

Memo

To

to whom it may concern

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Our reference

001

Number of pages

4

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Subject

SMART numerics: Atmospheric chemistry

1 Atmospheric chemistry

Example taken from **HundsdoerferAndVerwer2003**.

We illustrate the mass action law by the following three reactions between oxygen O_2 , atomic oxygen O , nitrogen oxide NO , and nitrogen dioxide NO_2 :



The corresponding ODE system reads

$$\frac{\partial u_1}{\partial t} = k_1 u_3 - k_2 u_1 \quad (4)$$

$$\frac{\partial u_2}{\partial t} = k_1 u_3 - k_3 u_2 u_4 + \sigma_2 \quad (5)$$

$$\frac{\partial u_3}{\partial t} = k_3 u_2 u_4 - k_1 u_3 \quad (6)$$

$$\frac{\partial u_4}{\partial t} = k_2 u_1 - k_3 u_2 u_4 \quad (7)$$

with $\mathbf{u}(0) = (0.0, 2.0 \times 10^{-1}, 2.0 \times 10^{-3}, 2.0 \times 10^{-1})^T$ and $\sigma_2 = 10^{-7}$, and the coefficients k are defined as (the given conditions for are different from the conditions as defined in **HundsdoerferAndVerwer2003**):

$$k_1 = \begin{cases} 10^{-5} \exp(7 g(t)) \\ 10^{-40}, \end{cases} \quad \text{during night} \quad (8)$$

$$k_2 = 2.0 \times 10^{-2} \quad (9)$$

$$k_3 = 1.0 \times 10^{-3} \quad (10)$$

with

$$g(t) = \left(\sin \left(\frac{\pi}{16} (t_h - 4) \right) \right)^{0.2}, \quad t_h = \frac{t}{3600}; \quad (11)$$

where t_h is the time in hours.

Some results are:

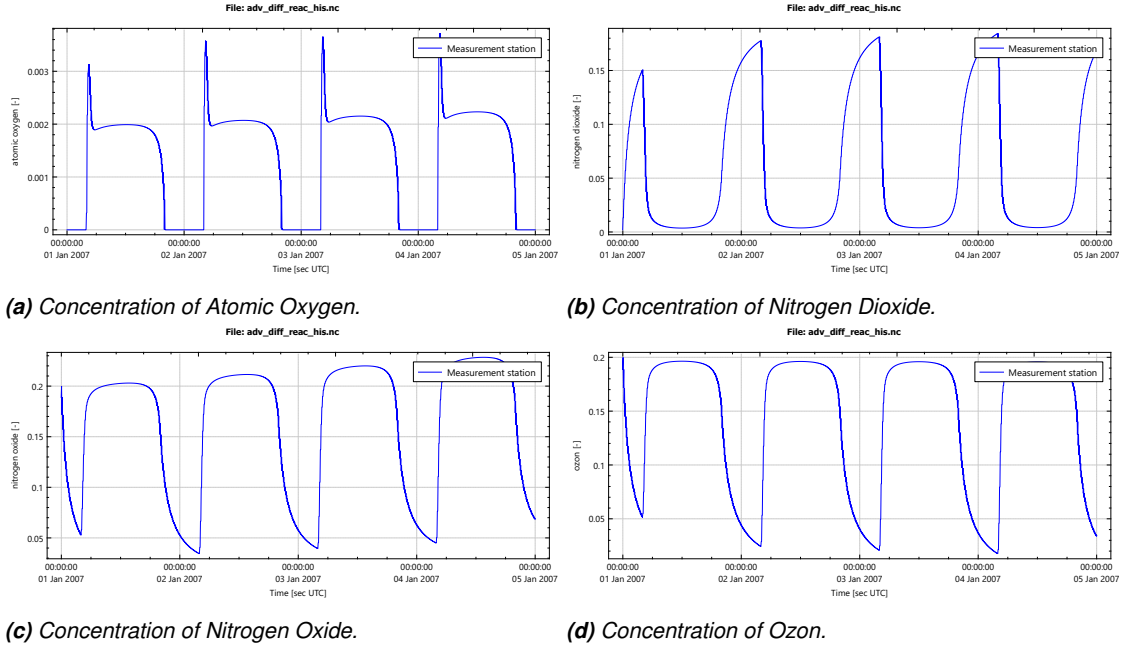


Figure 1: Result plots of the different constituents, compute with a Runge-Kutta 4 time integration with a timestep of 0.5[second].

2 Numerics

Discretized

$$\frac{1}{\Delta t} \Delta u_1^{n+1,p+1} = -\frac{1}{\Delta t} (u_1^{n+1,p} - u_1^n) + k_1(u_3^{n+\theta,p+1}) - k_2(u_1^{n+\theta,p+1}) \quad (12)$$

$$\frac{1}{\Delta t} \Delta u_2^{n+1,p+1} = -\frac{1}{\Delta t} (u_2^{n+1,p} - u_2^n) + k_1(u_3^{n+\theta,p+1}) - k_3(u_2^{n+\theta,p+1})(u_4^{n+\theta,p+1}) + \sigma_2 \quad (13)$$

$$\frac{1}{\Delta t} \Delta u_3^{n+1,p+1} = -\frac{1}{\Delta t} (u_3^{n+1,p} - u_3^n) + k_3(u_2^{n+\theta,p+1})(u_4^{n+\theta,p+1}) - k_1(u_3^{n+\theta,p+1}) \quad (14)$$

$$\frac{1}{\Delta t} \Delta u_4^{n+1,p+1} = -\frac{1}{\Delta t} (u_4^{n+1,p} - u_4^n) + k_2(u_1^{n+\theta,p+1}) - k_3(u_2^{n+\theta,p+1})(u_4^{n+\theta,p+1}) \quad (15)$$

