĂ**, *Modeling the Octanol-Water Partition Coefficient of Substituted Phenols by the Use of Structure Information*, International Journal of Quantum Chemistry, Wiley InterScience, ISSN 0020-7608, eISSN 1097-461X, New York, NY, USA, Volume 107, Issue 8 (Special Issue: Proceedings from the 3rd Humboldt Conference on Computational Chemistry. Issue Edited by Georgi N. Vayssilov, Tzonka Mineva), p. 1736-1744, **2007**.

- [id] => 127
- [recorddate] => 2007:05:02:13:30:46
- [lastupdate] => 2007:05:02:13:30:46
- [type] => article
- [place] => New York, NY, USA
- [subject] => chemistry - computational; chemistry - organic; chemistry - physical; informatics - models implementation; mathematics - modeling; mathematics - statistics
- [relatedworks] =>
  - 4 (some):
    - Structure-Property Based Model Estimation of Alkanes Boiling Points, [?id=145](#)
- [file] => [?f=127](#)
- [mime] => application/pdf
- [size] => 116714
- [pubname] => International Journal of Quantum Chemistry
- [pubinfo] => Wiley InterScience
- [pubkey] => ISSN 0020-7608, eISSN 1097-461X
- [workinfo] => Volume 107, Issue 8 (Special Issue: Proceedings from the 3rd Humboldt Conference on Computational Chemistry . Issue Edited by Georgi N. Vayssilov, Tzonka Mineva), p. 1736-1744
- [year] => 2007
- [title] => Modeling the Octanol-Water Partition Coefficient of Substituted Phenols by the Use of Structure Information
- [authors] => Lorentz JÄNTSCHI, Sorana-Daniela BOLBOACĂ
- [abstract] =>

This work presents the abilities in estimation and prediction of the octanol-water partition coefficient of some para-substituted phenols through the integration of complex structures information by the use of an original molecular descriptors family on the structure-property relationship approach.

The proposed approach uses the complex information obtained from para-substituted phenols structure in order to generate and calculate the molecular descriptors family. The structure-property relationship models were built based on the generated descriptors.

The obtained multi-varied models (model with two and four descriptors, respectively) were validated through the assessment of the cross-validation leave-one-out score. The comparison between the multi-varied model with two and four descriptors was performed using Steiger's Z-test. The analysis of the statistical characteristics of the

obtained models demonstrated that the model with four descriptors has greater ability to estimate and predict compared with the model with two descriptors. This observation was also sustained by the results of correlated-correlation analysis. The multi-varied model with four descriptors revealed that the octanol-water partition coefficient of studied parasubstituted phenols is likely to be of geometry nature, it is strongly dependent on the partial charges of compounds and group electronegativity, and it is in relation to the elastic force.

- [keywords] => molecular descriptors family on structure-property relationships (MDF-SPR); octanol-water partition coefficient; para-substituted phenols
- [acknowledgment] => The research was partly supported by UEFISCSU Romania through projects ET36/2005 and 108/2006.

**Sorana D. BOLBOACĂ, Lorentz JĂNTSCHI**, *Data Mining on Structure-Activity/Property Relationships Models*, ECC11- The 11th [Electronic Computational Chemistry Conference](#), online, Monmouth University, New Jersey, USA, N/A, www, Internet, paper #29, April 2-30, **2007**.

- [id] => 126
- [recorddate] => 2007:05:02:12:04:49
- [lastupdate] => 2007:05:02:12:05:01
- [type] => conference
- [place] => www, Internet
- [subject] => chemistry - computational; chemistry - general; informatics - applied; mathematics - applied; mathematics - statistics; medicine - informatics; research - management; research - methodology
- [relatedworks] => N/A
- [file] => [?f=126](#)
- [mime] => application/pdf
- [size] => 15899487
- [pubname] => ECC11- The 11th [Electronic Computational Chemistry Conference](#), online
- [pubinfo] => Monmouth University, New Jersey, USA
- [pubkey] => N/A
- [workinfo] => paper #29, Presentation located [here](#), April 2-30
- [year] => 2007
- [title] => Data Mining on Structure-Activity/Property Relationships Models
- [authors] => Sorana D. BOLBOACĂ, Lorentz JĂNTSCHI
- [abstract] =>

Molecular descriptors family on structure-activity/property relationships studies were carried out in order to identify the link between compounds structure and their activity/property.

