Solution of a Partial Differential Equations using the Method of Lines

Differential equations where there are several independent variables, such as in the equation:

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)$$

are called partial differential equations. To completely define a problem involving PDEs initial values and boundary conditions have to be specified, also.

The use of the "Method of Lines" for solving PDEs is demonstrated in this example.

Diffusion and Reaction in Falling Laminar Liquid Film of Finite Thickness

Steady state mass balance

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

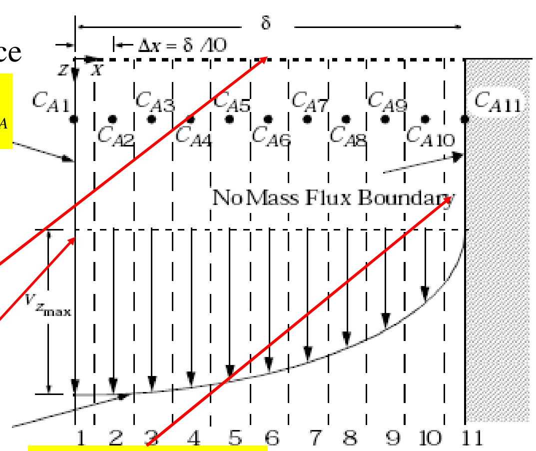
Laminar flow profile

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

Boundary conditions

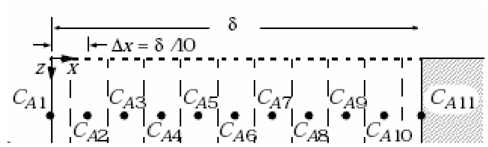
$$C_A |_{z=0} = 0;$$

$$C_A |_{x=0, z>0} = C_{AS} = 0.03$$



$$\frac{\partial C_A}{\partial z} |_{x=\delta, z>0} = 0$$

Discretization of the Partial Differential Equation in the x Direction



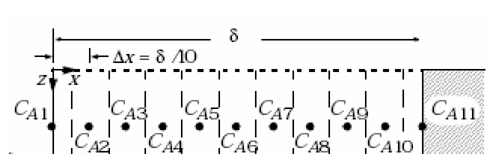
Central difference approximation for the 2nd derivative:

$$\frac{\partial C_{An}}{\partial z}=\left[\frac{D_{AB}}{(\Delta x)^2}\left(C_{A,n+1}-2C_{An}+C_{A,n-1}\right)-k' C_{A,n}\right]/v_{zn}\ \ for\left(2\le n\le 10\right)$$

Local velocity expression

$$v_{z,n}=v_{z,\max}\left[1-\left(\frac{(n-1)\Delta x}{\delta}\right)^2\right] for\left(2\le n\le 10\right)_A$$

Discretization of the Initial Values



$C_A\,|_{z=0}=0;$ $\qquad C_{An}=0;\ for\left(2\le n\le 10\right)$

$C_A\,|_{x=0,z>0}=C_{AS}=0.03$ $\qquad C_{A1}=0.03;\ for\ z>0$

$\frac{\partial C_A}{\partial z}\,|_{x=\delta,z>0}=0$

2nd order backward approximation

$$\frac{\partial C_{A11}}{\partial x}=\frac{3C_{A11}-4C_{A10}+C_{A9}}{2\Delta x}=0$$

Solving for C_{A11} $\qquad C_{A11}=\frac{4C_{A10}-C_{A9}}{3}$

Diffusion and Reaction in Falling Laminar Liquid Film of Finite Thickness - Solution by the Method of Lines

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d(CA2)/d(z)=(DAB*(CA3-2*CA2+CA1)/deltax^2-kprime*CA2)/(vmax*(1-((2-1)*deltax/delta)^2))
d(CA4)/d(z)=(DAB*(CA5-2*CA4+CA3)/deltax^2-kprime*CA4)/(vmax*(1-((4-1)*deltax/delta)^2))
d(CA5)/d(z)=(DAB*(CA6-2*CA5+CA4)/deltax^2-kprime*CA5)/(vmax*(1-((5-1)*deltax/delta)^2))
d(CA3)/d(z)=(DAB*(CA4-2*CA3+CA2)/deltax^2-kprime*CA3)/(vmax*(1-((3-1)*deltax/delta)^2))
d(CA6)/d(z)=(DAB*(CA7-2*CA6+CA5)/deltax^2-kprime*CA6)/(vmax*(1-((6-1)*deltax/delta)^2))
d(CA7)/d(z)=(DAB*(CA8-2*CA7+CA6)/deltax^2-kprime*CA7)/(vmax*(1-((7-1)*deltax/delta)^2))
d(CA8)/d(z)=(DAB*(CA9-2*CA8+CA7)/deltax^2-kprime*CA8)/(vmax*(1-((8-1)*deltax/delta)^2))
d(CA9)/d(z)=(DAB*(CA10-2*CA9+CA8)/deltax^2-kprime*CA9)/(vmax*(1-((9-1)*deltax/delta)^2))
d(CA10)/d(z)=(DAB*(CA11-2*CA10+CA9)/deltax^2-kprime*CA10)/(vmax*(1-((10-1)*deltax/delta)^2))
DAB=1.5E-9
kprime=0
vmax=0.6
delta=3.E-4
CA1=0.03
CA11=if(4*CA10<CA9)then(0)else((4*CA10-CA9)/3)
deltax=0.1*delta
vavg=(2/3)*vmax
z(0)=0
CA2(0)=0
CA4(0)=0
CA5(0)=0
CA3(0)=0
CA6(0)=0
CA7(0)=0
CA8(0)=0
CA9(0)=0
CA10(0)=0
z(f)=1
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No reaction

