Boundary value problems

Martin van Sint Annaland, Edwin Zondervan, Ivo Roghair

m.v.sintannaland@tue.nl

Chemical Process Intensification,
Process Systems Engineering,
Eindhoven University of Technology

Today's outline

1. Solution techniques in Excel
   - Solver and goal-seek
2. Boundary value problems
3. Shooting method
   - Example

Today's outline

1. Solution techniques in Excel
   - Solver and goal-seek
2. Boundary value problems
3. Shooting method
   - Example

Solver and goal-seek

Excel comes with a goal-seek and solver function. For Excel 2010:

- Install via Excel ⇒ File ⇒ Options ⇒ Add-Ins ⇒ Go (at the bottom) ⇒ Select solver add-in. You can now call the solver screen on the 'data' menu ('Oplosser' in Dutch)
- Select the goal-cell, and whether you want to minimize, maximize or set a certain value
- Enter the variable cells; Excel is going to change the values in these cells to get to the desired solution
- Specify the boundary conditions (e.g. to keep certain cells above zero)
- Click 'solve' (possibly after setting the advanced options).

Goal-seek: a simple example

Goal-Seek can be used to make the goal-cell to a specified value by changing another cell:

- Open Excel and type the following:

	A	B
1	x	3
2	f(x)	=–3*B1^2–5*B1+2
3		

- Go to Data ⇒ What-If Analysis ⇒ Goal Seek...
  - Set cell: B2
  - To value: 0
  - By changing cell: B1
- OK. You find a solution of 0.333 . . . .

Goal-seek: a simple example

Goal-Seek can be used to make the goal-cell to a specified value by changing another cell:

- Open Excel and type the following:

	A	B
1	x	3
2	f(x)	=–3*B1^2–5*B1+2
3		

- Go to Data ⇒ What-If Analysis ⇒ Goal Seek...
  - Set cell: B2
  - To value: 0
  - By changing cell: B1
- OK. You find a solution of 0.333 . . ..

Goal-seek: a simple example

Goal-Seek can be used to make the goal-cell to a specified value by changing another cell:

- Open Excel and type the following:

	A	B
1	x	3
2	f(x)	=–3*B1^2–5*B1+2
3		

- Go to Data ⇒ What-If Analysis ⇒ Goal Seek...
  - Set cell: B2
  - To value: 0
  - By changing cell: B1
- OK. You find a solution of 0.333 . . ..

Goal-seek: a simple example

Goal-Seek can be used to make the goal-cell to a specified value by changing another cell:

- Open Excel and type the following:

	A	B
1	x	3
2	f(x)	=–3*B1^2–5*B1+2
3		

- Go to Data ⇒ What-If Analysis ⇒ Goal Seek...
  - Set cell: B2
  - To value: 0
  - By changing cell: B1
- OK. You find a solution of 0.333 . . . .

Solver: a simple example

The solver is used to change the value in a goal-cell, by changing the values in 1 or more other cells while keeping boundary conditions:

- Use the following sheet:

	A	B	C
1		x	f(x)
2	x1	3	=2*B2*B3–B3+2
3	x2	4	=2*B3–4*B2-4

- Go to Data ⇒ Solver
  - Goalfunction: C1 (value of: 0)
  - Add boundary condition: C2 = 0
  - By changing cells: $B$1:$B$2 (you can just select the cells)
- Solve. You will find B1=0 and B2=2.

Solver: a simple example

The solver is used to change the value in a goal-cell, by changing the values in 1 or more other cells while keeping boundary conditions:

- Use the following sheet:

	A	B	C
1		x	f(x)
2	x1	3	=2*B2*B3–B3+2
3	x2	4	=2*B3–4*B2-4

- Go to Data ⇒ Solver
  - Goalfunction: C1 (value of: 0)
  - Add boundary condition: C2 = 0
  - By changing cells: $B$1:$B$2 (you can just select the cells)
- Solve. You will find B1=0 and B2=2.

Solver: a simple example

The solver is used to change the value in a goal-cell, by changing the values in 1 or more other cells while keeping boundary conditions:

- Use the following sheet:

	A	B	C
1		x	f(x)
2	x1	3	=2*B2*B3–B3+2
3	x2	4	=2*B3–4*B2-4

- Go to Data ⇒ Solver
  - Goalfunction: C1 (value of: 0)
  - Add boundary condition: C2 = 0
  - By changing cells: $B$1:$B$2 (you can just select the cells)
- Solve. You will find B1=0 and B2=2.

