Mass Conservation in ELM Advection Schemes for Water Quality Simulations with QSim-3D

What is the problem?

The basic ELM scheme, used in QSim-3D, is not exactly mass conservative.

In QSim-3D the advection part in a transport equation ist discretized with the ELM (Euler-Lagrange-Method), sometimes also called Method of Characteristics or Semi-Lagrangian Method.

The advected concentration difference in a timestep is taken as the difference between the actual value and the value at the origin of a backtracked streamline.

The hydraulic drivers used for Qsim-3d (casu, SCHISM) do backtracking for momentum advection anyway. These streamline origins can be stored and reused in subsequent (offline coupled) water quality simulations with Qsim-3D.

In 2D-depth averaged computaions a linear Interpolation of the conservative variable (concentration times depth) is used to evaluate the value at the streamline origin.

How large is the problem?

Method 1: Integral measures for mass conservation:

In QSim-3D a module was added that summs up tracer mass in each zone (in Qsim-3D the computational domain is subdiveded into zones used for the assignment of e. g. weather bondary condions). Together with this the evaluation of tracer fluxes across boundary lines and across cross sections was implemented.

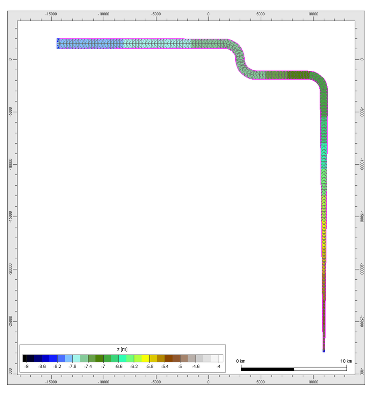


Figure 1 schematic estuary, mesh and bathymetry

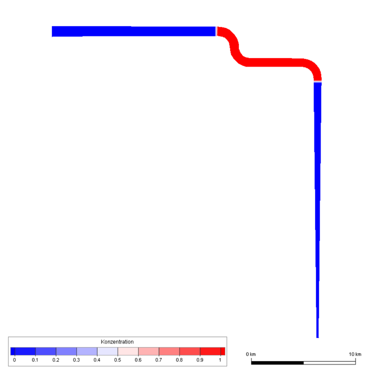


Figure 2 schematic estuary, initial tracer distribution

Boundary conditions: M2 tidal amplitude 1.5m prescribed at the sea boundary at upper left. Constant influx of 100 m³/s at inland boundary at lower left

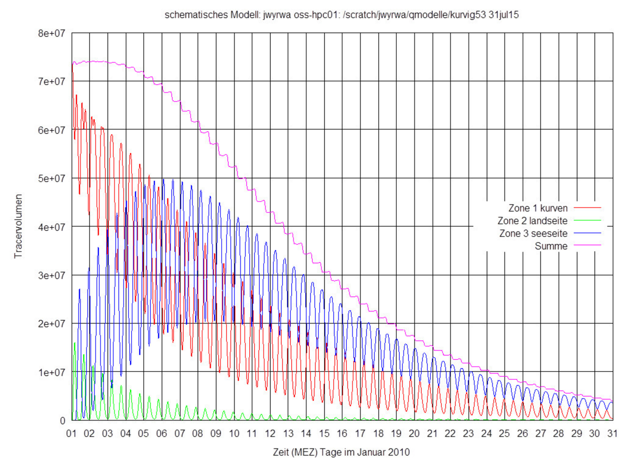


Figure 3 schematic estuary, evolution of tracer mass in the individual zones and the sum of all zones

In a schematic testcase with horizontal side walls Qsim-3D performs a good mass conservation during the first days of the „experiment“ when the tracer mass is advected within the domain. The wash out of the tracer caused by the riverine influx is plausible.

