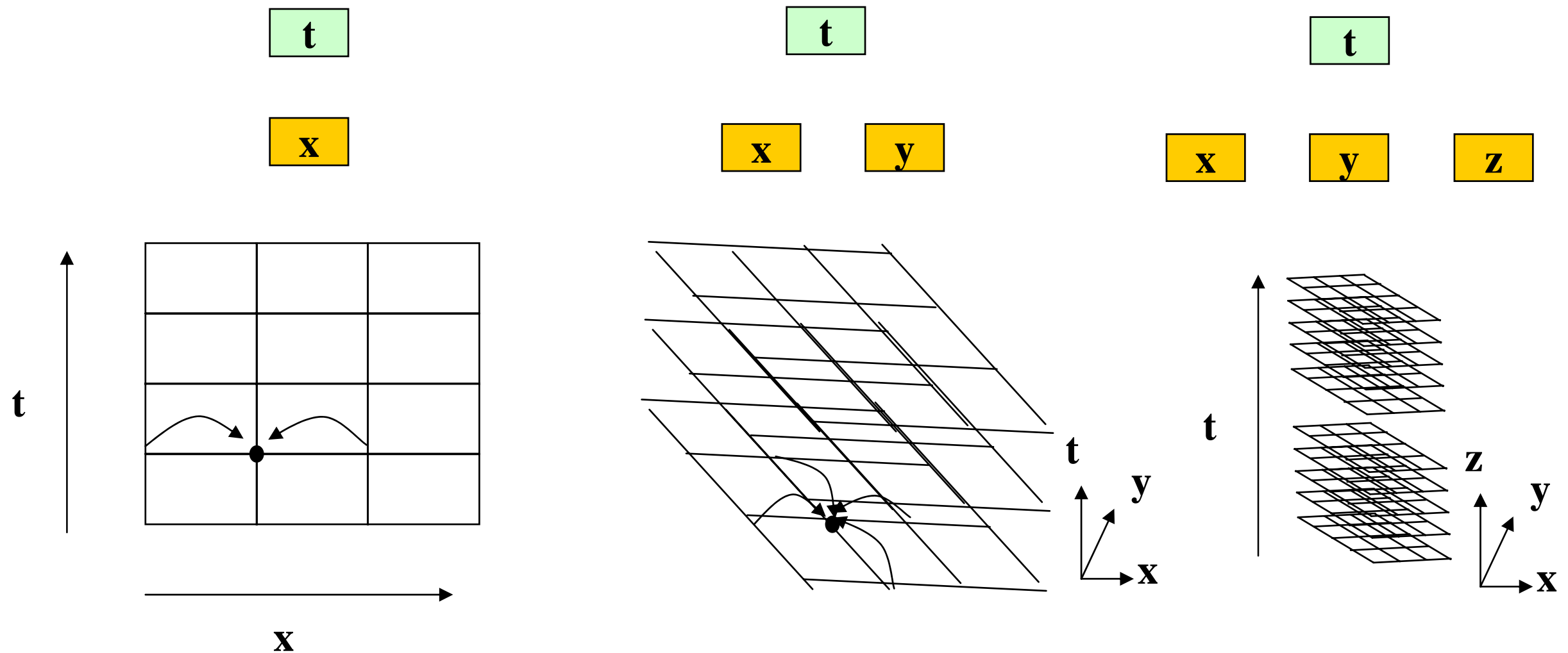


***Polymath***  
***for Partial***  
***Differential***  
***Equations***

# Partial Differential Equations (PDEs)

One dimensional problem :  $t$  and  $x$

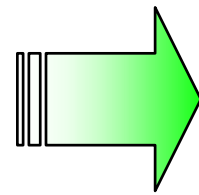
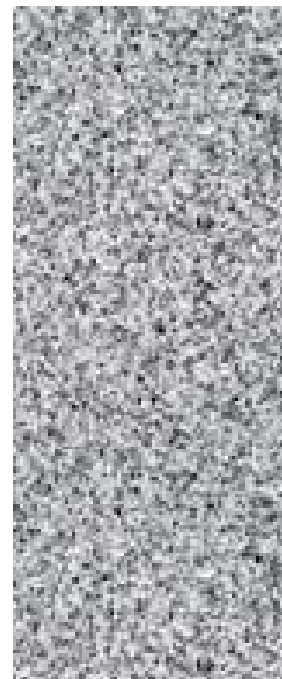
Two dimensional problem :  $t$ ,  $x$ , and  $y$





# *Unsteady state mass transfer in a slab*

Equation of continuity of A for constant  $\rho$  and  $D_{AB}$



$$\frac{\partial C_A}{\partial t} + (\cancel{v \cdot \nabla C_A}) = D_{AB} \nabla^2 C_A + \cancel{R_A}$$

$$\frac{\partial C_A}{\partial t} = D_{AB} \frac{d^2 C_A}{dx^2}$$

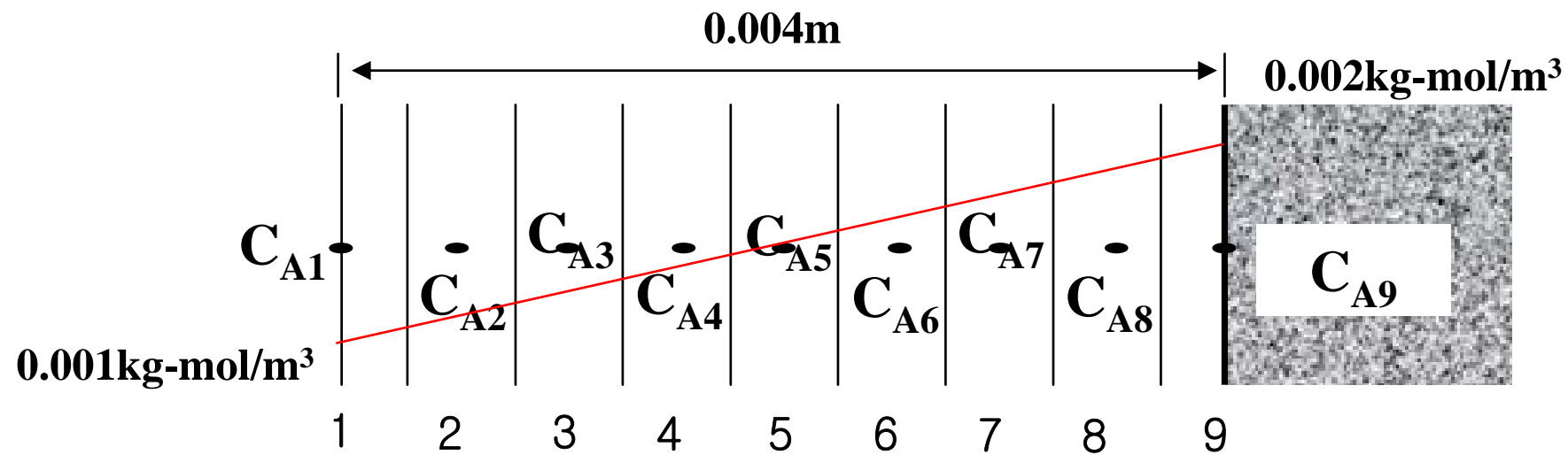
No mass transfer

Distribution coefficient, K

kc for external mass transfer

# Questions

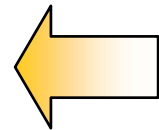
- 1. Concentration vs. Distance after 2500s  
( interval=0.0005)**
- 2. Concentration vs. time to 25000s  
at  $x=0.001, 0.002, 0.003$  and  $0.004$**
- 3. Concentration vs. Distance after 2500s  
( Interval=0.00025)**



$$\frac{\partial C_{A_n}}{\partial t} = \frac{D_{AB}}{(\Delta x)^2} (C_{A_{n+1}} - 2C_{A_n} + C_{A_{n-1}}) \text{ for } (2 \leq n \leq T-1)$$

**Boundary Condition**

**X=0.0**

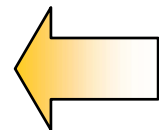


$$C_{A1} = \frac{C_{A0}}{K} \quad \text{for case (1)}$$

$$k_c(C_{A0} - KC_{A1}) = -D_{AB} \left. \frac{\partial C_A}{\partial x} \right|_{x=0} \quad \text{for case (2)}$$

$$\left. \frac{\partial C_A}{\partial x} \right|_{x=0} = \frac{-C_{A3} + 4C_{A2} - 3C_{A1}}{2\Delta x}$$

**X=0.004**



$$\left. \frac{\partial C_A}{\partial x} \right|_{x=0.004} = 0 \quad \frac{\partial C_{A9}}{\partial x} = \frac{3C_{A9} - 4C_{A8} + C_{A7}}{2\Delta x} = 0$$

$$C_{A9} = \frac{4C_{A8} - C_{A7}}{3}$$

**Initial Condition** : **linear concentration profile**



Solve system of nonlinear equations

Indep Var  Initial Value Solve with  Final Value 



 Comments









	Differential equations / explicit equations	Initial value	Comments
1	$d(CA2)/d(t) = DAB*(CA3-2*CA2+CA1)/deltax^2$	0.001125	
2	$d(CA3)/d(t) = DAB*(CA4-2*CA3+CA2)/deltax^2$	0.00125	
3	$d(CA4)/d(t) = DAB*(CA5-2*CA4+CA3)/deltax^2$	0.001375	
4	$d(CA5)/d(t) = DAB*(CA6-2*CA5+CA4)/deltax^2$	0.0015	
5	$d(CA6)/d(t) = DAB*(CA7-2*CA6+CA5)/deltax^2$	0.001625	
6	$d(CA7)/d(t) = DAB*(CA8-2*CA7+CA6)/deltax^2$	0.00175	
7	$d(CA8)/d(t) = DAB*(CA9-2*CA8+CA7)/deltax^2$	0.001825	
8	$DAB = 1.0e-9$	n.a.	
9	$deltax = 0.0005$	n.a.	
10	$CA9 = \text{if}(t==0)\text{then}(2.0e-3)\text{else}((4*CA8-CA7)/3)$	n.a.	
11	$CA0 = 6.0e-3$	n.a.	
12	$K = 1.5$	n.a.	
13	$CA1 = \text{if}(t==0)\text{then}(1.0e-3)\text{else}(CA0/K)$	n.a.	