A number of fifty-five classes of properties or activities of different compounds sets were investigated. Single and multi-varied linear regression models using molecular descriptors as variables were identified.

The models with estimation and prediction abilities and associated characteristics were stored into a database.

A data mining analysis using classification and clustering were applied on the obtained database for searching and extracting useful information.

The methodology applied in searching and extracting for information and the obtained results are presented.
- [keywords] => Knowledge-Discovery in Database (KDD); Cluster analysis; Structure-Activity/Property Relationships (SAR/SPR); Molecular Descriptors Family (MDF)
- [acknowledgment] => MEC/UEFISCSU Romania, Grants ET.46&108/2006

*Lorentz JÄNTSCHI, Sorana Daniela BOLBOACĂ, Processes Kinetics Modeling: A Numerical Study*, Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences [<http://sizemat.igic.bas.bg>], FP6: EC-INCO-CT-2005-016414 Specific Support Action, Plovdiv, Bulgaria, p. 72-73, April 19-21, **2007**.

- [id] => 125
- [recorddate] => 2007:04:30:17:12:14
- [lastupdate] => 2007:04:30:17:12:14
- [type] => conference
- [place] => Plovdiv, Bulgaria
- [subject] => chemistry - computational; chemistry - inorganic; chemistry - physical; informatics - applied; mathematics - analysis; mathematics - applied; mathematics - modeling; mathematics - optimization; mathematics - statistics; physics - optics; research - methodology
- [relatedworks] => N/A
- [file] => [?f=125](#)
- [mime] => application/pdf
- [size] => 841279
- [pubname] => Institute of General and Inorganic Chemistry
- [pubinfo] => Bulgarian Academy of Sciences [<http://sizemat.igic.bas.bg>]
- [pubkey] => FP6: EC-INCO-CT-2005-016414 Specific Support Action
- [workinfo] => p. 72-73, April 19-21
- [year] => 2007
- [title] => Processes Kinetics Modeling: A Numerical Study
- [authors] => Lorentz JÄNTSCHI, Sorana Daniela BOLBOACĂ
- [abstract] =>  
Introduction  
The kinetics study of the reaction between  $\text{Cu}^{2+}$  and  $\text{S}_2\text{O}_3^{2-}$  in solutions is not entirely studied, being reported into the specialty literature just few papers which refer the reaction in aqueous solutions.  
Aim  
By using of a set of experimental data obtained from stopped flow spectrophotometrical installation build at Technical University of Cluj-Napoca, to investigate the kinetic of the reaction.  
Assumption  
The general form of the reaction is  $\text{A} + \text{B} \rightleftharpoons \text{X} \rightarrow \text{P}$   
Experimental procedure  
The cooper and tiosulfate aqueous solutions were prepared in different concentrations varying from 0.001 M to 0.01 M. The reaction was detected to be a very fast one: the existence of the X intermediary was found to be below 25 ms. The wavelength of light detection diode was found (and is 430 nm) in order to prepare the detection of intermediary forming as the wavelength which assures the best stability of the light emission in time. A microampere meter was set in order to be used for recording of the signal from detector and the baud rate of the recording was choused to be 0.04 ms. A digital oscilloscope with buffer was used to plot and transfer the data to the computer. In order to minimize the experimental interferences such as dilution of the

intermediary, the size of the mixing chamber was varied; a small size one was selected and used for measurements. The mixing chamber has a volume equal to 0.35cm<sup>3</sup> and the length of optical pathway traversed by the beam through measurement chamber is 0.4 cm.

