Modeling of geochemical processes

Numeric methods

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Dynamic models

Numerical methods for solution of differential equations

Euler iteration method

Differential equation: $\frac{dy}{dx} = f(x)$

Substituting of differentials by differences gives: $\frac{\Delta y}{\Delta x} = f(x)$

$$\frac{y_{(k+1)} - y_k}{x_{k+1} - x_k} = f(x_k) \qquad \frac{y_{(k+1)} - y_k}{h} = f(x)$$

h is a step of iteration

It gives $$\boxed{y_{k+1} = y_k + h\, f(x_k)}$$

The precision of the method depends on the magnitude of ***h***

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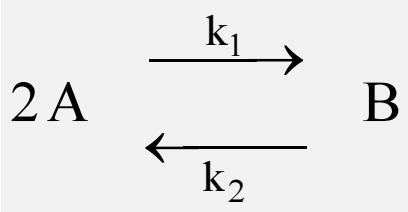
Example:



$$+\frac{dA}{dt} = 2k_2 B - 2k_1 A^2$$

$$+\frac{dB}{dt} = k_1 A^2 - k_2 B$$

$$k_1 = 300$$

$$k_2 = 0{,}15$$

$$A_{n+1} = A_n + 0{,}1\,(2\,k_2 B_n - 2\,k_1 A_n^2)$$

$$B_{n+1} = B_n + 0{,}1\,(k_1 A_n^2 - k_2 B_n)$$

t	A	B	S
0	1,00E-03	0	1,00E-03
0,1	9,40E-04	3,00E-05	1,00E-03
0,2	8,88E-04	5,61E-05	1,00E-03
0,3	8,42E-04	7,89E-05	1,00E-03
0,4	8,02E-04	9,90E-05	1,00E-03
…	…	…	…
…	…	…	…
…	…	…	…
9,4	3,91E-04	3,04E-04	1,00E-03
9,5	3,91E-04	3,04E-04	1,00E-03
9,6	3,91E-04	3,04E-04	1,00E-03
9,7	3,91E-04	3,04E-04	1,00E-03
9,8	3,91E-04	3,04E-04	1,00E-03
9,9	3,91E-04	3,04E-04	1,00E-03
10	3,91E-04	3,04E-04	1,00E-03

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Runge - Kutta method of 4th order

$$+\frac{dA}{dt} = 2k_2 B - 2k_1 A^2$$

$$+\frac{dB}{dt} = k_1 A^2 - k_2 B$$

$$A^{n+1} = A^n + \frac{1}{6}(p_1^{n+1} + 2p_2^{n+1} + 2p_3^{n+1} + p_4^{n+1})$$

$$B^{n+1} = B^n + \frac{1}{6}(q_1^{n+1} + 2q_2^{n+1} + 2q_3^{n+1} + q_4^{n+1})$$

$$p_1^{n+1} = h\, f\left(t^n,\ A^n,\ B^n\right)$$

$$p_2^{n+1} = h\, f\left(t^n + \frac{h}{2},\ A^n + \frac{p_1}{2},\ B^n + \frac{q_1}{2}\right)$$

$$p_3^{n+1} = h\, f\left(t^n + \frac{h}{2},\ A^n + \frac{p_2}{2},\ B^n + \frac{q_2}{2}\right)$$

$$p_4^{n+1} = h\, f\left(t^n + h,\ A^n + p_3,\ B^n + q_3\right)$$

$$q_1^{n+1} = h\, f\left(t^n,\ A^n,\ B^n\right)$$

$$q_2^{n+1} = h\, f\left(t^n + \frac{h}{2},\ A^n + \frac{p_1}{2},\ B^n + \frac{q_1}{2}\right)$$

$$q_3^{n+1} = h\, f\left(t^n + \frac{h}{2},\ A^n + \frac{p_2}{2},\ B^n + \frac{q_2}{2}\right)$$

$$q_4^{n+1} = h\, f\left(t^n + h,\ A^n + p_3,\ B^n + q_3\right)$$

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t	A	p_1	p_2	p_3	p_4	B	q_1	q_2	q_3	q_4	Σ
0	1,00E-3					0,00E+0					1,00E-3
0,1	9,44E-4	-6,00E-5	-5,60E-5	-5,63E-5	-5,26E-5	2,81E-5	3,00E-5	2,80E-5	2,81E-5	2,63E-5	1,00E-3
0,2	8,94E-4	-5,26E-5	-4,93E-5	-4,95E-5	-4,64E-5	5,28E-5	2,63E-5	2,46E-5	2,47E-5	2,32E-5	1,00E-3
0,3	8,51E-4	-4,64E-5	-4,36E-5	-4,38E-5	-4,12E-5	7,47E-5	2,32E-5	2,18E-5	2,19E-5	2,06E-5	1,00E-3
...	...	...	...	...	...	...	...	...	...	...	...
9,8	3,91E-4	-5,89E-8	-5,71E-8	-5,71E-8	-5,53E-0	3,04E-4	2,94E-8	2,85E-8	2,86E-8	2,77E-8	1,00E-3
9,9	3,91E-4	-5,53E-8	-5,36E-8	-5,37E-8	-5,20E-0	3,04E-4	2,77E-8	2,68E-8	2,68E-8	2,60E-8	1,00E-3
10	3,91E-4	-5,20E-8	-5,04E-8	-5,05E-8	-4,89E-0	3,04E-4	2,60E-8	2,52E-8	2,52E-8	2,44E-8	1,00E-3