Differential Equations: 7 Auxiliary Equations: 6

**POLYMATH Results**

7.13(a) Unsteady-state Mass Transfer in a Slab 06-02-2004, Rev5.1.225

**Calculated values of the DEQ variables**

Variable	initial value	minimal value	maximal value	final value
t	0	0	2500	2500
CA2	0.001125	0.001125	0.0035727	0.0035727
CA3	0.00125	0.00125	0.0031691	0.0031691
CA4	0.001375	0.001375	0.0028097	0.0028097
CA5	0.0015	0.0015	0.0025088	0.0025088
CA6	0.001625	0.0016185	0.0022742	0.0022742
CA7	0.00175	0.0016945	0.0021083	0.0021083
CA8	0.001825	0.0017171	0.0020099	0.0020099
DAB	1.0E-09	1.0E-09	1.0E-09	1.0E-09
deltax	5.0E-04	5.0E-04	5.0E-04	5.0E-04
CA9	0.002	0.0017145	0.002	0.001977
CA0	0.006	0.006	0.006	0.006
K	1.5	1.5	1.5	1.5
CA1	0.001	0.001	0.004	0.004

**ODE Report (RKF45)**

## Differential equations as entered by the user

- [1]  $d(CA2)/d(t) = DAB*(CA3-2*CA2+CA1)/deltax^2$
- [2]  $d(CA3)/d(t) = DAB*(CA4-2*CA3+CA2)/deltax^2$
- [3]  $d(CA4)/d(t) = DAB*(CA5-2*CA4+CA3)/deltax^2$
- [4]  $d(CA5)/d(t) = DAB*(CA6-2*CA5+CA4)/deltax^2$
- [5]  $d(CA6)/d(t) = DAB*(CA7-2*CA6+CA5)/deltax^2$
- [6]  $d(CA7)/d(t) = DAB*(CA8-2*CA7+CA6)/deltax^2$
- [7]  $d(CA8)/d(t) = DAB*(CA9-2*CA8+CA7)/deltax^2$

## Explicit equations as entered by the user

- [1]  $DAB = 1.0e-9$
- [2]  $deltax = 0.0005$
- [3]  $CA9 = \text{if}(t=0)\text{then}(2.0e-3)\text{else}((4*CA8-CA7)/3)$
- [4]  $CA0 = 6.0e-3$
- [5]  $K = 1.5$
- [6]  $CA1 = \text{if}(t=0)\text{then}(1.0e-3)\text{else}(CA0/K)$