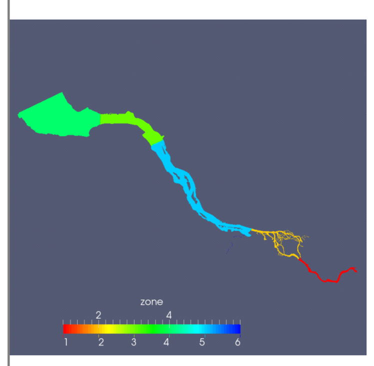


Figure 4 zones of Elbe estuary model

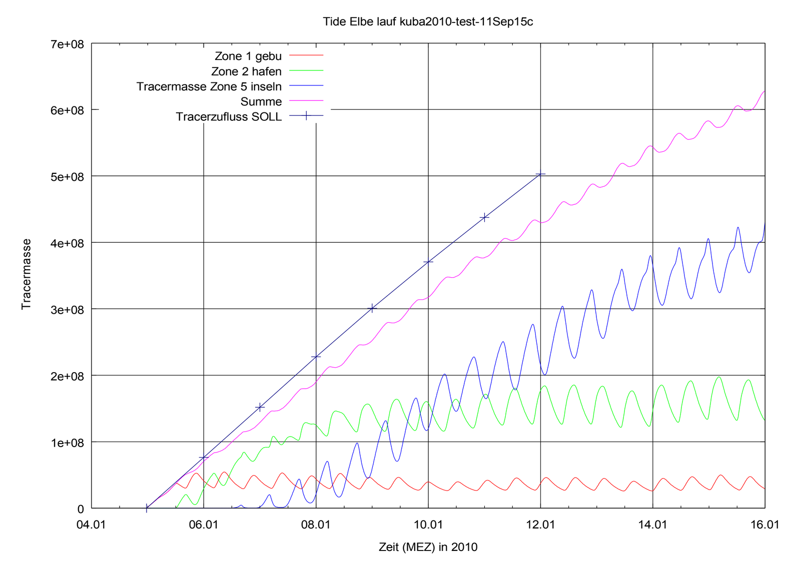
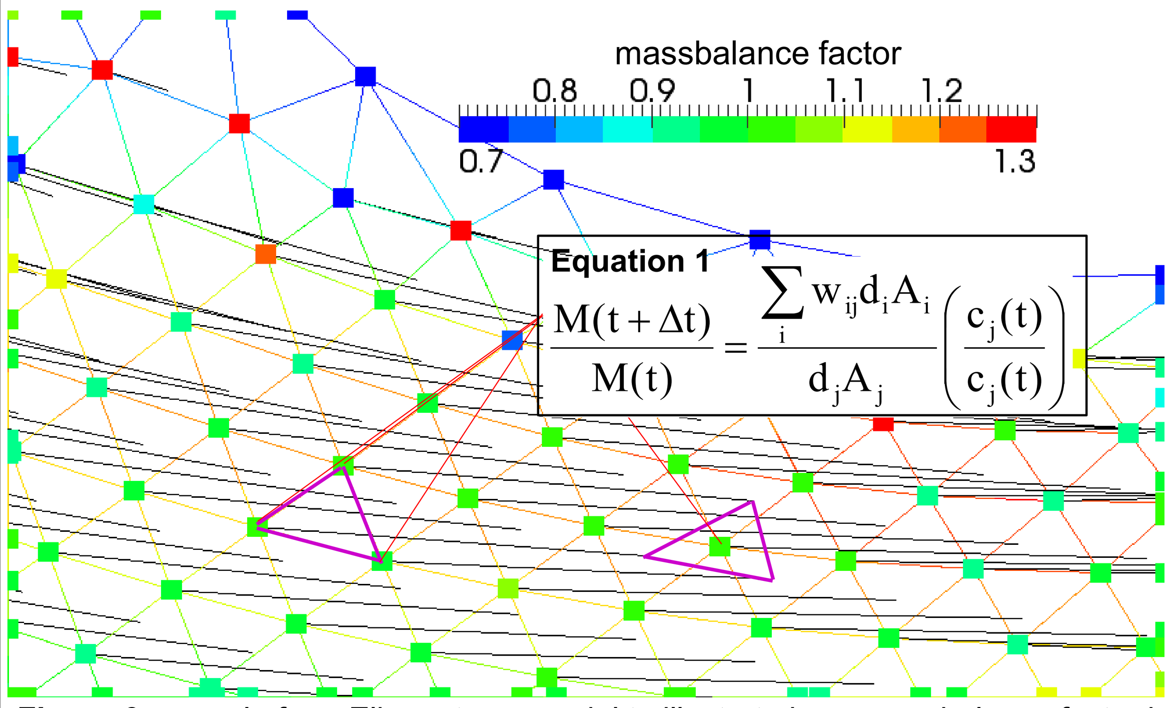


