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University of Natural Resources and Life Sciences, Vienna Department of Water, Atmosphere and Environment

# Levelling of connected tanks and mass transport

Daniel Wildt

SWARM Summer School 15 – 26 November 2021

15th November 2021

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### Outline I





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Finite Differences Method (FDM)

#### Leveling of two tanks

Analytical solution Numerical solution Summary

#### Mass transport

The Sandoz/Rhine accident 1986 Governing equations Boundary and initial conditions Analytical solution



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# FDM: Definition of the slope from the SW2 M





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## FDM: Approxima-tion of the derivative SW2 rM in Excel





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	A	В	С	D	E	F	G	н	1	J	К	L	м	N	0
1	х	1													
2	f(x)	6													
	1.1.1									Difference	Difference	Differnce	error	error	error
3						forward	backward	central		forward	backward	central	forward	backward	central
	<u>Δx</u>	x+∆x	x-∆x .	f(x+∆x) .	f(x-∆x)	differencing	differencing	differencing	f'(x) .	differencing	differencing	differencing	differencing	differencing	differencing .
4	2.000	3.000	-1.000	100.000	0.000	. 47,000	3.000	25.000	. 13.000	. 34.000	-10.000	12,000	. 34.000	10.000	12.000
5	1.000	2.000	0.000	33.000	1.000	27.000	5.000	16.000	13.000	14.000	-8.000	3.000	14.000	8.000	3.000
6	0.900	1.900	0.100	28.797	1.023	25.330	5.530	15.430	13.000	12.330	-7.470	2.430	12.330	7.470	2.430
7	0.800	1.800	0.200	24.976	1.104	23.720	6.120	14.920	13.000	10.720	-6.880	1.920	10.720	6.880	1.920
8	0.700	1.700	0.300	21.519	1.261	22.170	6.770	14.470	13.000	9.170	-6.230	1.470	9.170	6.230	1.470
9	0.600	1.600	0.400	18.408	1.512	20.680	7.480	14.080	13.000	7.680	-5.520	1.080	7.680	5.520	1.080
10	0.500	1.500	0.500	15.625	1.875	19.250	8.250	13.750	13.000	6.250	-4.750	0:750	6.250	4.750	0.750
11	0.400	1.400	0.600	13.152	2.368	17.880	9.080	13.480	· 13.000	4.880	-3.920	0:480	4.880	3.920	· 0.480
12	0.300	1.300	0.700	10.971	3.009	16.570	9.970	13.270	13.000	· · 3.570	-3.030	0.270	3.570	3.030	0.270
13	0.200	1.200	0.800	. 9.064	3.816	15.320	10.920	. 13.120	. 13.000	2.320	-2.080	0.120	2.320	. 2.080	0.120
14	0.100	1.100	. 0.900	. 7.413	.4.807	14.130		. 13.030	. 13.000	1.130	-1.070	. 0.030	1.130	. 1.070	0.030
15	0.050	1.050	0.950	6.678	5.377	13.558	12.458	13.008	13.000	0.558	-0.543	800.0	0.558	0.543	0.008
16	0.020	1.020	0.980	6.264	5.744	13.221	12.781	13.001	13.000	0.221	-0.219	0.001	0.221	0.219	0.001
17	0.010	1.010	0.990	6.131	5.871	13.110	12.890	13.000	13.000	0.110	-0.110	0.000	0.110	0.110	0.000
18	0.001	1.001	0.999	6.013	5.987	13.011	12.989	13.000	13.000	0.011	-0.011	0.000	0.011	0.011	0.000

Fig.: Exercise: Approximation of the derivative in Excel

#### Finite Differences (FDM): 💦 SW? M 💵 Method Order of Accuracy

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Forward and backward differencing:

- $\triangleright$  linear relation between  $\Delta x$  and error
- ▶ 1<sup>st</sup> order accuracy

central differencing:

 $\triangleright$  quadratic relation between  $\Delta x$ and error

2<sup>nd</sup> order accuracy



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## Leveling of two tanks: Problem SW2 M (

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• coefficient of resistance:  $\xi = 2,0$ 

inertia neglected





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energy conservation:

$$z = \frac{v^2}{2g} \cdot \xi = \frac{Q^2}{A^2 \cdot 2g} \cdot \xi$$
$$\Rightarrow Q = A \cdot \sqrt{\frac{2g \cdot z}{\xi}} \quad (9)$$