#### Experiments

Three experiments with equal concentration of reactants (0.001, 0.005 and 0.01 M) are the subject of this investigation. The recording of digital data was started always after the mixing moment but near to, because of limited memory buffer of the oscilloscope (64 Kb). The number of relevant measurements corresponding to the reaction time it varies in 1500-8000 range.

#### Mathematical Methods

The Lambert-Beer law was used to correlate extinction with concentration; the unknown parameter was the molar extinction coefficient. The mathematical model of the assumed reaction mechanism was numerically written; the unknown parameters were four partial reaction orders and three reaction rates constants. The subject of optimization was squared sum of differences between experimental extinction  $E$  and theoretical approach of extinction  $a[X]$ . Only a first part of the experimental data records entered into the optimization procedure (1100 for 0.001 M, 1300 for 0.005 M, and 6500 for 0.01M).

#### Results

The optimization procedure produced the best fit of the model to the experiment with 0.962, 0.955, and 0.980 respectively correlation coefficients. Not all unknown parameters were possible to be obtained. Reaction rates: only to the right ones. Partial orders: all, except one of intermediary for the left direction reaction. Extinction coefficient: 212 +/- 22 1/mol\*cm. For all obtained parameters is no significant difference between parameters values from one experiment to another with a 95% confidence.

#### Conclusion

Reaction kinetics was almost complete determined. Reaction rates: 2000 +/- 1000, N/A, 2200 +/- 200, partial orders: 0.789 +/- 0.05, 0.781 +/- 0.04, N/A, 1.55 +/- 0.04. The optimization procedure was proved to be a self consistent one, despite of the number of unknown parameters used.

- [keywords] => Process modeling; Mathematical modeling; Numerical optimization
- [acknowledgment] => Research supported in part by UEFISCSU Romania, Grant No. ET/108/2006. Thanks for providing the experimental data to Dr. Mihaela Ligia UNGUREȘAN from Technical University of Cluj-Napoca, Romania.

**Sorana Daniela BOLBOACĂ, Lorentz JÄNTSCHI**, *Modeling the Property of Compounds from Structure: Statistical Methods for Models Validation*, Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences [<http://sizemat.igic.bas.bg>], FP6: EC-INCO-CT-2005-016414 Specific Support Action, Plovdiv, Bulgaria, p. 71, April 19-21, 2007, *Environmental Chemistry Letters*, [DOI 10.1007/s10311-007-0119-9](https://doi.org/10.1007/s10311-007-0119-9)

- [id] => 124
- [recorddate] => 2007:04:30:17:08:30
- [lastupdate] => 2007:04:30:17:08:30
- [type] => conference
- [place] => Plovdiv, Bulgaria
- [subject] => chemistry - computational; informatics - applied; informatics - databases; mathematics - statistics; medicine - informatics; research - methodology
- [relatedworks] => N/A
- [file] => [?f=124](#)
- [size] => 1474294
- [pubname] => Institute of General and Inorganic Chemistry
- [pubinfo] => Bulgarian Academy of Sciences [<http://sizemat.igic.bas.bg>]
- [pubkey] => FP6: EC-INCO-CT-2005-016414 Specific Support Action
- [workinfo] => p. 71, April 19-21
- [year] => 2007
- [title] => Modeling the Property of Compounds from Structure: Statistical Methods for Models Validation
- [authors] => Sorana Daniela BOLBOACĂ, Lorentz JÄNTSCHI
- [abstract] =>

A molecular descriptors family on structure-property relationships study (MDF-SPR) was conducted in order to model the boiling points of alkanes using the compounds structure information.

The alkanes from C3 to C9 were included into study. Two MDF-SPR models, one with one descriptor and other with two descriptors, were identified. The estimation and prediction of the MDF-SPR models were analyzed. The methods used for validation of the obtained MDF-SPR models are presented.