Figure 5 Elbe estuary model, evolution of tracer mass in the individual zones and the sum of all zones. The tidal movement is prescribed by the water elevation at the see boundary (upper left fig.4) and the river inflow (lower right fig.4) during January 2010. starting from 5[th] Jan. a constant tracer concentration is inserted into the inflow. The time integration of this flux results in the dark blue curve. The purple curve shows the evolution of the sum of tracer contained in all zones. No tracer leaves the domain during the perion shown.

In the Elbe estuary model mass losses can be detected and sum up to ca. 15% within one week.

Method 2: Local measure for mass conservation

When the advection algorithm adds up the concentration mass, which a node (cell) is recieving, this mass can be added in the donating node as well. This donated mass can then be set into relation with the mass, the node had in the previous time step. This relation is called „mass balance factor“; values smaler or larger then 1 indicate mass loss or gain respectively.



Equation 1

$$\frac{M(t+\Delta t)}{M(t)} = \frac{\sum_i w_{ij} d_i A_i}{d_j A_j} \left(\frac{c_j(t)}{c_j(t)} \right)$$

$M(t+\Delta t)$ – Mass in current time step, summing up all contributions that node j gave to the nodes i

$M(t)$ – Mass in previous time step, when held by node j

w – weighting factors of ELM advection

d - water depth

A - Area of the cell associated with node

c – concentration

Figure 6 example from Elbe estuary model to illustrate how mass balance factor is formed. Mesh colored with velocity magnitude (scale not shown). Black lines connect nodes with the origin of their backtracked streamline. Nodes shown as square dots colored with mass balance factor. Purple triangel on the left highlights example of recieving nodes i. Purple triange on the right encircles the donation node j.

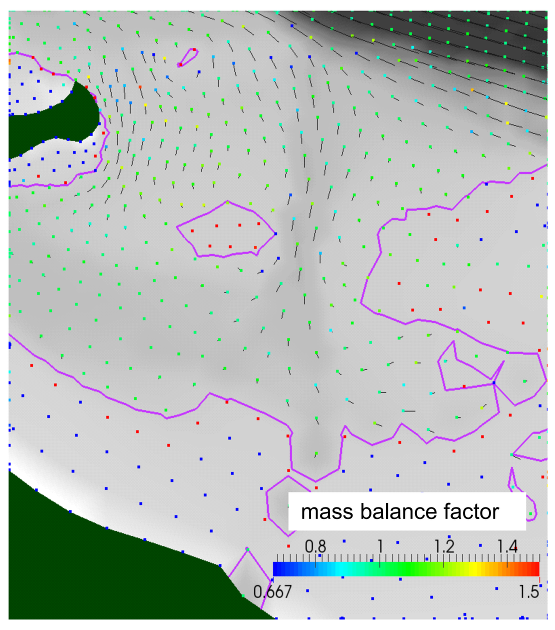


Figure 7 Mass balance factor in a small part of Elbe estuary model, ebb flow running down intertidal flats, fairway visible in the upper right corner. Gray shading shows bathymetry (without scale). Black lines symbolize backtracked streamlines. Purple line = shore line. Node coloring gives mass balance factor according to scale

Both examples (fig. 6 and 7) show that mass conservation is good in the fairway and less precise on slopes, side channels and intertidal flats.

Conclusion from both methods: Mass conservation is less exact in shallow water areas and intertidal flats.

How to cope with the problem?

Option 1:
Careful interpretation of results.

Metabolic processes, that „create“ and „destroy“ concentration, dominate in water quality processes. Mass losses caused by the advection scheme are comparably small in the context of some biochemical concentrations.

In models of estuarine water quality, boundary values are difficult to determine. Already salinity is hard to measure at extended sea boundaries.

Differences, detected in validation, can be checked with the methods described above. Enabeling the experinced modeller to distiguish possible origins.