Behälterausgleich Behälter B Behälter A ΔH  $\emptyset 1 \text{ m}^2$  $\nabla$ 5 m 10.000 m<sup>2</sup> 2 m

 $5.000 \text{ m}^2$ 

$$\Delta V = \int Q \, \mathrm{d}t = \int A \cdot \sqrt{\frac{2g \cdot z}{\xi}} \, \mathrm{d}t \quad .$$
(10)

Fig.: Leveling of two tanks connected through a pipe

# Leveling of two tanks: Analytical SW2 M (19)

Change of Water Surface elevation in

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# Leveling of two tanks: Analytical SW2 MORE



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 $\mathrm{d}z$  from equation 13 using equation 11 and 12:

$$dz = -(dx + dy) = -Q \cdot \left(\frac{1}{A_{A}} + \frac{1}{A_{B}}\right) dt = -\underbrace{A\sqrt{\frac{2g}{\xi}} \cdot \frac{A_{B} + A_{A}}{A_{A}A_{B}}}_{K} \sqrt{z} dt \quad (14)$$
$$dt = -\frac{1}{K}\frac{dz}{\sqrt{z}} \qquad (15)$$

integration of equation 15:

$$t(z) = -\frac{1}{K} \int_{\Delta H}^{z} \frac{1}{\sqrt{z}} \, \mathrm{d}z = -\frac{1}{K} \cdot 2\sqrt{z} \, \left|_{\Delta H}^{z} = 2 \cdot \frac{1}{K} \cdot \left(\sqrt{\Delta H} - \sqrt{z}\right)$$
(16)

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Time until water surface elevations in tanks A and B are fully leveled out (z = 0):

$$t(0) = 2 \cdot \frac{1}{K} \cdot \left(\sqrt{\Delta H} - \sqrt{z}\right)$$
$$= 2 \cdot \frac{1}{A\sqrt{\frac{2g}{\xi}} \cdot \frac{A_{\rm B} + A_{\rm A}}{A_{\rm A}A_{\rm B}}} \cdot \left(\sqrt{\Delta H} - 0\right)$$
$$= 3.687 \,\mathrm{s}$$



#### Leveling of two tanks: solution ۵۵

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conservation of mass:

 $\Delta V = Q \cdot \Delta t = A_{\rm A} \cdot \Delta h_{\rm A} = A_{\rm B} \cdot \Delta h_{\rm B}$ 

# Leveling of two tanks: Numerical SW2 M (1)

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Equations 20 and 21 using Behälterausgleich Behälter A Behälter B equations 18 and 19: ΔH  $h_{\mathrm{A}}^{n+1} = h_{\mathrm{A}}^n - \frac{\Delta V}{A_{\mathrm{A}}} = h_{\mathrm{A}}^n - \frac{Q \cdot \Delta t}{A_{\mathrm{A}}}$ øl m 5 m 10.000 m 2 m (22) $h_{\mathrm{B}}^{n+1} = h_{\mathrm{B}}^{n} + \frac{\Delta V}{A_{\mathrm{B}}} = h_{\mathrm{B}}^{n} + \frac{Q \cdot \Delta t}{A_{\mathrm{B}}}$  $5.000 \text{ m}^2$ Fig.: Leveling of two tanks connected (23) through a pipe

# Leveling of two tanks: Numerical SW2 MORE

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Q from energy conservation (equation 9)

$$Q = A \cdot \sqrt{\frac{2g \cdot z}{\xi}}$$

different methods to approximate z:

- backward differencing
- central differencing



## Leveling of two tanks: Numerical SW2 CM

backward differencing (Euler method):



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- $z=h_{
  m A}^n-h_{
  m B}^n$
- Zentrale Differenzen (Predictor-Correktor or Runge-Kutta method):

 $\Delta z^{n+\frac{1}{2}} = h_{\rm A}^{n+\frac{1}{2}} - h_{\rm B}^{n+\frac{1}{2}}$ (25)

mit : 
$$h_{\rm A}^{n+\frac{1}{2}} = \frac{h_{\rm A}^n + h_{\rm A}^{n+1\star}}{2}$$
  $h_{\rm B}^{n+\frac{1}{2}} = \frac{h_{\rm B}^n + h_{\rm B}^{n+1\star}}{2}$  (26)

with  $h_{\rm A}^{n+1\star}$  and  $h_{\rm B}^{n+1\star}$  estimated using backward differencing.