Solver: a simple example

The solver is used to change the value in a goal-cell, by changing the values in 1 or more other cells while keeping boundary conditions:

- Use the following sheet:

	A	B	C
1		x	f(x)
2	x1	3	=2*B2*B3–B3+2
3	x2	4	=2*B3–4*B2-4

- Go to Data ⇒ Solver
  - Goalfunction: C1 (value of: 0)
  - Add boundary condition: C2 = 0
  - By changing cells: $B$1:$B$2 (you can just select the cells)
- Solve. You will find B1=0 and B2=2.

Exercise

Use Excel functions to obtain the Antoine coefficients A, B and C for carbon monoxide following the equation:

$$\ln P = A - \frac{B}{T + C}$$

P in Pa, T in K. Experimental data is given:

P [mmHg]	T [°C]
1	-222.0
5	-217.2
10	-215.0
20	-212.8
40	-210.0
60	-208.1
100	-205.7
200	-201.3
400	-196.3
760	-191.3

Exercise

Use Excel functions to obtain the Antoine coefficients A, B and C for carbon monoxide following the equation:

$$\ln P = A - \frac{B}{T + C}$$

P in Pa, T in K. Experimental data is given:

P [mmHg]	T [°C]
1	-222.0
5	-217.2
10	-215.0
20	-212.8
40	-210.0
60	-208.1
100	-205.7
200	-201.3
400	-196.3
760	-191.3

1. Dedicate three separate cells for A, B and C. Give an initial guess
2. Convert all values to proper units (hint: use e.g. =CONVERT(A2,“mmHg”,“Pa”))

Exercise

Use Excel functions to obtain the Antoine coefficients A, B and C for carbon monoxide following the equation:

$$\ln P = A - \frac{B}{T + C}$$

P in Pa, T in K. Experimental data is given:

P [mmHg]	T [°C]
1	-222.0
5	-217.2
10	-215.0
20	-212.8
40	-210.0
60	-208.1
100	-205.7
200	-201.3
400	-196.3
760	-191.3

1. Dedicate three separate cells for A, B and C. Give an initial guess
2. Convert all values to proper units (hint: use e.g. =CONVERT(A2,“mmHg”,“Pa”))
3. Compute $\ln P_{exp}$ and $\ln P_{corr}$

Exercise

Use Excel functions to obtain the Antoine coefficients A, B and C for carbon monoxide following the equation:

$$\ln P = A - \frac{B}{T + C}$$

P in Pa, T in K. Experimental data is given:

P [mmHg]	T [°C]
1	-222.0
5	-217.2
10	-215.0
20	-212.8
40	-210.0
60	-208.1
100	-205.7
200	-201.3
400	-196.3
760	-191.3

1. Dedicate three separate cells for A, B and C. Give an initial guess
2. Convert all values to proper units (hint: use e.g. =CONVERT(A2,“mmHg”,“Pa”))
3. Compute $\ln P_{\text{exp}}$ and $\ln P_{\text{corr}}$
4. Compute $(\ln P_{\text{exp}} - \ln P_{\text{corr}})^2$, and sum this column

Exercise

Use Excel functions to obtain the Antoine coefficients A, B and C for carbon monoxide following the equation:

$$\ln P = A - \frac{B}{T + C}$$

P in Pa, T in K. Experimental data is given:

P [mmHg]	T [°C]
1	-222.0
5	-217.2
10	-215.0
20	-212.8
40	-210.0
60	-208.1
100	-205.7
200	-201.3
400	-196.3
760	-191.3

1. Dedicate three separate cells for A, B and C. Give an initial guess
2. Convert all values to proper units (hint: use e.g. =CONVERT(A2,“mmHg”,“Pa”))
3. Compute $\ln P_{\text{exp}}$ and $\ln P_{\text{corr}}$
4. Compute $(\ln P_{\text{exp}} - \ln P_{\text{corr}})^2$, and sum this column
5. Start the solver, and minimize the sum by changing cells for A, B and C.

Exercise

Use Excel functions to obtain the Antoine coefficients A, B and C for carbon monoxide following the equation:

$$\ln P = A - \frac{B}{T + C}$$

P in Pa, T in K. Experimental data is given:

P [mmHg]	T [°C]
1	-222.0
5	-217.2
10	-215.0
20	-212.8
40	-210.0
60	-208.1
100	-205.7
200	-201.3
400	-196.3
760	-191.3

1. Dedicate three separate cells for A, B and C. Give an initial guess
2. Convert all values to proper units (hint: use e.g. =CONVERT(A2,"mmHg","Pa"))
3. Compute $\ln P_{\mathrm{exp}}$ and $\ln P_{\mathrm{corr}}$
4. Compute $(\ln P_{\mathrm{exp}} - \ln P_{\mathrm{corr}})^2$, and sum this column
5. Start the solver, and minimize the sum by changing cells for A, B and C.

What is an ODE?