## Independent variable

variable name : t

initial value : 0

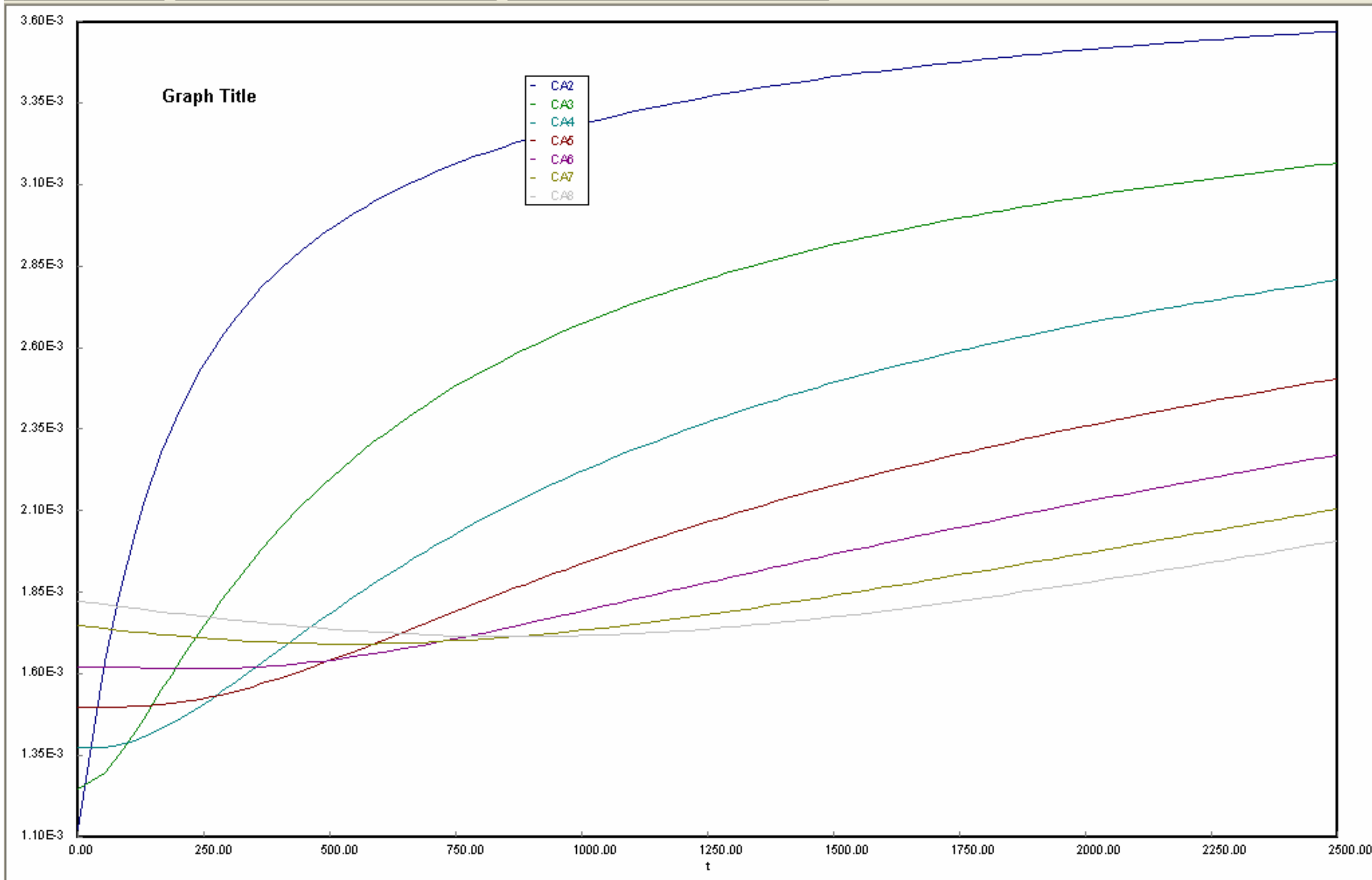
Final value : 2500

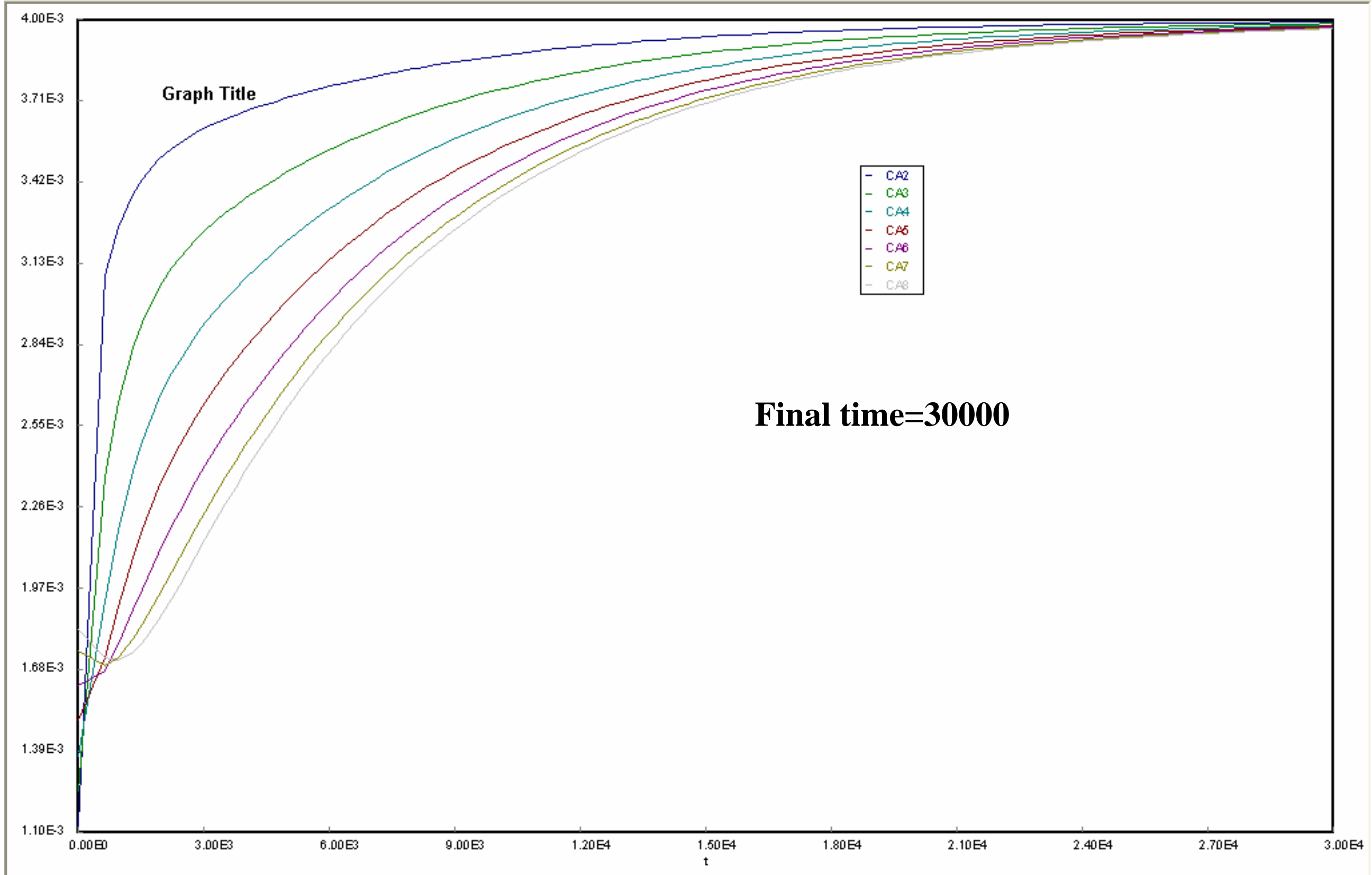


Open Save LEQ NLE DEQ REG Calculate Units Const Setup

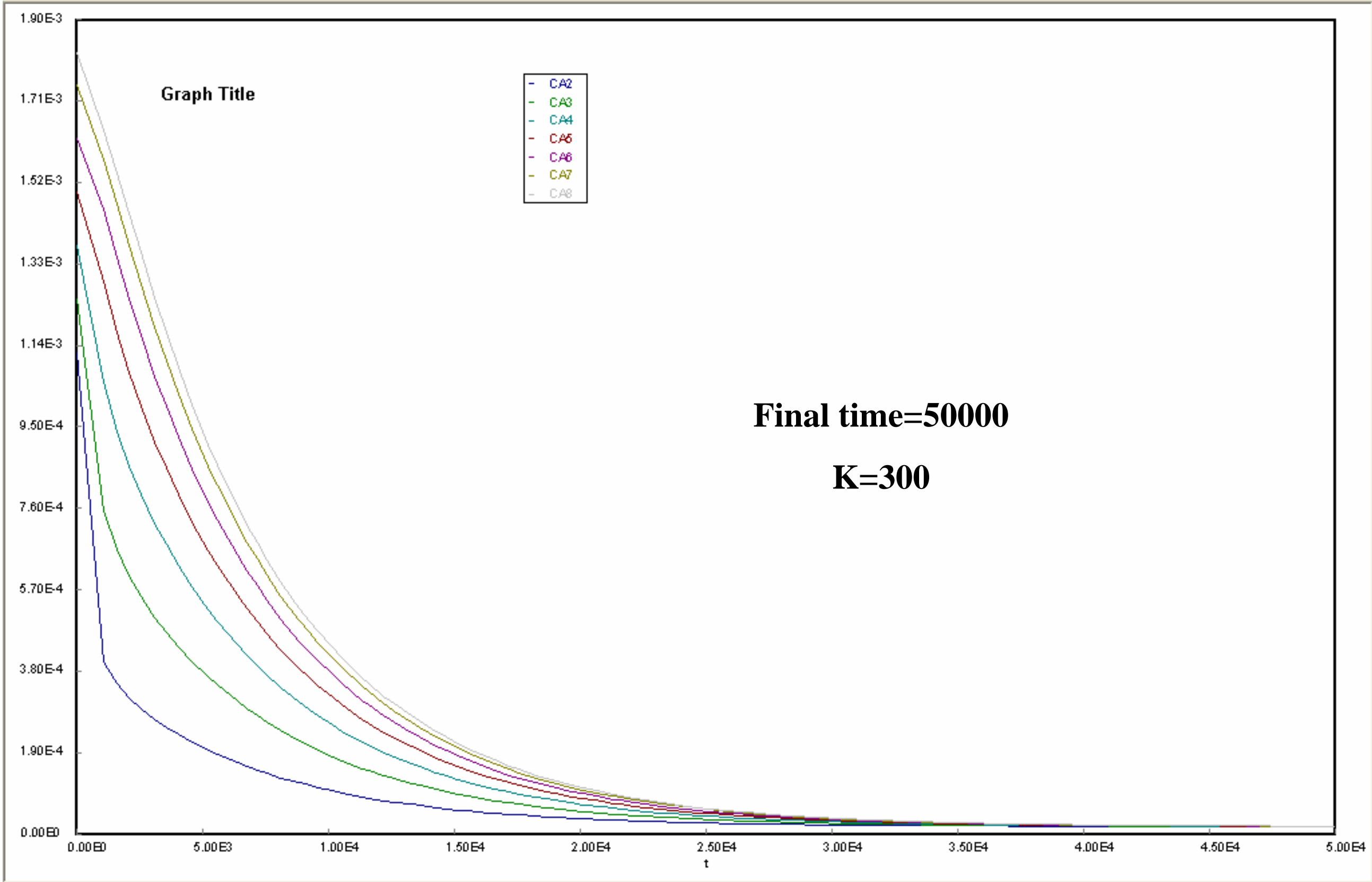
R018 : C011 = 0.0017627

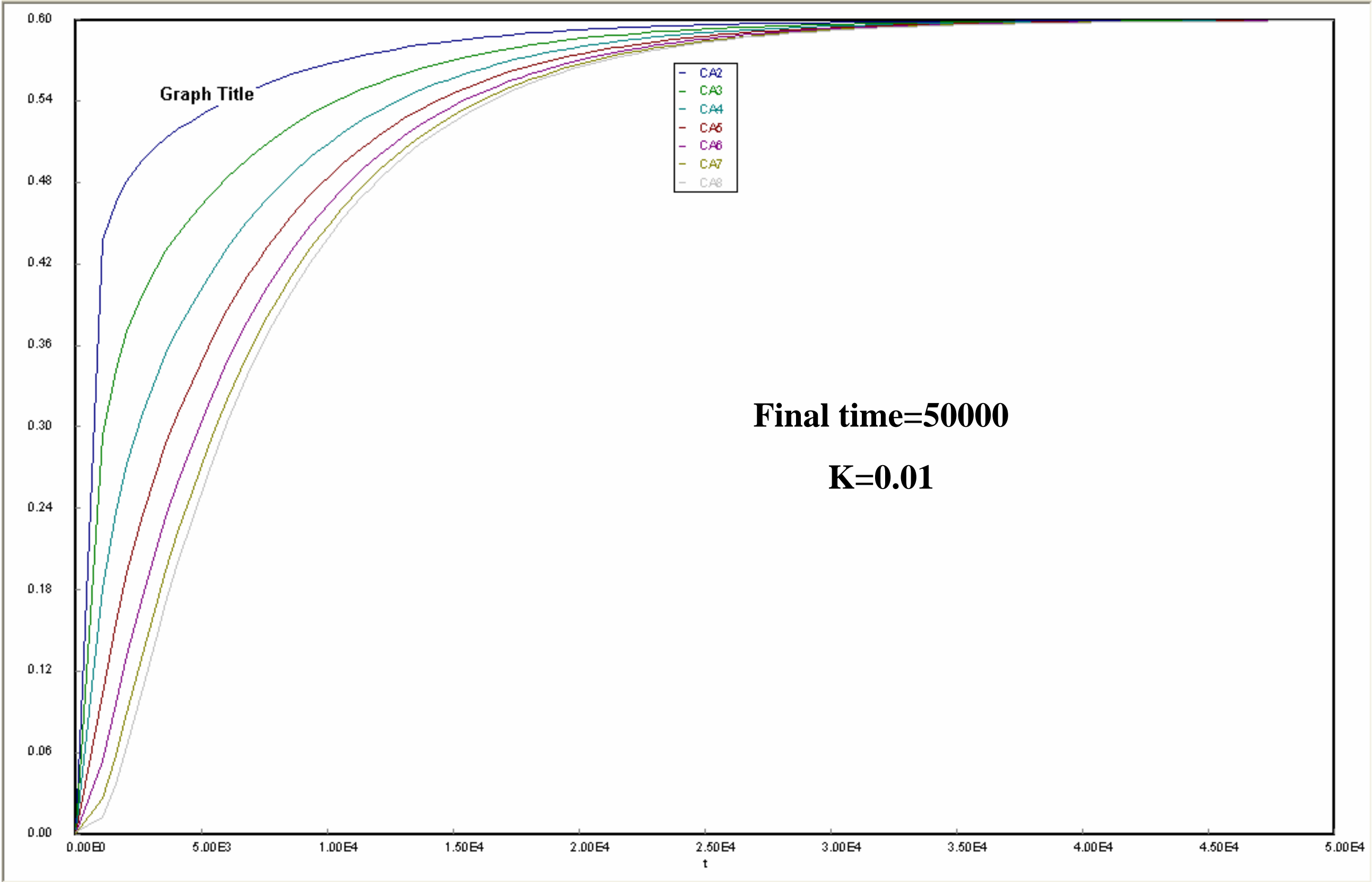
	t	CA2	CA3	CA4	CA5	CA6	CA7	CA8	DAB	deltax	CA9	CA0	K	
1	0	0.001125	0.00125	0.001375	0.0015	0.001625	0.00175	0.001825	1.0E-09	5.0E-04	0.002	0.006	1.5	0.00
2	52.349347	0.0016416	0.0013003	0.0013784	0.0015001	0.0016241	0.0017404	0.0018146	1.0E-09	5.0E-04	0.0018407	0.006	1.5	0.00
3	81.031595	0.0018512	0.0013552	0.0013857	0.0015006	0.0016231	0.0017358	0.0018089	1.0E-09	5.0E-04	0.0018348	0.006	1.5	0.00
4	112.24666	0.0020378	0.0014252	0.0013991	0.0015021	0.0016218	0.001731	0.0018029	1.0E-09	5.0E-04	0.0018285	0.006	1.5	0.00
5	128.95345	0.0021235	0.0014649	0.0014084	0.0015034	0.0016211	0.0017285	0.0017997	1.0E-09	5.0E-04	0.0018252	0.006	1.5	0.00
6	164.9258	0.0022815	0.0015525	0.0014334	0.0015077	0.0016197	0.0017235	0.001793	1.0E-09	5.0E-04	0.001818	0.006	1.5	0.00
7	184.36358	0.0023545	0.0015997	0.0014492	0.001511	0.0016192	0.0017208	0.0017894	1.0E-09	5.0E-04	0.0018142	0.006	1.5	0.00
8	204.36358	0.0024222	0.0016477	0.0014668	0.0015151	0.0016187	0.0017182	0.0017858	1.0E-09	5.0E-04	0.0018102	0.006	1.5	0.00
9	244.36358	0.0025389	0.0017404	0.0015057	0.0015254	0.0016185	0.0017133	0.0017787	1.0E-09	5.0E-04	0.0018024	0.006	1.5	0.00
10	264.36358	0.0025896	0.0017848	0.0015264	0.0015316	0.0016188	0.001711	0.0017752	1.0E-09	5.0E-04	0.0017985	0.006	1.5	0.00
11	284.36358	0.002636	0.0018278	0.0015478	0.0015385	0.0016193	0.0017088	0.0017718	1.0E-09	5.0E-04	0.0017947	0.006	1.5	0.00
12	304.36358	0.0026787	0.0018693	0.0015697	0.001546	0.0016202	0.0017068	0.0017685	1.0E-09	5.0E-04	0.0017909	0.006	1.5	0.00
13	344.36358	0.0027545	0.0019479	0.0016144	0.0015628	0.0016228	0.0017031	0.0017621	1.0E-09	5.0E-04	0.0017835	0.006	1.5	0.00
14	364.36358	0.0027884	0.001985	0.001637	0.001572	0.0016246	0.0017014	0.0017589	1.0E-09	5.0E-04	0.0017799	0.006	1.5	0.00
15	384.36358	0.0028199	0.0020208	0.0016596	0.0015816	0.0016267	0.0017	0.0017559	1.0E-09	5.0E-04	0.0017763	0.006	1.5	0.00
16	404.36358	0.0028494	0.0020551	0.0016823	0.0015916	0.0016291	0.0016987	0.001753	1.0E-09	5.0E-04	0.0017728	0.006	1.5	0.00
17	444.36358	0.0029029	0.00212	0.0017271	0.0016128	0.0016348	0.0016966	0.0017474	1.0E-09	5.0E-04	0.001766	0.006	1.5	0.00
18	464.36358	0.0029273	0.0021506	0.0017493	0.0016239	0.0016382	0.0016958	0.0017447	1.0E-09	5.0E-04	0.0017627	0.006	1.5	0.00
19	484.36358	0.0029503	0.0021801	0.0017713	0.0016352	0.0016418	0.0016952	0.0017422	1.0E-09	5.0E-04	0.0017594	0.006	1.5	0.00
20	504.36358	0.0029721	0.0022085	0.001793	0.0016467	0.0016457	0.0016948	0.0017397	1.0E-09	5.0E-04	0.0017562	0.006	1.5	0.00
21	544.36358	0.0030122	0.0022621	0.0018354	0.0016703	0.0016542	0.0016945	0.0017351	1.0E-09	5.0E-04	0.0017502	0.006	1.5	0.00
22	564.36358	0.0030307	0.0022875	0.0018562	0.0016822	0.0016588	0.0016946	0.001733	1.0E-09	5.0E-04	0.0017473	0.006	1.5	0.00
23	584.36358	0.0030484	0.0023121	0.0018766	0.0016943	0.0016637	0.0016949	0.001731	1.0E-09	5.0E-04	0.0017444	0.006	1.5	0.00
24	604.36358	0.0030652	0.0023357	0.0018967	0.0017065	0.0016687	0.0016954	0.0017292	1.0E-09	5.0E-04	0.0017417	0.006	1.5	0.00
25	644.36358	0.0030966	0.0023806	0.0019358	0.001731	0.0016794	0.0016969	0.0017258	1.0E-09	5.0E-04	0.0017367	0.006	1.5	0.00
26	664.36358	0.0031113	0.0024019	0.0019548	0.0017432	0.001685	0.0016979	0.0017243	1.0E-09	5.0E-04	0.0017343	0.006	1.5	0.00
27	684.36358	0.0031253	0.0024226	0.0019735	0.0017555	0.0016908	0.001699	0.001723	1.0E-09	5.0E-04	0.0017321	0.006	1.5	0.00
28	704.36358	0.0031388	0.0024425	0.0019918	0.0017677	0.0016967	0.0017004	0.0017218	1.0E-09	5.0E-04	0.0017299	0.006	1.5	0.00
29	744.36358	0.0031641	0.0024806	0.0020274	0.0017921	0.0017089	0.0017035	0.0017198	1.0E-09	5.0E-04	0.0017261	0.006	1.5	0.00
30	764.36358	0.0031761	0.0024987	0.0020446	0.0018043	0.0017152	0.0017053	0.001719	1.0E-09	5.0E-04	0.0017243	0.006	1.5	0.00
31	784.36358	0.0031876	0.0025163	0.0020616	0.0018163	0.0017216	0.0017073	0.0017183	1.0E-09	5.0E-04	0.0017227	0.006	1.5	0.00
32	804.36358	0.0031987	0.0025334	0.0020782	0.0018283	0.0017281	0.0017094	0.0017178	1.0E-09	5.0E-04	0.0017213	0.006	1.5	0.00
33	844.36358	0.0032197	0.002566	0.0021104	0.0018521	0.0017413	0.001714	0.0017172	1.0E-09	5.0E-04	0.0017188	0.006	1.5	0.00
34	864.36358	0.0032296	0.0025816	0.002126	0.0018639	0.001748	0.0017165	0.0017171	1.0E-09	5.0E-04	0.0017177	0.006	1.5	0.00
35	884.36358	0.0032393	0.0025968	0.0021413	0.0018755	0.0017548	0.0017191	0.0017171	1.0E-09	5.0E-04	0.0017168	0.006	1.5	0.00