The correlated correlation analysis was using in order to compare the performances of the obtained MDF-SPR models and of the MDF-SPR models comparing with previous reported model. The Steiger's Z test [1] at a significance level of 5% was applied.

The statistical analysis of the obtained MDF-SPR models demonstrated that the model with two descriptors has greater abilities in estimation and prediction compared with the model with one descriptor. More, the MDF-SPR model with two descriptors has greater abilities in estimation comparing with previous reported model. These observations were also sustained by the results of correlated-correlation analysis.

The multi-varied MDF-SPR model can be used in order to predict the property of interest of studied alkanes without any experiments and measurements, by using the MDF SPR Predictor application [2].
- [keywords] => Structure-activity relationships (SARs); Method validation; Method evaluation; Molecular Descriptors Family (MDF)
- [acknowledgment] => The research was partly supported by UEFISCSU Romania through projects ET36/2005 & ET108/2006.

**Carmen Elena STOENOIU, Sorana Daniela BOLBOACĂ, Lorentz JÄNTSCHI,**  
*Characterization of Marine Sediments Toxicity based on Structural Information*, Institute of  
 General and Inorganic Chemistry, Bulgarian Academy of Sciences  
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- [authors] => Carmen Elena STOENOIU, Sorana Daniela BOLBOACĂ, Lorentz JÄNTSCHI
- [abstract] =>

The marine sediment toxicity was previously studied for eight ordnance compounds: 2,4,6-trinitrotoluene (2,4,6-TNT), 2,4-dinitrotoluene (2,4-DNT), 2,6-dinitrotoluene (2,6-DNT), 1,3-dinitrobenzene (1,3-DNB), 1,3,5-trinitrobenzene (1,3,5-TNB), Royal Demolition Explosive (RDE), tetryl, and picric acid [1]. Based on the obtained experimental data, the lethal concentration to 50% of the test organisms (LC50) and the effective concentration to 50% of the test organisms (EC50) have been modeled by using the molecular descriptors family on structure activity relationships (MDF-SAR) approach [2].

For five organisms and nine endpoints, the MDF-SAR models with two variables were obtained. The statistical characteristics of the obtained MDF-SAR models are:

No.	Organism	EndPoint	r <sup>2</sup>	s	F	Γ <sub>cv-loo</sub> <sup>2</sup>	n
1	sea urchin( <i>Arbacia punctulata</i> )	fertilization	0.9999	3.83·10 <sup>-5</sup>	9.16·10 <sup>8†</sup>	0.9999	5
2		embryological development	0.9999	8.64·10 <sup>-3</sup>	5.86·10 <sup>4†</sup>	0.9998	7
3		germination	0.9991	3.75·10 <sup>-2</sup>	2.95·10 <sup>3†</sup>	0.9976	8
4	green macro-alga ( <i>Ulva fasciata</i> )	zoospore germination	0.9998	1.74·10 <sup>-2</sup>	1.13·10 <sup>4†</sup>	0.9984	8

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

5		germling length	0.9992	$3.33 \cdot 10^{-2}$	$3.13 \cdot 10^{3\dagger}$	0.9984	8
6		Germling cell number	0.9999	$5.88 \cdot 10^{-3}$	$1.08 \cdot 10^{5\dagger}$	0.9999	7
7	polychaete ( <i>Dinophilus gyrociliatus</i> )	survival and reproductive success	0.9996	$2.70 \cdot 10^{-2}$	$6.31 \cdot 10^{3\dagger}$	0.9991	8
8	redfish ( <i>Sciaenops ocellatus</i> )	larvae survival	0.9999	$6.13 \cdot 10^{-3}$	$4.59 \cdot 10^{4\dagger}$	0.9999	7
9	opossum shrimp ( <i>Mysidopsis bahia</i> )	juveniles survival	0.9999	$5.24 \cdot 10^{-3}$	$2.13 \cdot 10^{4\dagger}$	0.9997	7
<p>r<sup>2</sup> = squared correlation coefficient; s = standard error of estimated; F = Fisher parameter; rcv-loo2 = cross-validation leave-one-out score; n = sample size; †:p &lt; 0.001</p>							

- The analysis of the obtained models with two descriptors revealed that the MDF-SAR approach is able to provide valid and reliable model for marine sediments toxicity characterization.