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## Leveling of two tanks: Numerical SW2 CM (19) solution



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### Numerical solution in Excel applying the Euler method:

	Α	B	С
1	g	m/s <sup>2</sup>	9.81
2	А	m <sup>2</sup>	1
3	AA	m²	10000
4	AB	m²	5000
5	zeta	1	2
6	Delta t	s	100

Fig.: Leveling of two tanks input

	A N	D				- F	0			J J
1	n	t	hA	hB	z	Q	Delta V	hA_(n+1)	hB_(n+1)	t analytisch
2		s	m	m	m	m³/s	m <sup>3</sup>	m	m	s
3	0	0	5.000	2.000	3.000	5.425	542.494	4.946	2.108	(
4	1	100	4.946	2.108	2.837	5.276	527.574	4.893	2.214	101
5	2	200	4.893	2.214	2.679	5.126	512.648	4.842	2.317	203
6	3	300	4.842	2.317	2.525	4.977	497.715	4.792	2.416	304
7	4	400	4.792	2.416	2.376	4.828	482.776	4.744	2.513	406
8	5	500	4.744	2.513	2.231	4.678	467.830	4.697	2.606	507
9	6	600	4.697	2.606	2.091	4.529	452.876	4.652	2.697	609
10	7	700	4.652	2.697	1.955	4.379	437.914	4.608	2.784	71:
11	8	800	4.608	2.784	1.823	4.229	422.943	4.566	2.869	812
12	9	900	4.566	2.869	1.697	4.080	407.963	4.525	2.951	914
13	10	1000	4.525	2.951	1.574	3.930	392.972	4.485	3.029	1016
14	11	1100	4.485	3.029	1.456	3.780	377.971	4.448	3.105	1118
15	12	1200	4.448	3.105	1.343	3.630	362.958	4.411	3.177	1220
16	13	1300	4.411	3.177	1.234	3.479	347.932	4.377	3.247	1322
17	14	1400	4.377	3.247	1.130	3.329	332.892	4.343	3.313	1424
18	15	1500	4.343	3.313	1.030	3.178	317.836	4.311	3.377	152
19	16	1600	4.311	3.377	0.934	3.028	302.764	4.281	3.438	1629
20	17	1700	4.281	3.438	0.844	2.877	287.673	4.252	3.495	1732
21	18	1800	4.252	3.495	0.757	2.726	272.561	4.225	3.550	1834

Fig.: Numerical solution in Excel applying the Euler method

## Leveling of two tanks: Numerical SW2 rm (1990) solution



Numerical solution in Excel applying the Predictor-Corrector frethod:

	A	В	C	D	E	F	G	Н	1	J	К	L	M	N	0	Р	Q
1	n t		hA	hB	z	Q	Delta V	hA_(n+1)*	hB_(n+1)*	t analytisch	hA_(n+0.5)	hB_(n+0.5)	z PrädKorr.	Q	Delta V	hA_(n+1)	hB_(n+1)
2		5	m	m	m	m³/s	m <sup>3</sup>	m	m	s	m	m	m	m³/s	m <sup>3</sup>	m	m
3	0	0	5.000	2.000	3.000	5.425	542.494	4.946	2.108	0	4.973	2.054	2.919	5.351	535.086	4.946	2.107
-4	1	100	4.946	2.107	2.839	5.278	527.781	4.894	2.213	100	4.920	2.160	2.760	5.204	520.371	4.894	2.211
5	2	200	4.894	2.211	2.683	5.131	513.067	4.843	2.314	200	4.869	2.262	2.606	5.057	505.656	4.844	2.312
6	3	300	4.844	2.312	2.532	4.984	498.354	4.794	2.412	300	4.819	2.362	2.457	4.909	490.941	4.795	2.410
7	4	400	4.795	2.410	2.384	4.836	483.640	4.746	2.507	400	4.771	2.459	2.312	4.762	476.226	4.747	2.506
8	5	500	4.747	2.506	2.242	4.689	468.927	4.700	2.599	500	4.724	2.553	2.171	4.615	461.511	4.701	2.598
9	6	600	4.701	2.598	2.103	4.542	454.214	4.656	2.689	600	4.678	2.643	2.035	4.468	446.796	4.656	2.687
10	7	700	4.656	2.687	1.969	4.395	439.501	4.612	2.775	700	4.634	2.731	1.903	4.321	432.081	4.613	2.774
11	8	800	4.613	2.774	1.839	4.248	424.788	4.571	2.859	800	4.592	2.816	1.776	4.174	417.366	4.571	2.857
12	9	900	4.571	2.857	1.714	4.101	410.076	4.530	2.939	900	4.551	2.898	1.653	4.027	402.651	4.531	2.938
13	10	1000	4.531	2.938	1.593	3.954	395.363	4.492	3.017	1000	4.511	2.977	1.534	3.879	387.936	4.492	3.015
14	11	1100	4.492	3.015	1.477	3.807	380.651	4.454	3.091	1100	4.473	3.053	1.420	3.732	373.221	4.455	3.090
15	12	1200	4.455	3.090	1.365	3.659	365.939	4.418	3.163	1200	4.437	3.127	1.310	3.585	358.506	4.419	3.162
16	13	1300	4.419	3.162	1.257	3.512	351.227	4.384	3.232	1300	4.402	3.197	1.205	3.438	343.791	4.385	3.230
17	14	1400	4.385	3.230	1.154	3.365	336.515	4.351	3.298	1400	4.368	3.264	1.104	3.291	329.076	4.352	3.296
18	15	1500	4.352	3.296	1.056	3.218	321.804	4.320	3.361	1500	4.336	3.328	1.007	3.144	314.360	4.320	3.359
19	16	1600	4.320	3.359	0.961	3.071	307.093	4.290	3.421	1600	4.305	3.390	0.915	2.996	299.645	4.290	3.419
20	17	1700	4.290	3.419	0.871	2.924	292.383	4.261	3.478	1700	4.276	3.448	0.828	2.849	284.930	4.262	3.476
21	18	1800	4.262	3.476	0.786	2.777	277.673	4.234	3.532	1800	4.248	3.504	0.744	2.702	270.215	4.235	3.530