- Algebraic equation:

$$f(y(x), x) = 0 \qquad \text{e.g.} \ -\ln(K_{eq}) = (1-\zeta)$$

- First order ODE:

$$f\left(\frac{dy}{dx}(x), y(x), x\right) = 0 \quad \text{e.g.} \ \frac{dc}{dt} = -kc^n$$

- Second order ODE:

$$f\left(\frac{d^2y}{dx^2}(x), \frac{dy}{dx}(x), y(x), x\right) = 0 \quad \text{e.g.} \quad \mathcal{D}\frac{d^2c}{dx^2} = -\frac{kc}{1+Kc}$$

About second order ODEs

Very often a second order ODE can be rewritten into a system of first order ODEs (whether it is handy depends on the boundary conditions!)

About second order ODEs

Very often a second order ODE can be rewritten into a system of first order ODEs (whether it is handy depends on the boundary conditions!)

In general

Consider the second order ODE:

$$\frac{d^2y}{dx^2} + q(x)\frac{dy}{dx} = r(x)$$

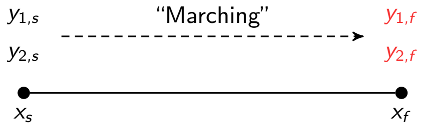
Now define and solve using z as a new variable:

$$\frac{dy}{dx} = z(x)$$
$$\frac{dz}{dx} = r(x) - q(x)z(x)$$

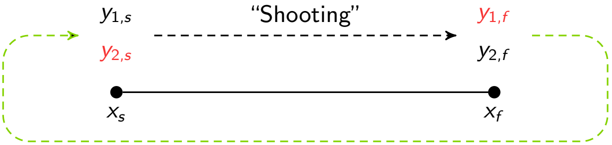
Importance of boundary conditions

The nature of boundary conditions determines the appropriate numerical method. Classification into 2 main categories:

- *Initial value problems (IVP)*
  We know the values of all y_i at some starting position x_s, and it is desired to find the values of y_i at some final point x_f.

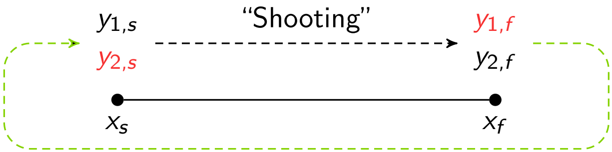


- *Boundary value problems (BVP)*
  Boundary conditions are specified at more than one x. Typically, some of the BC are specified at x_s and the remainder at x_f.



Shooting method

How to solve a BVP using the shooting method:



- Define the system of ODEs
- Provide an initial guess for the unknown boundary condition
- Solve the system and compare the resulting boundary condition to the expected value
- Adjust the guessed boundary value, and solve again. Repeat until convergence.
  - Of course, you can subtract the expected value from the computed value at the boundary, and use a non-linear root finding method

BVP: example in Excel

Consider a chemical reaction in a liquid film layer of thickness δ:

$$\mathcal{D}\frac{d^2c}{dx^2} = k_R c \text{ with } \quad \begin{aligned} &c(x=0) = C_{A,i,L} = 1 && \text{(interface concentration)} \\ &c(x=\delta) = 0 && \text{(bulk concentration)} \end{aligned}$$

Question: compute the concentration profile in the film layer.

BVP: example in Excel

Consider a chemical reaction in a liquid film layer of thickness δ:

$$\mathcal{D}\frac{d^2c}{dx^2} = k_R c \text{ with } \begin{array}{ll} c(x=0) = C_{A,i,L} = 1 & \text{(interface concentration)} \\ c(x=\delta) = 0 & \text{(bulk concentration)} \end{array}$$

Question: compute the concentration profile in the film layer.

Step 1: Define the system of ODEs

This second-order ODE can be rewritten as a system of first-order ODEs, if we define the flux q as:

$$q = -\mathcal{D}\frac{dc}{dx}$$

Now, we find:

$$\frac{dc}{dx} = -\frac{1}{\mathcal{D}}q$$
$$\frac{dq}{dx} = -k_R c$$

BVP: example in Excel

Consider a chemical reaction in a liquid film layer of thickness δ:

$$\mathcal{D}\frac{d^2c}{dx^2} = k_R c \text{ with } \quad \begin{array}{ll} c(x=0) = C_{A,i,L} = 1 & \text{(interface concentration)} \\ c(x=\delta) = 0 & \text{(bulk concentration)} \end{array}$$

Question: compute the concentration profile in the film layer.

Step 2: Set the boundary conditions

The boundary conditions for the concentrations at $x = 0$ and $x = \delta$ are known.