Final time=30000






 Indep Var  Initial Value 

 Solve with  Final Value 


Table

Graph

Report

 Comments

Add DE

Add EE

Remove

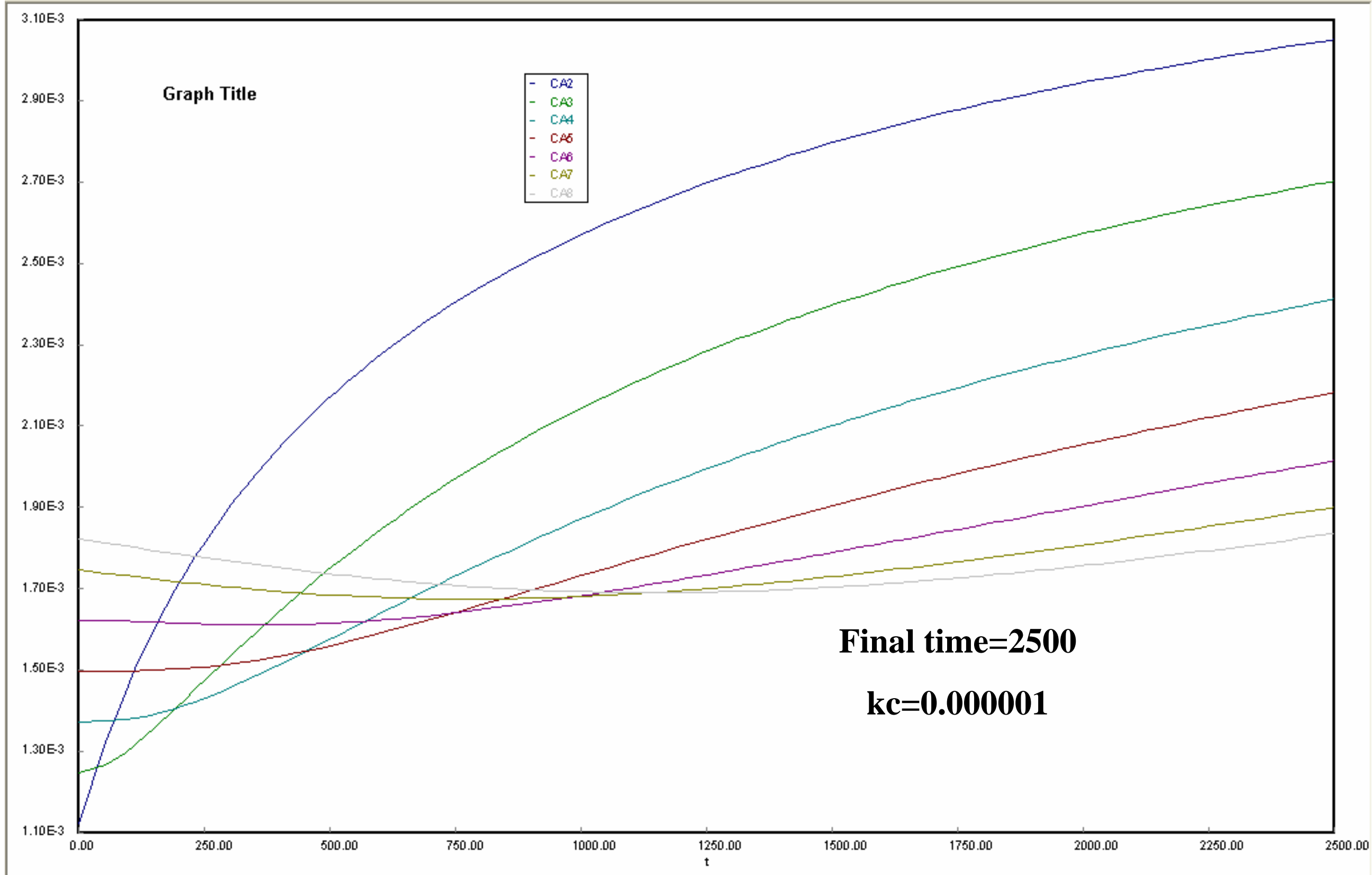
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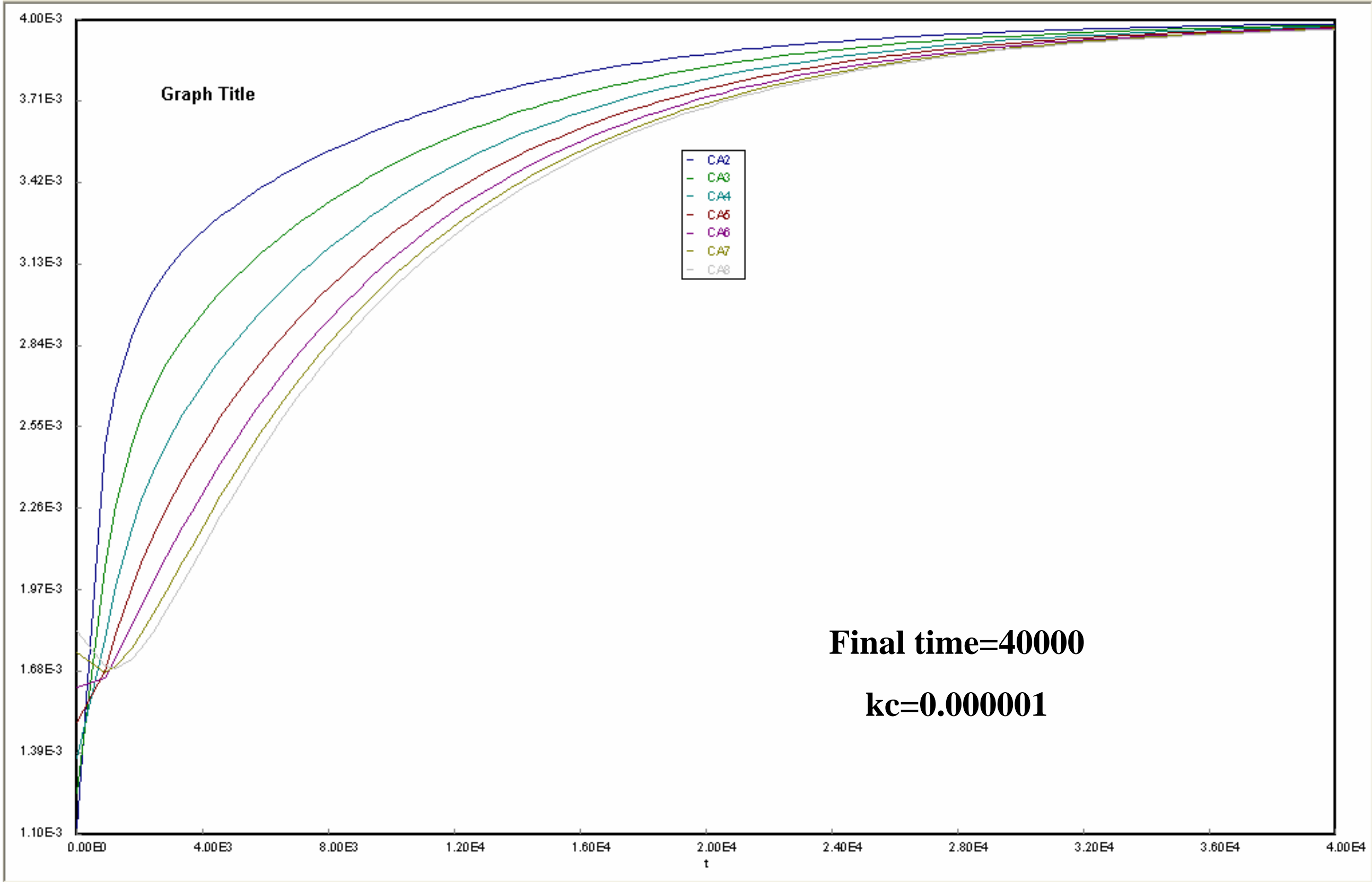


	Differential equations / explicit equations	Initial value	Comments
1	$d(CA2)/dt = DAB*(CA3-2*CA2+CA1)/deltax^2$	0.001125	
2	$d(CA3)/dt = DAB*(CA4-2*CA3+CA2)/deltax^2$	0.00125	
3	$d(CA4)/dt = DAB*(CA5-2*CA4+CA3)/deltax^2$	0.001375	
4	$d(CA5)/dt = DAB*(CA6-2*CA5+CA4)/deltax^2$	0.0015	
5	$d(CA6)/dt = DAB*(CA7-2*CA6+CA5)/deltax^2$	0.001625	
6	$d(CA7)/dt = DAB*(CA8-2*CA7+CA6)/deltax^2$	0.00175	
7	$d(CA8)/dt = DAB*(CA9-2*CA8+CA7)/deltax^2$	0.001825	
8	$CA9 = \text{if}(t==0)\text{then}(2.0e-3)\text{else}((4*CA8-CA7)/3)$	n.a.	
9	$DAB = 1.0e-9$	n.a.	
10	$deltax = 0.0005$	n.a.	
11	$CA0 = 6.0e-3$	n.a.	
12	$K = 1.5$	n.a.	
13	$CA1 = \text{if}(t==0)\text{then}(1.0e-3)\text{else}((2*kc*CA0*deltax-DAB*CA3+4*DAB*CA2)/(3*DAB+2*kc*K*deltax))$	n.a.	
14	$kc = 0.000001$	n.a.	