Fig.: Numerical solution in Excel applying the Predictor-Corrector method

# Leveling of two tanks: Numerical SW2 M ()

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Leveling of two containers

Fig.: Levelling of two containers: comparison of solutions

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Solution using the prepared Excel-Worksheet by Maurer (2010) Behaelterausgleich\_Maurer.xlsm note: access VBA-code via Developer Tools > VBA tasks:

- Which convergence criteria is used?
- How long does it take for the water surfaces in the tanks to level out?
- How long does it take for the water surfaces in the tanks to level out when the pipe diameter is doubled?
- How can the difference between the Euler and the Predictor-Corrector method be explained?



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Tab.: Comparison between an analytical and a numerical solution

analytical solution	numerical solution			
available in special cases only no discretization necessary	can be derived for any problem suitable discretization necessary for accurate results			
function can be evaluated at indi- vidual points	function needs to be solved for the entire domain			

Mass transport: The Sandoz/Rhine accident 1986





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

Mass transport: The dent 1986





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

- 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)

Mass transport: The Sandoz/Rhine acci- SW2MM (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-verifikatiRhine-Alarm model





report of the

(Mazijk et al., 1991)



# Mass





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Advection equation:

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

Advection-Diffusion equation:

$$\frac{\partial c}{\partial t} + u \cdot \frac{\partial c}{\partial x} + D_0 \frac{\partial^2 c}{\partial x^2} = 0$$
(29)

for comparison: diffusion only

$$\frac{\partial \phi}{\partial t} + \Gamma \frac{\partial^2 \phi}{\partial x^2} = 0 \tag{30}$$

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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)

# Mass transport: **Coverning equations**

Semi-empirical calculation of the coefficient of dispersion  $D_0$ :

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$$D_0 = \alpha \cdot \frac{u^2 \cdot B_5^2}{\bar{h} \cdot u_\star} \qquad \text{mit } u_\star = \frac{u \cdot \sqrt{g}}{C} = \frac{u \cdot g^{\frac{1}{2}}}{k_{\text{St}} \cdot \sqrt[3]{\bar{h}}} \tag{31}$$

Dispersion has the same effect as diffusion, but the coefficient of dispersion can be several orders of magnitudes higher than the coefficient of diffusion.

