Transport processes

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Outline

The Sandoz/Rhine accident 1986

Fig.: Plainly Difficult: "A Brief History of: The Sandoz Chemical Disaster (Short Documentary)" https://www.youtube.com/watch?v=6RjTvN2QhSY (7:08 min)

The Sandoz/Rhine accident 1986

- one of the severest environmental disasters caused by humans in Europe
- chemically polluted water from discharged into the Rhine river
- Rhine polluted over a length of 400 km
- initiation of new developments in water protection
- amongst others development of the Rhine-Alarm model (Mazijk et al., 1991)

(IKSR, 2016)

Fig.: source: Badische Zeitung/dapd (IKSR, 2016)

The Sandoz/Rhine accident 1986

Aim of the model is to predict

- time of arrival of the polluted water
- maximum concentration of pollutants
- end of contamination

on any point along the river length (Mazijk et al., 1991).
allows to warn e. g.:

- waterworks
- fishers

https://www.chr-khr.org/de/veroffentlichung/rheinalarmmodell-version-20-kalibrierung-und-verifikation

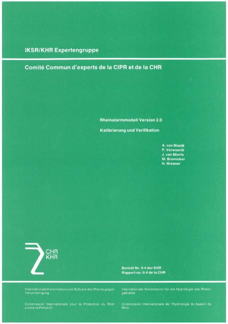


Fig.: Validation report of the Rhine-Alarm model (Mazijk et al., 1991)

Advection equation

Example: Advection-equation:

$$\frac{\partial \phi}{\partial t} + u \cdot \frac{\partial \phi}{\partial x} = 0 \tag{1}$$

Initial condition:

$$\phi(x,0) = \begin{cases} 1 & \text{für } 0 < x \leq 1 \\ 0 & \text{else} \end{cases} \tag{2}$$

to solve on $x = [0, 20]$ with boundary conditions:

$$\phi(0,t) = f(20,t) = 0 \tag{3}$$

Advection equation

Forward in time and backward in space (upwind):

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u \cdot \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x} = 0 \Rightarrow \phi_i^{n+1} = \phi_i^n - \Delta t \cdot u \cdot \frac{\phi_i^n - \phi_{i-1}^n}{\Delta x} \quad (4)$$

Forward time, central space (FTCS):

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + u \cdot \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2 \cdot \Delta x} = 0 \Rightarrow \phi_i^{n+1} = \phi_i^n - \Delta t \cdot u \cdot \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2 \cdot \Delta x} \quad (5)$$

Advection equation

	A	B
1	u	1
2	Delta t	0.5
3	Delta x	1
4	CFL R	0.5

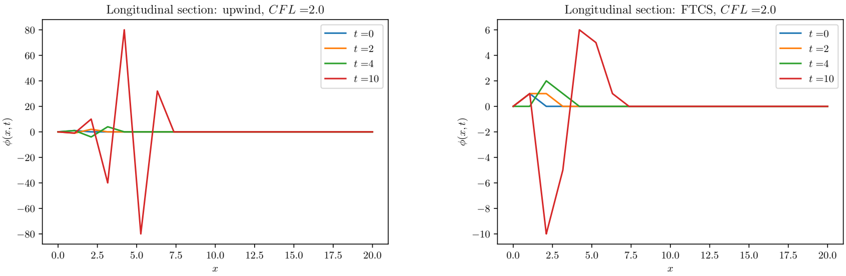
(a) input

	A	B	C	D	E	F	G
1	n/i		0	1	2	3	4
2		t/x	0	1.000	2.000	3.000	4.000
3	0	0.0	0	1.000	0.000	0.000	0.000
4	1	0.5	0	0.500	0.500	0.000	0.000
5	2	1.0	0	0.250	0.500	0.250	0.000
6	3	1.5	0	0.125	0.375	0.375	0.125
7	4	2.0	0	0.063	0.250	0.375	0.250
8	5	2.5	0	0.031	0.156	0.313	0.313
9	6	3.0	0	0.016	0.094	0.234	0.313
10	7	3.5	0	0.008	0.055	0.164	0.273
11	8	4.0	0	0.004	0.031	0.109	0.219
12	9	4.5	0	0.002	0.018	0.070	0.164
13	10	5.0	0	0.001	0.010	0.044	0.117
14	11	5.5	0	0.000	0.005	0.027	0.081
15	12	6.0	0	0.000	0.003	0.016	0.054
16	13	6.5	0	0.000	0.002	0.010	0.035
17	14	7.0	0	0.000	0.001	0.006	0.022
18	15	7.5	0	0.000	0.000	0.003	0.014