The flux at the interface, however, is not known, and should be solved for.

$$\frac{dc}{dx} = -\frac{1}{\mathcal{D}}q$$

$$\frac{dq}{dx} = -k_R c$$

BVP: example in Excel

Solving the two first-order ODEs in Excel. First, the cells with constants:

	A	B	C
1	CAiL	1	ml/m3
2	D	1e–8	m2/s
3	kR	10	1/s
4	delta	1e–4	m
5	N	100	
6	dx	=B4/B5	

$$\frac{dc}{dx} = -\frac{1}{\mathcal{D}} q$$

$$\frac{dq}{dx} = -k_R c$$

BVP: example in Excel

Solving the two first-order ODEs in Excel. First, the cells with constants:

	A	B	C
1	CAiL	1	ml/m3
2	D	1e–8	m2/s
3	kR	10	1/s
4	delta	1e–4	m
5	N	100	
6	dx	=B4/B5	

$$\frac{dc}{dx} = -\frac{1}{\mathcal{D}}q$$

$$\frac{dq}{dx} = -k_R c$$

Now, we program the forward Euler (explicit) schemes for c and q below:

	A	B	C
10	x	c	q
11	0	=B1	10
12	=A11+$B$6	=B11+$B$6*(–1/$B$2*C11)	=C11+$B$6*(-$B$3*B11)
13	=A12+$B$6	=B12+$B$6*(–1/$B$2*C12)	=C12+$B$6*(-$B$3*B12)
...	...	...	...
111	=A110+$B$6	=B110+$B$6*(–1/$B$2*C110)	=C110+$B$6*(-$B$3*B110)

BVP: example in Excel

- We now have profiles for c and q as a function of position x.
- The concentration $c(x = \delta)$ depends (eventually) on the boundary condition at the interface $q(x = 0)$
- We can use the solver to change $q(x = 0)$ such that the concentration at the bulk meets our requirement: $c(x = \delta) = 0$

BVP: example in Matlab

We first program the system of ODEs in a separate function:

$$\frac{dc}{dx} = -\frac{1}{\mathcal{D}}q$$
$$\frac{dq}{dx} = -k_R c$$

```
function [dxdt] = BVPODE(t,x,ps)
dxdt(1)=-1/ps.D*x(2);
dxdt(2)=-ps.kR*x(1);
dxdt=dxdt';
return
```

BVP: example in Matlab

We first program the system of ODEs in a separate function:

$$\frac{dc}{dx} = -\frac{1}{\mathcal{D}}q$$
$$\frac{dq}{dx} = -k_R c$$

```
function [dxdt] = BVPODE(t,x,ps)
dxdt(1)=-1/ps.D*x(2);
dxdt(2)=-ps.kR*x(1);
dxdt=dxdt';
return
```

Note that we pass a variable (type: struct) that contains required parameters: `ps`.

BVP: example in Matlab

The ODE function is solved via ode45, after setting a number of initial and boundary conditions:

```
function f = RunBVP(bcq,ps)
[x,cq] = ode45(@BVPODE,[0 ps.delta],[1 bcq], [], ps);
f = cq(end,1) - 0;
plotyy(x,cq(:,1),x,cq(:,2));
return;
```

BVP: example in Matlab

The ODE function is solved via ode45, after setting a number of initial and boundary conditions:

```
function f = RunBVP(bcq,ps)
[x,cq] = ode45(@BVPODE,[0 ps.delta],[1 bcq], [], ps);
f = cq(end,1) - 0;
plotyy(x,cq(:,1),x,cq(:,2));
return;
```

Note the following:

- We use the interval $0 \leq x \leq \delta$
- Boundary conditions are given as: $c(x = 0) = 1$ and $q(x = 0) =$ `bcq`, which is given as an argument to the function (i.e. changable from 'outside'!)
- The function returns `f`, the difference between the computed and desired concentration at $x = \delta$.

BVP: example in Matlab

Finally, we should solve the system so that we obtain the right boundary condition $q = \texttt{bcq}$ such that $c(x = \delta) = 0$. We can use the built-in function `fzero` to do this

```
% Parameter definition
ps.D=1e-8;
ps.kR=10;
ps.delta=1e-4;

% Solve for flux boundary condition (initial guess: 0)
opt = optimset('Display','iter');
flux = fzero(@RunBVP,0,opt,ps);
```

BVP example: analytical solution

Compare with the analytical solution:

$$q = k_L E_A C_{A,i,L} \quad \text{with}$$

$$E_A = \frac{Ha}{\tanh Ha} \qquad \text{(Enhancement factor)}$$

$$Ha = \frac{\sqrt{k_R \mathcal{D}}}{k_L} \qquad \text{(Hatta number)}$$

$$k_L = \frac{\mathcal{D}}{\delta} \qquad \text{(mass transfer coefficient)}$$