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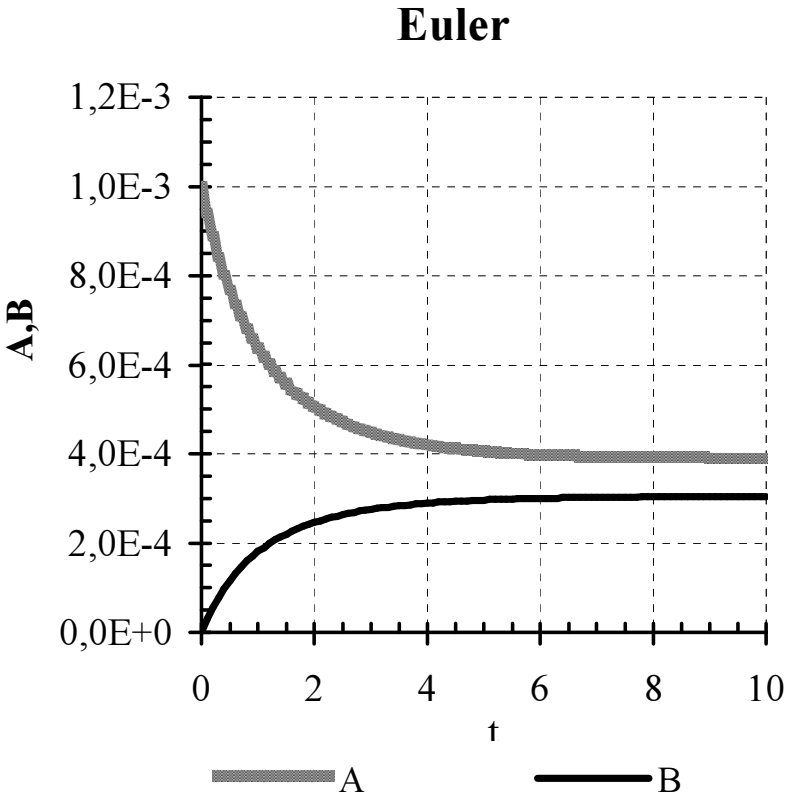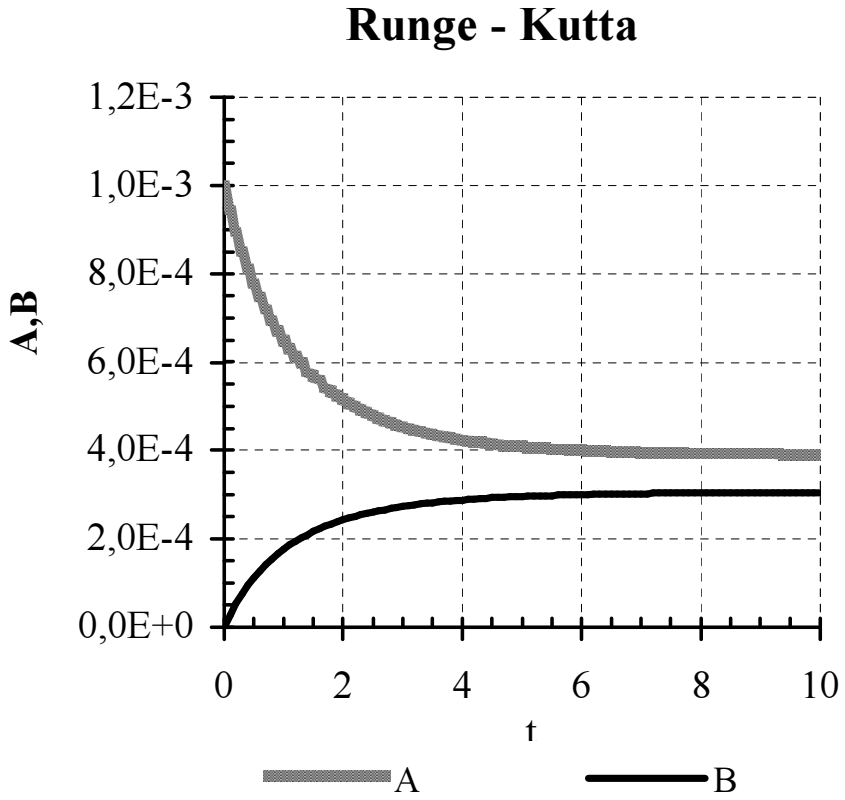
Dynamic models