Differential Equations: 7 Auxiliary Equations: 7

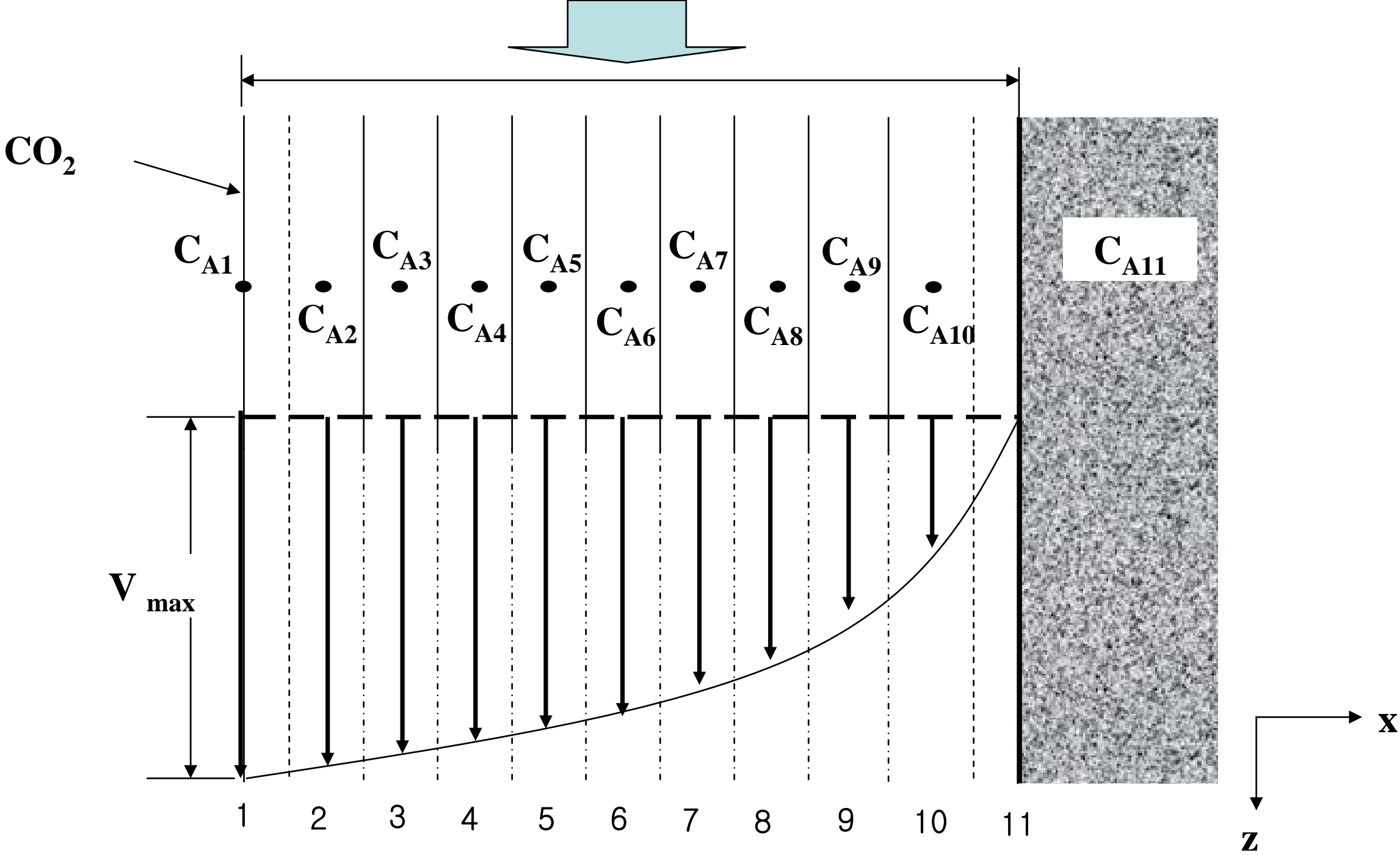
Open Save LEQ NLE DEQ REG Calculate Units Const Setup







# *Diffusion and Reaction in Falling Liquid Film*



$$\frac{\partial C_A}{\partial t} + (v \cdot \nabla C_A) = D_{AB} \nabla^2 C_A + R_A$$

$$v_z \frac{\partial C_A}{\partial z} = D_{AB} \frac{d^2 C_A}{dx^2} - k' C_A$$

$$v_z = \frac{\rho g \delta^2}{2\mu} \left[ 1 - \left( \frac{x}{\delta} \right)^2 \right] = v_{max} \left[ 1 - \left( \frac{x}{\delta} \right)^2 \right]$$

$$v_{z,c} = v_{max} \left[ 1 - \left( \frac{(n-1)\Delta x}{\delta} \right)^2 \right]$$

$$\frac{\partial C_{A,n}}{\partial z} = \left\{ \frac{D_{AB}}{(\Delta x)^2} (C_{A,n+1} - 2C_{A,n} + C_{A,n-1}) - k' C_{A,n} \right\} / v_{z,n}$$

$$C_{A,n} = 0 \text{ at } Z=0$$

$$C_{A1} = 0.03 \text{ for } z \geq 0$$

$$C_{A11} = (4C_{A10} - C_{A9})/3$$

## Questions

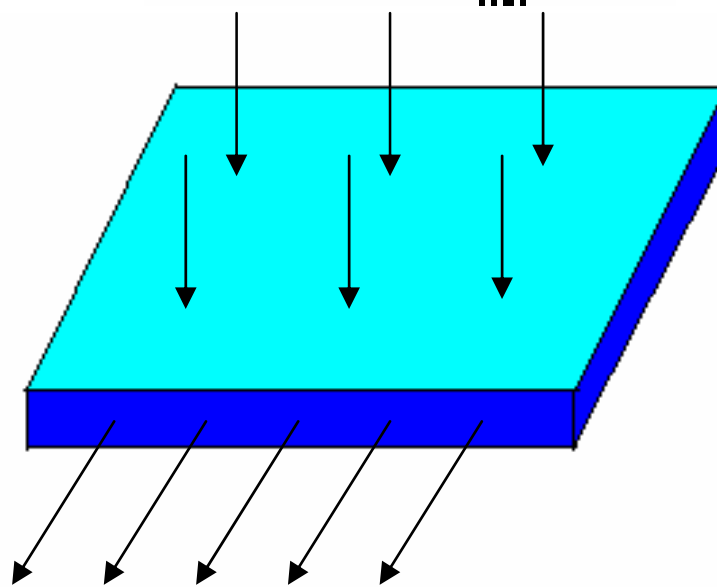
- 1. Concentration of dissolved A within the solution at  $z=1\text{m}$ , no reaction**
- 2. Average flux of A**
- 3. Concentration vs  $z$**
- 4. Compare adsorbed A with exiting A value**
- 5. Reaction constant,  $k=1\text{s}^{-1}$**
- 6. Compare 1 with 5**

$$N_{A_{cm}} = \frac{\int_0^H \left( -D_{AB} \frac{dC_A}{dx} \Big|_{x=0,2} \right) dz}{H}$$

$$\frac{dN_{A_{cm}}}{dz} = \frac{\left( -D_{AB} \frac{dC_A}{dx} \Big|_{x=0,2} \right)}{H}$$

$$\frac{dN_{A_{cm}}}{dz} = - \frac{D_{AB}}{H} \frac{(-3C_{A1} + 4C_{A2} - C_{A3})}{2\Delta x}$$