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

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

$$C_{A1} = 0.03$$

$$C_{A11} = \frac{4C_{A10} - C_{A9}}{3}$$

$$C_{An} = 0; \; for \left(2 \le n \le 10 \right)$$

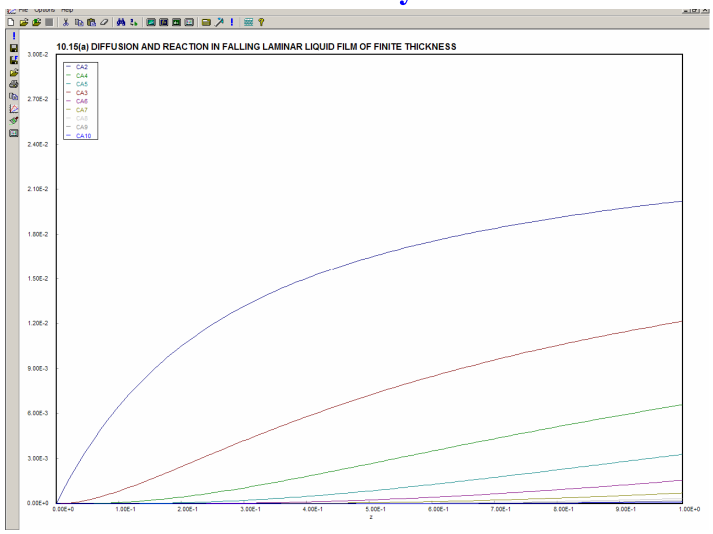
Diffusion and Reaction in Falling Laminar Liquid Film of Finite Thickness - Solution by the Method of Lines

POLYMATH Report
Ordinary Differential Equations

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	CA1	0.03	0.03	0.03	0.03
2	CA10	0	0	0.0001302	0.0001302
3	CA11	0	0	0.0001102	0.0001102
4	CA2	0	0	0.0202344	0.0202344
5	CA3	0	0	0.0121765	0.0121765
6	CA4	0	0	0.006606	0.006606
7	CA5	0	0	0.0032975	0.0032975
8	CA6	0	0	0.001558	0.001558
9	CA7	0	0	0.0007235	0.0007235
10	CA8	0	0	0.0003486	0.0003486
11	CA9	0	0	0.0001902	0.0001902
12	DAB	1.5E-09	1.5E-09	1.5E-09	1.5E-09
13	delta	0.0003	0.0003	0.0003	0.0003
14	deltax	3.0E-05	3.0E-05	3.0E-05	3.0E-05
15	kprime	0	0	0	0
16	vavg	0.4	0.4	0.4	0.4
17	vmax	0.6	0.6	0.6	0.6
18	z	0	0	1.	1.

Diffusion and Reaction in Falling Laminar Liquid Film of Finite Thickness - Solution by the Method of Lines



Calculation of the Average Flux of A absorbed by the Film

The average flux of A (*NAavg)* to a liquid film of height H is given by

$$N_{A_{avg}} = \frac{\int_0^H \left(-D_{AB} \frac{dC_A}{dx} \bigg|_{x=0,\,z} \right) dz}{H} \quad \text{or} \quad \frac{dN_{A_{avg}}}{dz} = \frac{\left(-D_{AB} \frac{dC_A}{dx} \bigg|_{x=0,\,z} \right)}{H} \quad N_{Aavg} = 0 \text{ at } z = 0$$

Where N_{Aavg} is in kg-mol/m^2*s and H is in m.

Rewriting the equation using second-order forward difference approximation yields

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

Adding to the Polymath program

d(NAavg)/d(z)=-(DAB/H)*(-3*CA1+4*CA2-CA3)/(2*deltax)

NAavg(0)=0

Balance on *A* Absorbed and *A* Exiting by Flow

For a film of height H in m and width W in m, the input is given by

$$M_A = NAavg\ H\ W$$

where M_A is in kg-mol/s

The output of A that exits the film of height H is

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

In which v_z and C_A are determined by the profile obtained from the numerical solution at height *H*.

To calculate the integral the values of C_A at 11 node location are entered into the data table of Polymath where the Analysis -> Integration options are used to carry out the integration