Linearization of $\mathbf{u}^{n+\theta,p+1}$:

$$\frac{1}{\Delta t} \Delta u_1^{n+1,p+1} = -\frac{1}{\Delta t} (u_1^{n+1,p} - u_1^n) + \quad (16)$$

$$+ k_1(u_3^{n+\theta,p} + \theta \Delta u_3^{n+1,p+1}) - k_2(u_1^{n+\theta,p} + \theta \Delta u_1^{n+1,p+1}) \quad (17)$$

$$\frac{1}{\Delta t} \Delta u_2^{n+1,p+1} = -\frac{1}{\Delta t} (u_2^{n+1,p} - u_2^n) + \quad (18)$$

$$+ k_1(u_3^{n+\theta,p} + \theta \Delta u_3^{n+1,p+1}) - k_3(u_2^{n+\theta,p} + \theta \Delta u_2^{n+1,p+1})(u_4^{n+\theta,p} + \theta \Delta u_4^{n+1,p+1}) + \sigma_2 \quad (19)$$

$$\frac{1}{\Delta t} \Delta u_3^{n+1,p+1} = -\frac{1}{\Delta t} (u_3^{n+1,p} - u_3^n) + \quad (20)$$

$$+ k_3(u_2^{n+\theta,p} + \theta \Delta u_2^{n+1,p+1})(u_4^{n+\theta,p} + \theta \Delta u_4^{n+1,p+1}) - k_1(u_3^{n+\theta,p} + \theta \Delta u_3^{n+1,p+1}) \quad (21)$$

$$\frac{1}{\Delta t} \Delta u_4^{n+1,p+1} = -\frac{1}{\Delta t} (u_4^{n+1,p} - u_4^n) + \quad (22)$$

$$+ k_2(u_1^{n+\theta,p} + \theta \Delta u_1^{n+1,p+1}) - k_3(u_2^{n+\theta,p} + \theta \Delta u_2^{n+1,p+1})(u_4^{n+\theta,p} + \theta \Delta u_4^{n+1,p+1}) \quad (23)$$

Rearrange to $\mathbf{Ax} = \mathbf{b}$

$$\frac{1}{\Delta t} \Delta u_1^{n+1,p+1} - k_1 \theta \Delta u_3^{n+1,p+1} + k_2 \theta \Delta u_1^{n+1,p+1} = \quad (24)$$

$$= -\frac{1}{\Delta t} (u_1^{n+1,p} - u_1^n) + k_1 u_3^{n+\theta,p} - k_2 u_1^{n+\theta,p} \quad (25)$$

$$\frac{1}{\Delta t} \Delta u_2^{n+1,p+1} - k_1 \theta \Delta u_3^{n+1,p+1} + k_3 \theta u_4^{n+1,p} \Delta u_2^{n+1,p+1} + k_3 \theta u_2^{n+1,p} \Delta u_4^{n+1,p+1} = \quad (26)$$

$$= -\frac{1}{\Delta t} (u_2^{n+1,p} - u_2^n) + k_1 u_3^{n+\theta,p} - k_3 u_2^{n+\theta,p} u_4^{n+\theta,p} + \sigma_2 \quad (27)$$

$$\frac{1}{\Delta t} \Delta u_3^{n+1,p+1} - k_3 u_2^{n+\theta,p} \theta \Delta u_4^{n+1,p+1} - k_3 u_4^{n+\theta,p} \theta \Delta u_2^{n+1,p+1} + k_1 \theta \Delta u_3^{n+1,p+1} = \quad (28)$$

$$= -\frac{1}{\Delta t} (u_3^{n+1,p} - u_3^n) + k_3 u_2^{n+\theta,p} u_4^{n+\theta,p} - k_1 u_3^{n+\theta,p} \quad (29)$$

$$\frac{1}{\Delta t} \Delta u_4^{n+1,p+1} - k_2 \theta \Delta u_1^{n+1,p+1} + k_3 u_2^{n+\theta,p} \theta \Delta u_4^{n+1,p+1} + k_3 u_4^{n+\theta,p} \theta \Delta u_2^{n+1,p+1} = \quad (30)$$

$$= -\frac{1}{\Delta t} (u_4^{n+1,p} - u_4^n) + k_2 u_1^{n+\theta,p} - k_3 u_2^{n+\theta,p} u_4^{n+\theta,p} \quad (31)$$

3 Numerical experiment

Table 1: Light blue theme of table

	Time step [sec]	Euler Explicit	Runge-Kutta 4	Fully Implicit Δ -formulation
1	0.5	-	✓	-
2	60	✓	✓	✓
3	120	Unstable	✓	✓
4	180	-	Unstable	✓
5	240	-	-	✓
6	300	-	-	✓
7	900	-	-	✓
8	1800	-	-	✓
9	3600	-	-	✓