$$M_A = N_{A_{cm}} HW$$



$$M_A = W \int_0^{\delta} u_x C_A dx$$

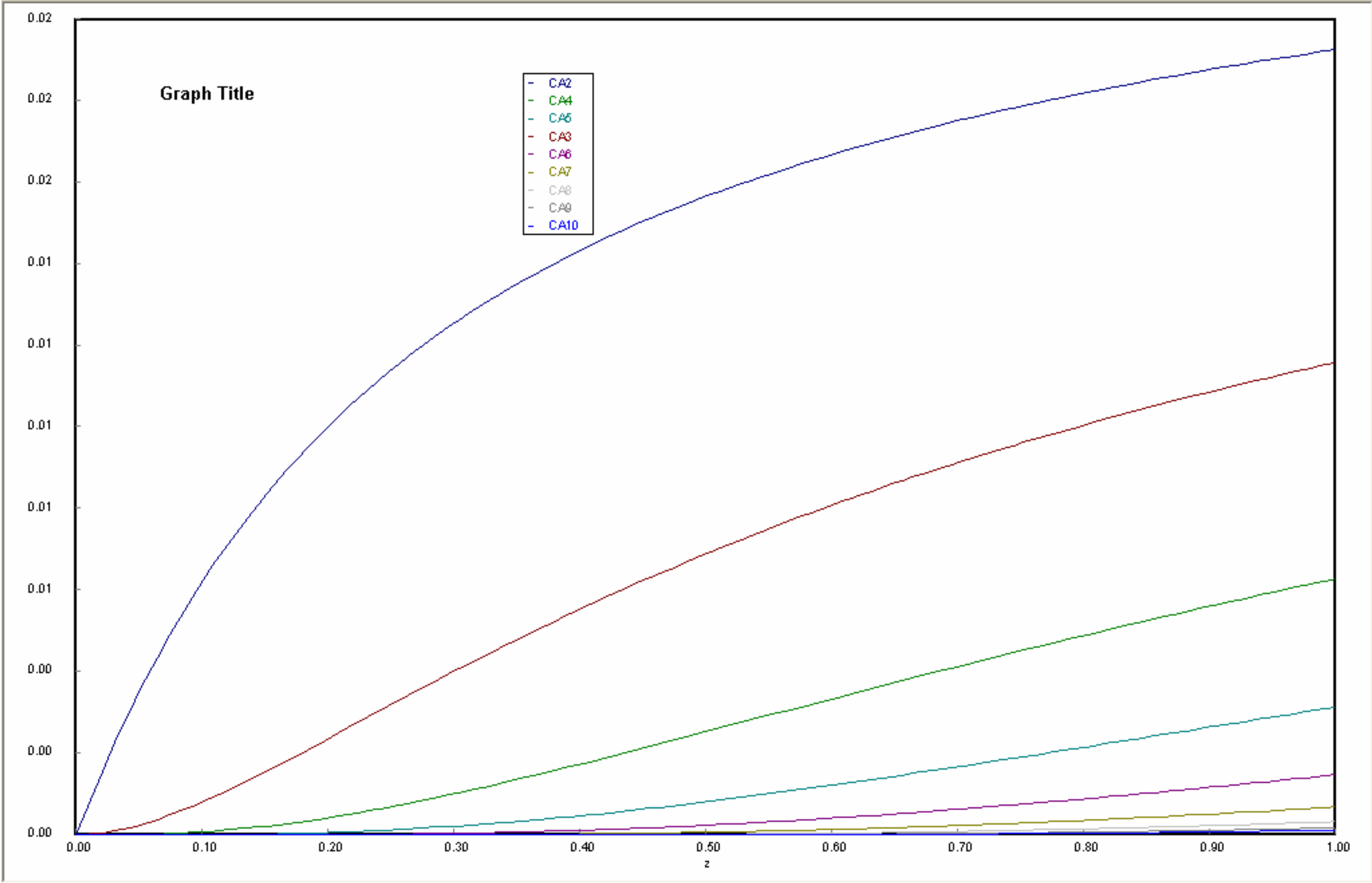

 Indep Var  Initial Value 

 Solve with  Final Value 

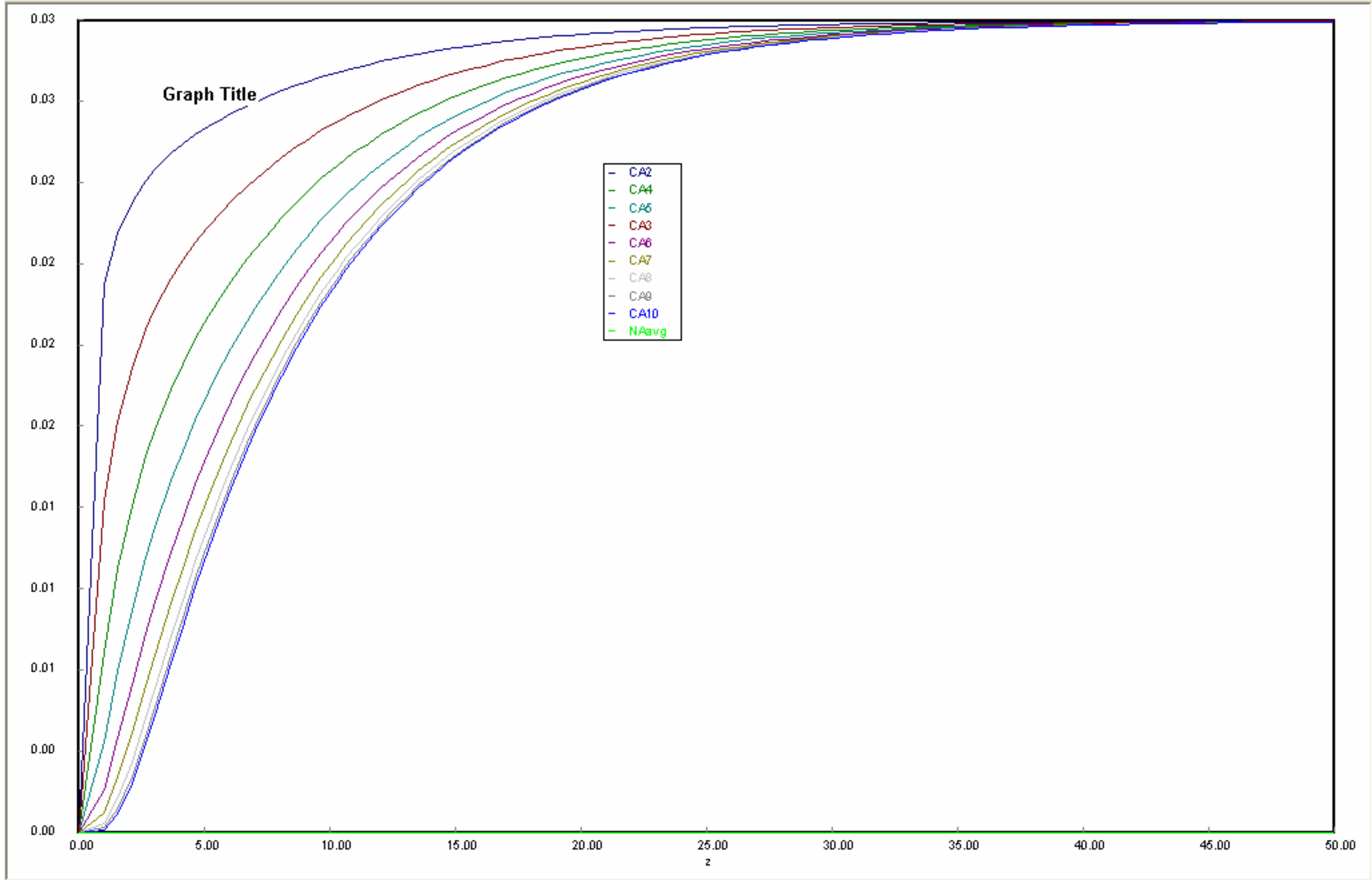
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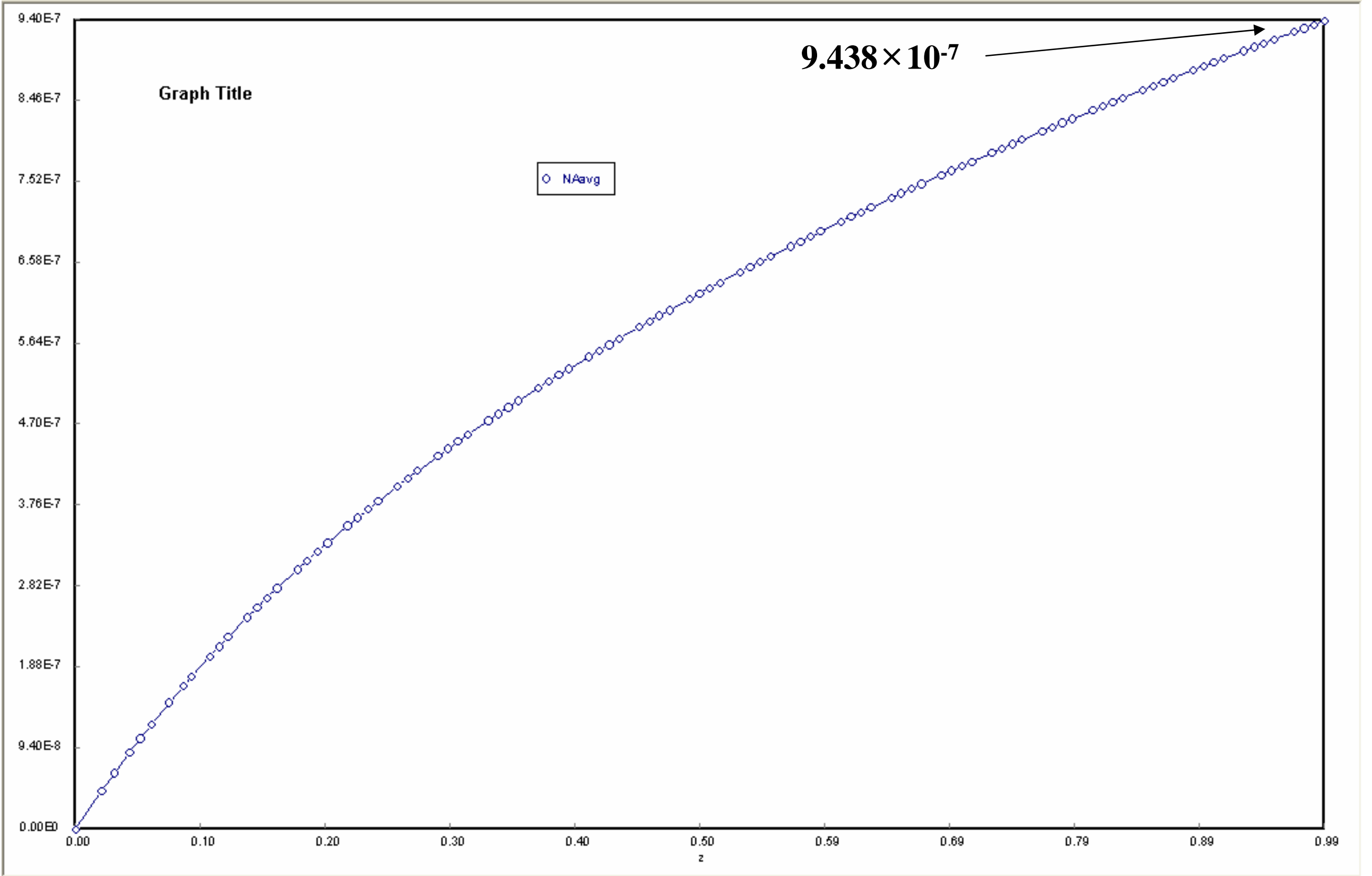
       

	Differential equations / explicit equations	Initial value	Comments
1	$d(CA2)/d(z) = (DAB*(CA3-2*CA2+CA1)/\text{deltax}^2 - kprime*CA2)/(vmax*(1-((2-1)*\text{deltax}/\text{delta})^2))$	0	
2	$d(CA4)/d(z) = (DAB*(CA5-2*CA4+CA3)/\text{deltax}^2 - kprime*CA4)/(vmax*(1-((4-1)*\text{deltax}/\text{delta})^2))$	0	
3	$d(CA5)/d(z) = (DAB*(CA6-2*CA5+CA4)/\text{deltax}^2 - kprime*CA5)/(vmax*(1-((5-1)*\text{deltax}/\text{delta})^2))$	0	
4	$d(CA3)/d(z) = (DAB*(CA4-2*CA3+CA2)/\text{deltax}^2 - kprime*CA3)/(vmax*(1-((3-1)*\text{deltax}/\text{delta})^2))$	0	
5	$d(CA6)/d(z) = (DAB*(CA7-2*CA6+CA5)/\text{deltax}^2 - kprime*CA6)/(vmax*(1-((6-1)*\text{deltax}/\text{delta})^2))$	0	
6	$d(CA7)/d(z) = (DAB*(CA8-2*CA7+CA6)/\text{deltax}^2 - kprime*CA7)/(vmax*(1-((7-1)*\text{deltax}/\text{delta})^2))$	0	
7	$d(CA8)/d(z) = (DAB*(CA9-2*CA8+CA7)/\text{deltax}^2 - kprime*CA8)/(vmax*(1-((8-1)*\text{deltax}/\text{delta})^2))$	0	
8	$d(CA9)/d(z) = (DAB*(CA10-2*CA9+CA8)/\text{deltax}^2 - kprime*CA9)/(vmax*(1-((9-1)*\text{deltax}/\text{delta})^2))$	0	
9	$d(CA10)/d(z) = (DAB*(CA11-2*CA10+CA9)/\text{deltax}^2 - kprime*CA10)/(vmax*(1-((10-1)*\text{deltax}/\text{delta})^2))$	0	
10	DAB = 1.5e-9	n.a.	
11	kprime = 0	n.a.	
12	vmax = 0.6	n.a.	
13	delta = 3.e-4	n.a.	
14	CA1 = 0.03	n.a.	
15	CA11 = if(4*CA10 < CA9) then 0 else (4*CA10 - CA9)/3	n.a.	
16	deltax = 0.1*delta	n.a.	
17	vavg = (2/3)*vmax	n.a.	