(b) upwind scheme

Fig.: Solution of the advection equation (1) with $\Delta t = 0{,}5$ in Excel

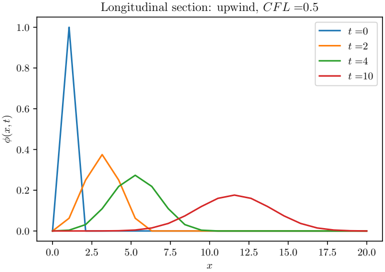
Advection equation



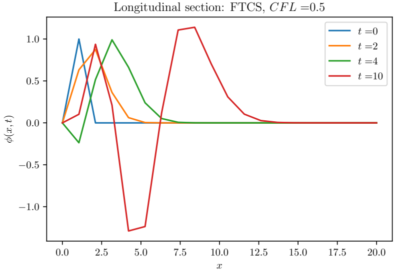
(a) upwind scheme (b) FTCS scheme

Fig.: Lösung der Advektionsgleichung (1) mit $\Delta t = 2{,}0$

Advection equation



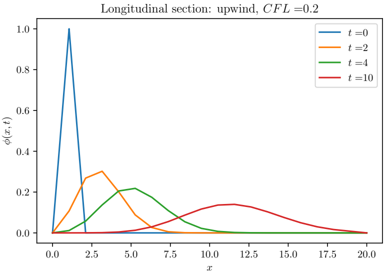
(a) upwind scheme



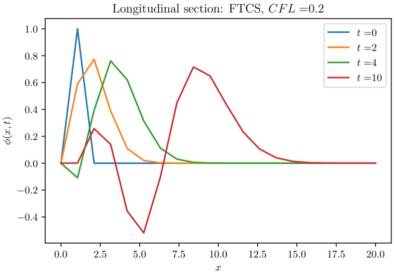
(b) FTCS scheme

Fig.: Lösung der Advektionsgleichung (1) mit $\Delta t = 0{,}5$

Advection equation



(a) upwind scheme



(b) FTCS scheme

Fig.: Lösung der Advektionsgleichung (1) mit $\Delta t = 0{,}2$

Numerical stability and the Courant-Friedrichs-Levy Criterion

Explicit numerical schemes require that the Courant number falls below a certain value < 1:

$$CFL = R = \frac{\Delta t}{\Delta x} \cdot \sup_i |f'(u_i)| \tag{6}$$

Simplification of equation (6) for one-dimensional advection equation with constant u:

$$CFL = R = \frac{\Delta t}{\Delta x} \cdot u \tag{7}$$

Numerical stability and the Courant-Friedrichs-Levy Criterion

Example:

- $u = 2\,\mathrm{m\,s^{-1}}$
- $\Delta x = 3\,\mathrm{m}$
- $\Delta t = 2\,\mathrm{s}$

Equation (7):

$$CFL = \frac{\Delta t}{\Delta x} \cdot u = 1{,}3$$

required timestep for $CFL < 1$:

$$\rightarrow \Delta t < CFL \cdot \frac{\Delta x}{u} \Rightarrow \Delta t < 1{,}5\,\mathrm{s}$$

Other transport processes

Examples:

- advection only: transport of a solid
- diffusion only: heat transport in a solid
- advection and diffusion: dissolved substance in a fluid

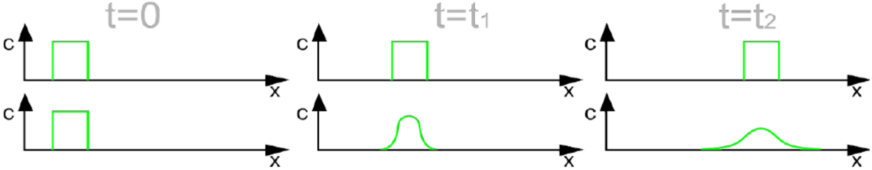


Fig.: Scheme of mass transport without diffusion (top) and with diffusion (bottom) (Maurer, 2010)

Other transport processes

- Advection equation:

$$\frac{\partial c}{\partial t} + \boldsymbol{u} \cdot \nabla c = 0 \tag{8}$$

$$\frac{\partial c}{\partial t} + u \cdot \frac{\partial c}{\partial x} = 0 \tag{9}$$

- Advection-Diffusion equation:

$$\frac{\partial c}{\partial t} + u \cdot \frac{\partial c}{\partial x} + D_0 \frac{\partial^2 c}{\partial x^2} = 0 \tag{10}$$

for comparison: diffusion only

$$\frac{\partial \phi}{\partial t} + \Gamma \frac{\partial^2 \phi}{\partial x^2} = 0 \tag{11}$$

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Mazijk, A. van, P. Verwoerdt, J. van Mierlo, M. Bremicker and H. Wiesner (1991). *Rheinalarmmodell Version 2.0 Kalibrierung und Verifikation*. Internationale Kommission zum Schutze des Rheins gegen Verunreinigung. URL: https://www.chr-khr.org/de/veroffentlichung/rheinalarmmodell-version-20-kalibrierung-und-verifikation.