Option 2:
Change to „classical“ finite volume algorithms with exact mass conservation.

Finite volume algorithm are exactly mass conservative but they have to obay the Courant criteria. This considerably limits the time step and increases computation time.

First order upwind schemes furthermore exibit substantial numerical diffusion.

Higher order schemes are less diffusive but need to implement limiters to make the solution total variation diminishing (TVD). This slows down the computation even further. Especially in water quality simulation where the limiter needs to be applied to each of the large number of concentrations individually.

For details see:

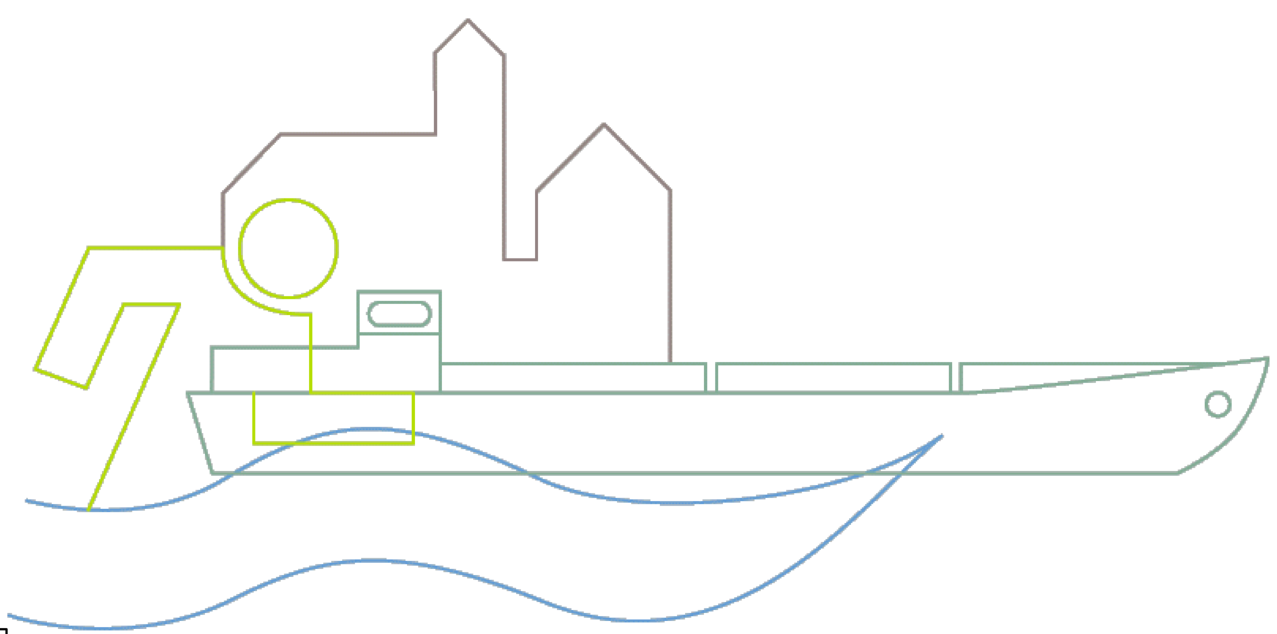
Zhang et al.
A new vertical coordinate system for a 3D unstructured-grid model
Ocean Modellig 85 (2015) 16-31.

Option 3:
Change to „advanced“ mass-conservative ELM's

A recent proposal by M. Lentine et al. utilizes the information gained in method 2 (see above) to correct mass conservation in a second step.

No experience regarding computaional speed and stability has yet been gained by the author.

Lentine, M., Gretarsson, J. and Fedkiw, R.,
An Unconditionally Stable Fully Conservative Semi-Lagrangian Method, Journal of Computational Physics 230, 2857-2879 (2011).



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Dr.-Ing. Jens Wyrwa

Federal Institute of Hydrology
(Part of German waterways)
Division U, Ecology
Am Mainzer Tor 1; 56068 Koblenz
Tel.: (0049) 261 / 1306 - 5254
wyrwa@bafg.de ; www.bafg.de

www.wyrwa.de