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- [keywords] => Toxicity; Marine organisms; Ordnance compounds; SAR
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**Lorentz JÄNTSCHI, Sorana BOLBOACĂ**, *Results from the Use of Molecular Descriptors*

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- [authors] => Lorentz JÄNTSCHI, Sorana BOLBOACĂ
- [abstract] =>

The aim of the paper is to present the results obtained by utilization of an original approach called Molecular Descriptors Family on Structure-Property (MDF-SPR) and Structure-Activity Relationships (MDF-SAR) applied on classes of chemical compounds and its usefulness as precursors of models elaboration of new compounds with better properties and/or activities and low production costs. The MDF-SPR/MDF-SAR methodology integrates the complex information obtained from compound's structure in unitary efficient models in order to explain properties/activities. The methodology has been applied on a number of thirty sets of chemical compounds. The best subsets of molecular descriptors family members able to estimate and predict property/activity of interest were identified and were statistically and visually analyzed. The MDF-SPR/MDF-SAR models were validated through internal and/or external validation methods. The estimation and prediction abilities of the MDF-SPR/MDF-SAR models were compared with previous reported models by applying of correlated correlation analysis, which revealed that the MDF-SPR/MDF-SAR methodology is reliable. The MDF-SPR/MDF-SAR methodology opens a new pathway in understanding the relationships between compound's structure and property/activity, in property/activity prediction, and in discovery, investigation and characterization of new chemical compounds, more competitive as costs and property/activity, being a method less expensive comparative with experimental methods.

*ET108/2006 – Et. Finală/2007 – Lucrare in extenso*

- [keywords] => Molecular Descriptors Family (MDF); Structure Property Relationships (SPR); Structure Activity Relationships (SAR); Activity/Property Modeling; Chemical Compounds; Open System
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## Concluzii

O concluzie îmbucurătoare este că nu se observă diferențe semnificative între soluțiile produse de modelul cu 6 și modelul cu 7 termeni, la optimizarea fazei mobile pentru amestecuri de 3 solvenți în cromatografia planară și de lichide de înaltă performanță, de unde rezultă că în designul experimental se poate reduce numărul de experimente preliminare procedurii de optimizare a compoziției fazei mobile la doar 6 experimente.

Integrarea informațiilor complexe provenite din experiment este permise efectuarea de predicții foarte bune în ceea ce privește comportamentul substanțelor chimice cu structură chimică bine definită.

Pentru fenomenele care se petrec la interfața fazelor, așa cum este cazul la cromatografia pe strat subțire, integrarea mai multor modele, așa cum face funcția obiectiv, aduce un supliment de certitudine în predicțiile efectuate.

Următoarele aplicații realizate și-au dovedit capabilitatea predictivă:

- Optimizarea fazei mobile la amestecuri de 3 solvenți în cromatografia planară și de lichide de înaltă performanță:

[http://l.academicdirect.org/Engineering/hptlc/mobile\\_phase\\_opt/](http://l.academicdirect.org/Engineering/hptlc/mobile_phase_opt/)

- Cinetica reacțiilor simple și complexe:

[http://vl.academicdirect.org/molecular\\_dynamics/reaction\\_kinetics/](http://vl.academicdirect.org/molecular_dynamics/reaction_kinetics/)

- Modelarea activității biologice prin descriptorii de natură cuantică semiempirici:

[http://vl.academicdirect.org/molecular\\_topology/mdf\\_findings/](http://vl.academicdirect.org/molecular_topology/mdf_findings/)

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<http://lori.academicdirect.org>

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