$\alpha$	 dimensionless constant $[\alpha] = 1$
$B_S$	 effective river width $[B_S] = m$
ħ	 average water depth $[ar{h}]={\sf m}$
u <sub>*</sub>	 shear stress velocity $[u_\star] = { m ms}^{-1}$
g	 gravitational acceleration $[g] = m s^{-2}$
С	 Chézy-Coefficient $[C] = m^{1/2} s^{-1}$
$k_{ m St}$	 Strickler-Coefficient $[k_{\rm St}] = m^{1/3} s^{-1}$



# Mass transport: **SW2rM**

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stagnant water zones: extension for non-uniform velocity distributions along the river width (Chatwin, 1980)



# Mass





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Transport velocity  $c_v$ :

$$c_{v} = \frac{u}{1+\beta}$$
 mit  $\beta = \kappa \cdot \frac{A_{b}}{A_{s}}$ 

C <sub>v</sub>	 mass transport velocity $[c_v] = m  \mathrm{s}^{-1}$
$\beta$	 portion of stagnant water zones $[eta]=1$
$\kappa$	 exchange coefficient $[\kappa]=1$
$A_b$	 storing cross sectional area $[A_b] = m^2$
$A_s$	 effective cross sectional area $[A_s] = m^2$

ad  $\kappa$  (exchange between stagnant and effective water zones): set  $\kappa = 1$  for complete exchange

Mass transport: Boundary and initial SW2 MORE ( conditions

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Boundary and initial conditions:

- total mass added at one particular instance in time and at one particular point along the river
- steady-state and uniform flow<sup>1</sup>
- initially no-substance in the river

<sup>1</sup>extension for non-uniform flow already implemented in the Rhine-Alarm model

# Mass transport: Analytical solution



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Equation 29 using boundary and initial conditions from above can be solved analytically using Taylor-polynomials (Fischer et al., 1979).

$$c(x,t) = \frac{\frac{M}{Q}}{\sqrt{4\pi D_0 \frac{t}{u_s^2}}} \cdot \exp\left(-\frac{\left(t - \frac{x}{u_s}\right)^2}{4D_0 \frac{t}{u_s^2}}\right)$$
(33)

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### Mass transport: Analytical solution



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Taking stagnant water zones into account results in the following equation:

$$c(x,t) = \frac{\frac{M}{Q}}{\sqrt{4\pi D_0 \frac{t}{c_v^2}}} \cdot \exp\left(-\frac{\left(t - \frac{x}{c_v}\right)^2}{4D_0 \frac{t}{c_v^2}}\right) \cdot \left(1 + \frac{G_t}{6} \cdot H_3 \cdot \frac{t - \frac{x}{c_v}}{\sqrt{2D_0 \frac{t}{c_v^2}}}\right) (34)$$

$$H_3[z] = z^3 - 3z \quad \text{Hermitian polynomial } (z = \frac{t - \mu_t}{\sigma_t})$$

$$\mu_t \quad \dots \quad \text{mean } [\mu_t] = s$$

$$\sigma_t \quad \dots \quad \text{variance } [\sigma_t] = s^2$$

$$G_t = \frac{|g_t|}{|\sigma_t^3|} \quad \dots \quad \text{skewness } [G_t] = 1$$

$$g_t \quad \dots \quad 3. \quad \text{moment } [g_t] = s^3$$

### Mass transport: Analytical solution





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Solution using the prepared Excel-Worksheet by Maurer (20 Compared Water, Atmosphere masstransport.xlsm note: access VBA-code via Developer Tools > VBA Input values river:

- length of the river section: L = 80 km
- Mannings' coeffecient:  $\frac{1}{n} = k_{St} = 35 \text{ m}^{1/3} \text{ s}^{-1}$
- discharge  $Q = 1\,800\,\mathrm{m}^3\,\mathrm{s}^{-1}$
- effective cross sectional area:  $A_s = 750 \text{ m}^2$
- effective river width:  $B_s = 75 \text{ m}$
- storing cross sectional area:  $A_D = 120 \text{ m}^2$
- water depth: h = 5 m

## Mass transport: Analytical solution





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Input values substance:

- mass of added substance: m = 2 kg
- coefficient  $\kappa = 1$
- coefficient of dispersion: α = 1
- Skewness:  $G_t = 1$

#### Tasks masstransport.xlsm

- When is the maximum concentration occuring in the middle of the river section?
- How high is the maximum concentration in the middle of the river section
- What would be the respective values when stagnant water zones are neglected?

Daniel Wildt 15/11/2021 Summer School Levelling of connected tanks and mass transport





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University of Natural Resources and Life Sciences, Vienna Department of Water, Atmosphere and Environment

University of Natural Resources and Life Science, Vienna

Department of Water, Atmosphere and Environment

Institut of Hydraulic Engineering and River Research

Daniel Wildt, MSc

Muthgasse 107, A - 1190 Wien Tel.: 01-47654-81935 daniel.wildt@boku.ac.at http://www.wau.boku.ac.at/iwa/

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University of Natural Resources and Life Sciences, Vienna Department of Water, Atmosphere and Environment

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