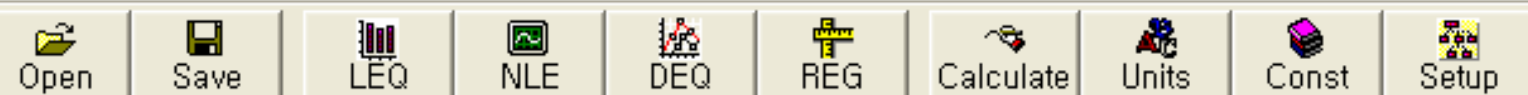


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Indep Var  Initial Value

Solve with  Final Value



Comments

	Differential equations / explicit equations	Initial value	Comments
15	delta = 3.e-4	n.a.	
16	CA1 = 0.03	n.a.	
17	CA11 = if(4*CA10<CA9)then(0)else((4*CA10-CA9)/3)	n.a.	
18	deltax = 0.1*delta	n.a.	
19	vavg = (2/3)*vmax	n.a.	
20	H = 1	n.a.	
21	W = 1	n.a.	
22	vz1 = vmax	n.a.	
23	vz2 = vmax*(1-((2-1)*deltax/delta)^2)	n.a.	
24	vz3 = vmax*(1-((3-1)*deltax/delta)^2)	n.a.	
25	vz4 = vmax*(1-((4-1)*deltax/delta)^2)	n.a.	
26	vz5 = vmax*(1-((5-1)*deltax/delta)^2)	n.a.	
27	vz6 = vmax*(1-((6-1)*deltax/delta)^2)	n.a.	
28	vz7 = vmax*(1-((7-1)*deltax/delta)^2)	n.a.	
29	vz8 = vmax*(1-((8-1)*deltax/delta)^2)	n.a.	
30	vz9 = vmax*(1-((9-1)*deltax/delta)^2)	n.a.	
31	vz10 = vmax*(1-((10-1)*deltax/delta)^2)	n.a.	
32	vz11 = 0	n.a.	
33	vc1 = vz1*CA1	n.a.	
34	vc2 = vz2*CA2	n.a.	
35	vc3 = vz3*CA3	n.a.	
36	vc4 = vz4*CA4	n.a.	
37	vc5 = vz5*CA5	n.a.	
38	vc6 = vz6*CA6	n.a.	
39	vc7 = vz7*CA7	n.a.	
40	vc8 = vz8*CA8	n.a.	
41	vc9 = vz9*CA9	n.a.	
42	vc10 = vz10*CA10	n.a.	
43	vc11 = vz11*CA11	n.a.	

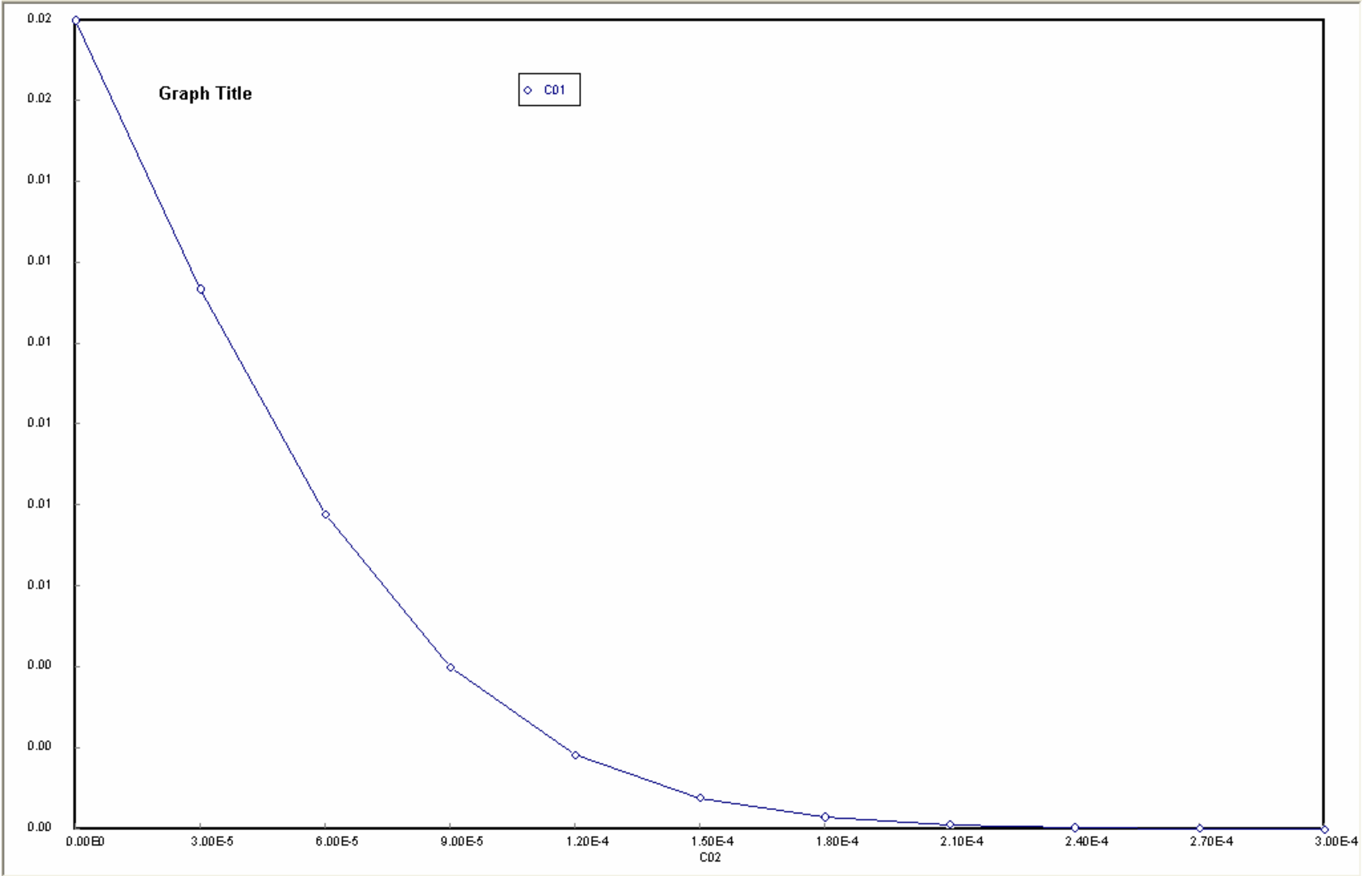
Differential Equations: 10 Auxiliary Equations: 33

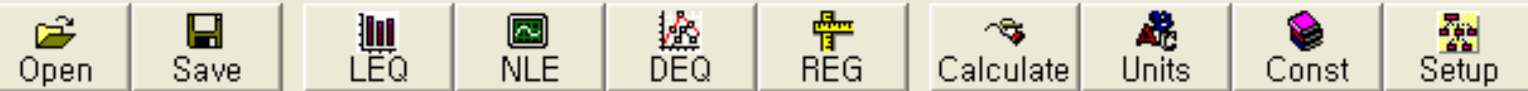
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R100 : C034 =

	vz8	vz9	vz10	vz11	vc1	vc2	vc3	vc4	vc5	vc6	vc7	vc8	vc9	vc10	vc11
67	0.306	0.216	0.114	0	0.018	0.0107759	0.0053315	0.0022246	8.067E-04	2.63E-04	7.979E-05	2.339E-05	6.892E-06	1.973E-06	0
68	0.306	0.216	0.114	0	0.018	0.0108539	0.0054293	0.0022966	8.458E-04	2.803E-04	8.648E-05	2.578E-05	7.723E-06	2.246E-06	0
69	0.306	0.216	0.114	0	0.018	0.0108921	0.0054774	0.0023324	8.655E-04	2.891E-04	8.994E-05	2.703E-05	8.164E-06	2.392E-06	0
70	0.306	0.216	0.114	0	0.018	0.0109296	0.005525	0.0023681	8.852E-04	2.98E-04	9.347E-05	2.832E-05	8.622E-06	2.545E-06	0
71	0.306	0.216	0.114	0	0.018	0.0109665	0.0055721	0.0024037	9.051E-04	3.071E-04	9.709E-05	2.965E-05	9.098E-06	2.705E-06	0
72	0.306	0.216	0.114	0	0.018	0.0110387	0.005665	0.0024745	9.451E-04	3.255E-04	1.045E-04	3.243E-05	1.01E-05	3.046E-06	0
73	0.306	0.216	0.114	0	0.018	0.011074	0.0057107	0.0025098	9.652E-04	3.349E-04	1.084E-04	3.387E-05	1.064E-05	3.228E-06	0
74	0.306	0.216	0.114	0	0.018	0.0111088	0.0057559	0.0025448	9.854E-04	3.444E-04	1.123E-04	3.536E-05	1.119E-05	3.418E-06	0
75	0.306	0.216	0.114	0	0.018	0.0111431	0.0058007	0.0025798	0.0010056	3.541E-04	1.163E-04	3.689E-05	1.176E-05	3.616E-06	0
76	0.306	0.216	0.114	0	0.018	0.0112102	0.005889	0.0026493	0.0010463	3.736E-04	1.245E-04	4.007E-05	1.295E-05	4.036E-06	0
77	0.306	0.216	0.114	0	0.018	0.011243	0.0059325	0.0026838	0.0010667	3.835E-04	1.287E-04	4.172E-05	1.358E-05	4.259E-06	0
78	0.306	0.216	0.114	0	0.018	0.0112754	0.0059755	0.0027182	0.0010872	3.935E-04	1.33E-04	4.341E-05	1.423E-05	4.49E-06	0
79	0.306	0.216	0.114	0	0.018	0.0113073	0.0060181	0.0027525	0.0011078	4.036E-04	1.373E-04	4.514E-05	1.49E-05	4.73E-06	0
80	0.306	0.216	0.114	0	0.018	0.0113698	0.0061021	0.0028206	0.001149	4.241E-04	1.462E-04	4.873E-05	1.63E-05	5.237E-06	0
81	0.306	0.216	0.114	0	0.018	0.0114004	0.0061435	0.0028544	0.0011697	4.345E-04	1.508E-04	5.059E-05	1.704E-05	5.504E-06	0
82	0.306	0.216	0.114	0	0.018	0.0114306	0.0061845	0.002888	0.0011904	4.45E-04	1.554E-04	5.249E-05	1.779E-05	5.781E-06	0
83	0.306	0.216	0.114	0	0.018	0.0114604	0.0062251	0.0029216	0.0012111	4.555E-04	1.602E-04	5.443E-05	1.857E-05	6.067E-06	0
84	0.306	0.216	0.114	0	0.018	0.0115188	0.0063051	0.0029882	0.0012527	4.769E-04	1.698E-04	5.845E-05	2.019E-05	6.669E-06	0
85	0.306	0.216	0.114	0	0.018	0.0115475	0.0063445	0.0030212	0.0012735	4.877E-04	1.747E-04	6.052E-05	2.104E-05	6.985E-06	0
86	0.306	0.216	0.114	0	0.018	0.0115757	0.0063836	0.0030542	0.0012944	4.986E-04	1.797E-04	6.263E-05	2.191E-05	7.312E-06	0
87	0.306	0.216	0.114	0	0.018	0.0116037	0.0064223	0.0030869	0.0013153	5.096E-04	1.848E-04	6.478E-05	2.28E-05	7.648E-06	0
88	0.306	0.216	0.114	0	0.018	0.0116584	0.0064986	0.003152	0.0013571	5.318E-04	1.951E-04	6.922E-05	2.465E-05	8.353E-06	0
89	0.306	0.216	0.114	0	0.018	0.0116853	0.0065362	0.0031843	0.001378	5.43E-04	2.003E-04	7.151E-05	2.561E-05	8.722E-06	0
90	0.306	0.216	0.114	0	0.018	0.0117119	0.0065735	0.0032165	0.001399	5.542E-04	2.057E-04	7.383E-05	2.66E-05	9.101E-06	0
91	0.306	0.216	0.114	0	0.018	0.0117381	0.0066105	0.0032485	0.0014199	5.656E-04	2.111E-04	7.62E-05	2.761E-05	9.491E-06	0
92	0.306	0.216	0.114	0	0.018	0.0117896	0.0066833	0.003312	0.0014619	5.885E-04	2.22E-04	8.107E-05	2.97E-05	1.031E-05	0
93	0.306	0.216	0.114	0	0.018	0.0118148	0.0067193	0.0033436	0.0014828	6.0E-04	2.276E-04	8.357E-05	3.078E-05	1.073E-05	0
94	0.306	0.216	0.114	0	0.018	0.0118398	0.0067549	0.003375	0.0015038	6.116E-04	2.333E-04	8.611E-05	3.189E-05	1.117E-05	0
95	0.306	0.216	0.114	0	0.018	0.0118645	0.0067902	0.0034062	0.0015248	6.233E-04	2.39E-04	8.87E-05	3.303E-05	1.161E-05	0
96	0.306	0.216	0.114	0	0.018	0.011913	0.0068598	0.0034682	0.0015667	6.468E-04	2.506E-04	9.4E-05	3.537E-05	1.254E-05	0
97	0.306	0.216	0.114	0	0.018	0.0119369	0.0068942	0.003499	0.0015877	6.587E-04	2.564E-04	9.671E-05	3.658E-05	1.303E-05	0
98	0.306	0.216	0.114	0	0.018	0.0119604	0.0069283	0.0035296	0.0016086	6.706E-04	2.624E-04	9.947E-05	3.781E-05	1.352E-05	0
99	0.306	0.216	0.114	0	0.018	0.0119837	0.006962	0.0035601	0.0016296	6.825E-04	2.684E-04	1.023E-04	3.907E-05	1.403E-05	0
100	0.306	0.216	0.114	0	0.018	0.0120192	0.0070137	0.0036069	0.0016619	7.011E-04	2.778E-04	1.067E-04	4.107E-05	1.484E-05	0

