**To** : ???
**From** : Jan Mooiman
**Subject** : Brusselator
**Date** : 2025-01-13 08:56:23

# 1 Brusselator

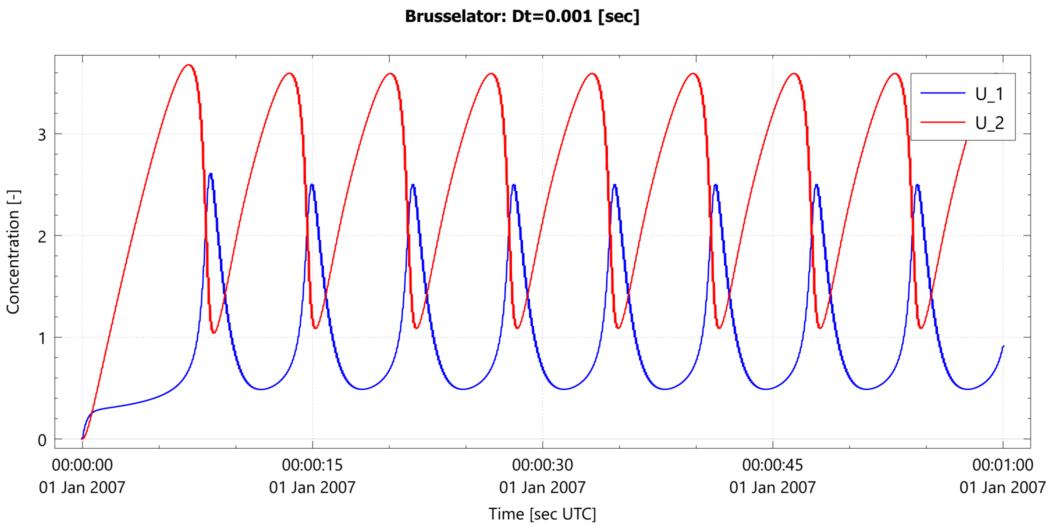
The Brusselator is taken as example to see the behaviour or the fully implicit $\Delta$-formulation for reaction terms only. This particularly of interest for the water quality computations with lots of processes. Example taken from Ault and Holmgreen (2003).

The ODE system reads:

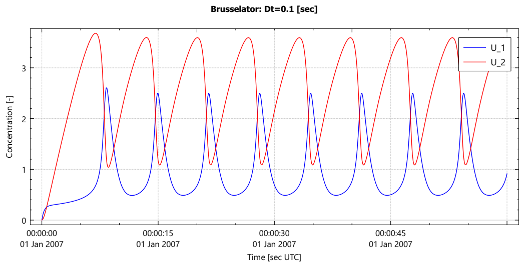
$$\frac{\partial u_1}{\partial t} = 1 - (k_2 + 1)u_1 + k_1 u_1^2 u_2, \quad (1)$$

$$\frac{\partial u_2}{\partial t} = k_2 u_1 - k_1 u_1^2 u_2 \quad (2)$$

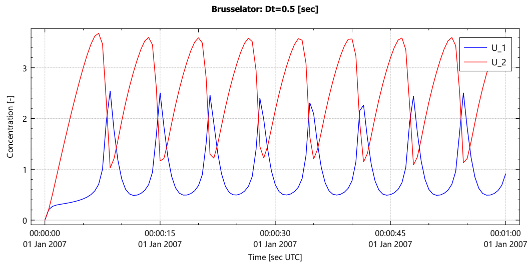
with $k_1 = 1$ and $k_2 = 2.5$ and initial values $u_1(0) = 0$ and $u_2(0) = 0$. Some results are:



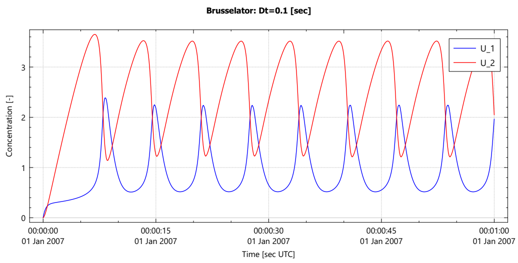

***(a)** Runge-Kutta 4:* $\Delta t = 0.001$, $k_1 = 1$, $k_2 = 2.5$



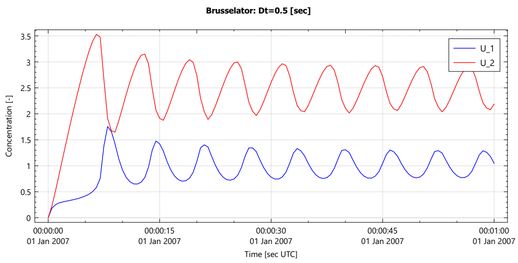

***(b)*** *Runge-Kutta 4:* $\Delta t = 0.1$, $k_1 = 1$, $k_2 = 2.5$




***(c)*** *Runge-Kutta 4:* $\Delta t = 0.5$, $k_1 = 1$, $k_2 = 2.5$



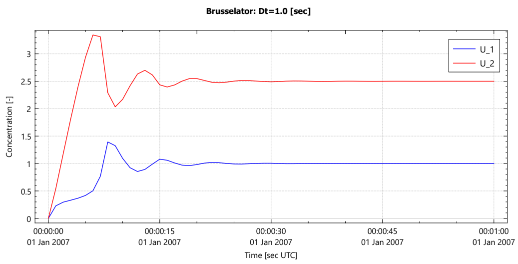

***(d)*** *Fully Implicit:* $\Delta t = 0.1$, $k_1 = 1$, $k_2 = 2.5$



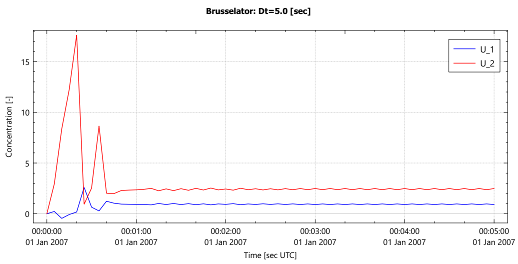

***(e)*** *Fully Implicit:* $\Delta t = 0.5$, $k_1 = 1$, $k_2 = 2.5$

***Figure 1:*** *Result plots for constant value of* $k_1 = 1$ *and* $k_2 = 2.5$*, computed with a Runge-Kutta 4 and fully implicit (*$\Delta$*-formulation) time integration method for different time steps* $\Delta t = 0.1, 0.5$.

Extra attention needed for the Fully Implicit time integration with larger time step:




***(a)*** *Fully Implicit:* $\Delta t = 1.0$, $k_1 = 1$, $k_2 = 2.5$




***(b)*** *Fully Implicit:* $\Delta t = 5.0$, $k_1 = 1$, $k_2 = 2.5$

***Figure 2:*** *Result plots for constant value of* $k_1 = 1$ *and* $k_2 = 2.5$*, computed with a fully implicit (*$\Delta$*-formulation) time integration method for different time steps* $\Delta t = 1.0, 5.0$.

Figure 2a converge to the equilibrium state $(u_1, u_2) = (1.0, 2.5)$ and Figure 2b looks to converge to the equilibrium state $(u_1, u_2) = (1.0, 2.5)$ but is still wiggling after 5 min of simulation time (even after one day — not presented).

## 2 Numerical experiment

***Table 1:*** *Stability of different time integrators for the Brusselator.*

| | **Time step [s]** | **Runge-Kutta 4** | **Fully Implicit $\Delta$-formulation** |
|---|---|---|---|
| **1** | 0.1 | ✓ | ✓ |
| **2** | 0.2 | ✓ | ✓ |
| **3** | 0.5 | ✓ | ✓ |
| **4** | 1.0 | Unstable | ✓ |
| **5** | 2.0 | | ✓ |
| **6** | 5.0 | | ✓ |

## References

Ault, Shaun and Erik Holmgreen (2003). *Dynamics of the Brusselator*. URL: https://mate.unipv.it/~boffi/teaching/download/Brusselator.pdf.