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Interpolation	Differentiation	Integration
		<div style="display: flex; justify-content: space-between;"> <div style="text-align: center;"> <input type="text" value="0.0003"/>  <math>\int</math>  <input type="text" value="0"/> </div> <div style="text-align: center;"> <math>C01 \, d \, C02 =</math> </div> <div style="text-align: center;"> <input type="text" value="1.018E-06"/> </div> </div> <div style="margin-top: 10px;">           Solve with <input type="text" value="SIMPSON"/> </div>
		Independent var <input type="text" value="C02"/> Dependent var <input type="text" value="C01"/> N = 11 Dev = 0.00%

$$MA1 = N_{avg} * H * W = 9.438 \times 10^{-7}$$

$$MA2 = H \int v_z C_A dx = 1.108 \times 10^{-6}$$

$$(MA2/MA1) = 117.4\%, \quad \text{error} = 17.4\%$$


 Indep Var  Initial Value 

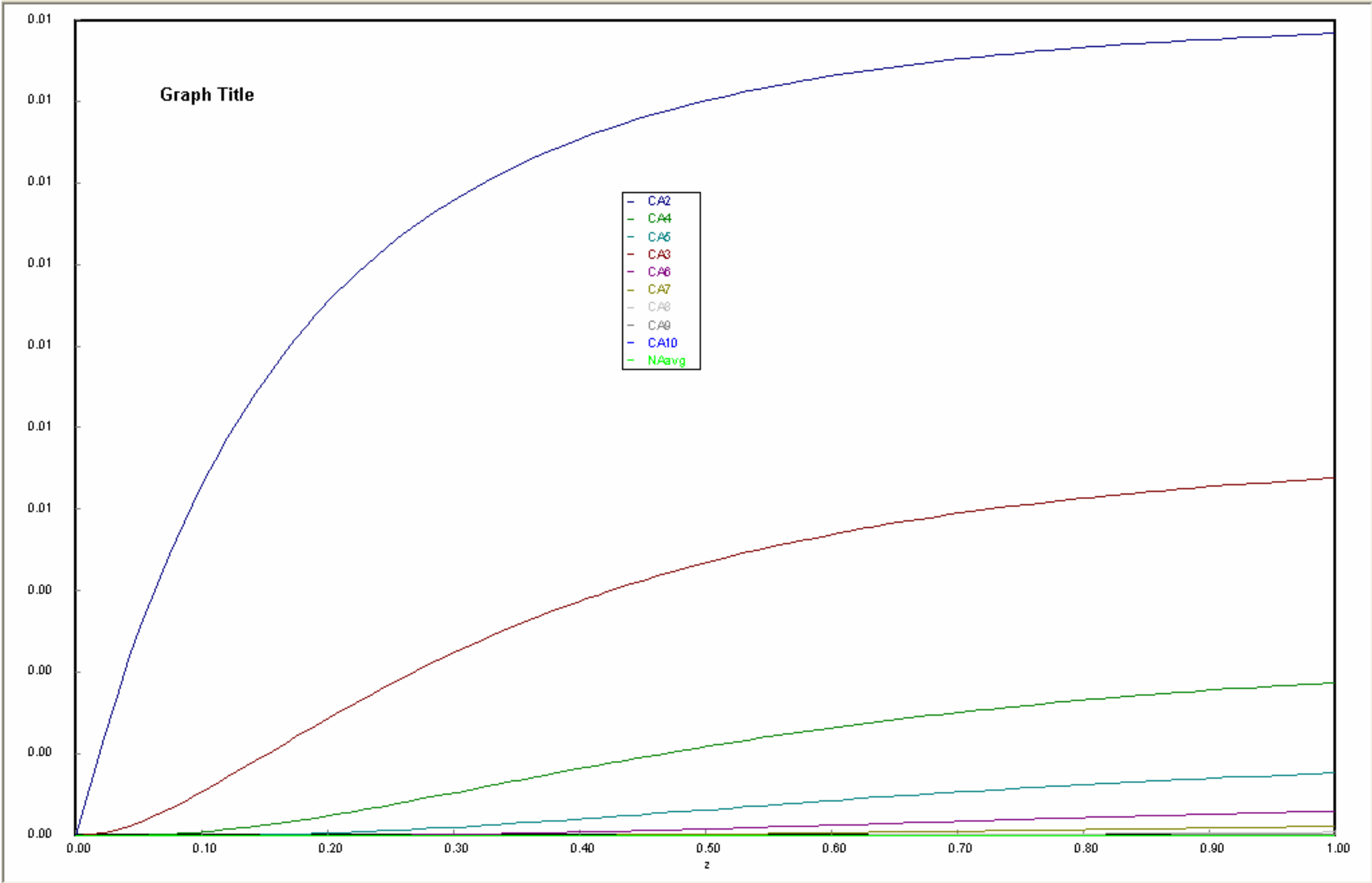
 Solve with  Final Value 

    Comments

	Differential equations / explicit equations	Initial value	Comments
1	$d(CA2)/d(z) = (DAB*(CA3-2*CA2+CA1)/\text{deltax}^2 - k_{\text{prime}}*CA2)/(v_{\text{max}}*(1-((2-1)*\text{deltax}/\text{delta})^2))$	0	
2	$d(CA4)/d(z) = (DAB*(CA5-2*CA4+CA3)/\text{deltax}^2 - k_{\text{prime}}*CA4)/(v_{\text{max}}*(1-((4-1)*\text{deltax}/\text{delta})^2))$	0	
3	$d(CA5)/d(z) = (DAB*(CA6-2*CA5+CA4)/\text{deltax}^2 - k_{\text{prime}}*CA5)/(v_{\text{max}}*(1-((5-1)*\text{deltax}/\text{delta})^2))$	0	
4	$d(CA3)/d(z) = (DAB*(CA4-2*CA3+CA2)/\text{deltax}^2 - k_{\text{prime}}*CA3)/(v_{\text{max}}*(1-((3-1)*\text{deltax}/\text{delta})^2))$	0	
5	$d(CA6)/d(z) = (DAB*(CA7-2*CA6+CA5)/\text{deltax}^2 - k_{\text{prime}}*CA6)/(v_{\text{max}}*(1-((6-1)*\text{deltax}/\text{delta})^2))$	0	
6	$d(CA7)/d(z) = (DAB*(CA8-2*CA7+CA6)/\text{deltax}^2 - k_{\text{prime}}*CA7)/(v_{\text{max}}*(1-((7-1)*\text{deltax}/\text{delta})^2))$	0	
7	$d(CA8)/d(z) = (DAB*(CA9-2*CA8+CA7)/\text{deltax}^2 - k_{\text{prime}}*CA8)/(v_{\text{max}}*(1-((8-1)*\text{deltax}/\text{delta})^2))$	0	
8	$d(CA9)/d(z) = (DAB*(CA10-2*CA9+CA8)/\text{deltax}^2 - k_{\text{prime}}*CA9)/(v_{\text{max}}*(1-((9-1)*\text{deltax}/\text{delta})^2))$	0	
9	$d(CA10)/d(z) = (DAB*(CA11-2*CA10+CA9)/\text{deltax}^2 - k_{\text{prime}}*CA10)/(v_{\text{max}}*(1-((10-1)*\text{deltax}/\text{delta})^2))$	0	
10	$d(NA_{\text{avg}})/d(z) = (-DAB/H)*(-3*CA1+4*CA2-CA3)/(2*\text{deltax})$	0	
11	$MA = NA_{\text{avg}}*H*W$	n.a.	
12	$DAB = 1.5e-9$	n.a.	
13	$k_{\text{prime}} = 1$	n.a.	
14	$v_{\text{max}} = 0.6$	n.a.	
15	$\text{delta} = 3.e-4$	n.a.	
16	$CA1 = 0.03$	n.a.	
17	$CA11 = \text{if}(4*CA10 < CA9) \text{then}(0) \text{else}((4*CA10 - CA9)/3)$	n.a.	
18	$\text{deltax} = 0.1*\text{delta}$	n.a.	
19	$v_{\text{avg}} = (2/3)*v_{\text{max}}$	n.a.	
20	$H = 1$	n.a.	
21	$W = 1$	n.a.	
22	$v_{z1} = v_{\text{max}}$	n.a.	
23	$v_{z2} = v_{\text{max}}*(1-((2-1)*\text{deltax}/\text{delta})^2)$	n.a.	
24	$v_{z3} = v_{\text{max}}*(1-((3-1)*\text{deltax}/\text{delta})^2)$	n.a.	
25	$v_{z4} = v_{\text{max}}*(1-((4-1)*\text{deltax}/\text{delta})^2)$	n.a.	
26	$v_{z5} = v_{\text{max}}*(1-((5-1)*\text{deltax}/\text{delta})^2)$	n.a.	
27	$v_{z6} = v_{\text{max}}*(1-((6-1)*\text{deltax}/\text{delta})^2)$	n.a.	
28	$v_{z7} = v_{\text{max}}*(1-((7-1)*\text{deltax}/\text{delta})^2)$	n.a.	
29	$v_{z8} = v_{\text{max}}*(1-((8-1)*\text{deltax}/\text{delta})^2)$	n.a.	
30	$v_{z9} = v_{\text{max}}*(1-((9-1)*\text{deltax}/\text{delta})^2)$	n.a.	

Differential Equations: 10 Auxiliary Equations: 33



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