Processing statistical parameters of concentration along a river network

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In-stream water quality modelling – state of the art

Driving forces of WQ modeling:

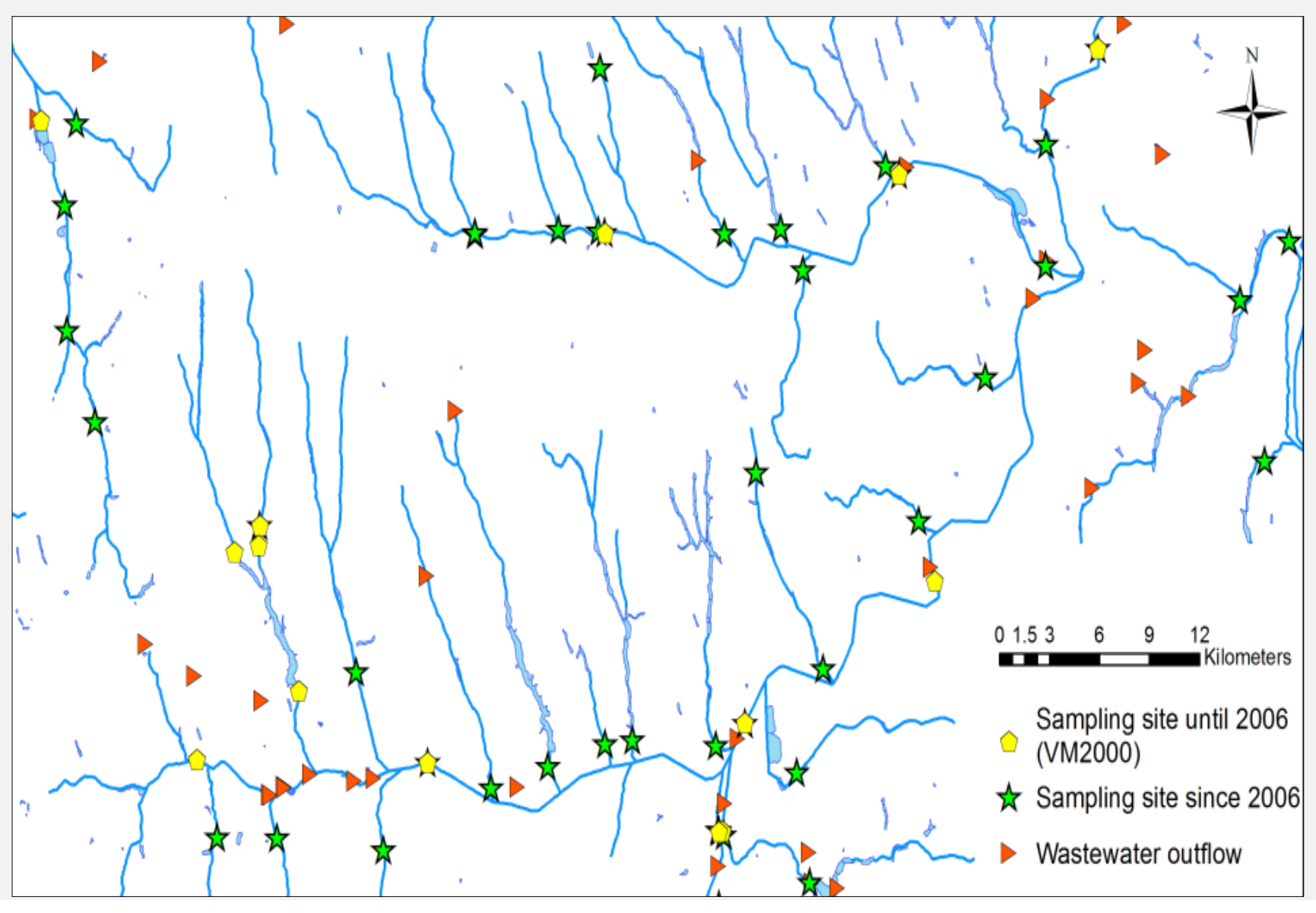
- contamination of waters (diffuse and point-sources)
- legislation (EU Directives, other international legislation,…)
- water uses (agricultural, domestic, industrial, recreational,…)
- scientific curiosity

Types of WQ models:

- the first step is always a hydrologic/ hydraulic model
- stochastic vs. process-based
- transient vs. stationary

Calibration/validation is problematic

- against extra measurements
- against another WQ model
- no calibration



Regular WQ monitoring in Hungary

Huge amount of data covering long period:
~ 50 years, > 1000 sampling sites, > 200 parameters

Time-shift between adjacent sampling stations

Data can be used for modelling purposes:

- long-term trends
- regional patterns

No use of the database to model ranges of concentrations in a longer time period with high spatial resolution!

Figure: Part of WQ monitoring network of Hungary

Modelling concept

- „steady-state" modelling of water quality in large spatial scale for „average" situtation
- time variation accounted for with momentums (average, variance, covariances) of the time series
- make use of the regular monitoring data
- traditional parameters (BOD, DO, N, P)
- changes assigned to edges, mixing processes, diffuse and point-source loads and monit. points represented by nodes
- simplified process representation
  - second order second moment approximation of equations

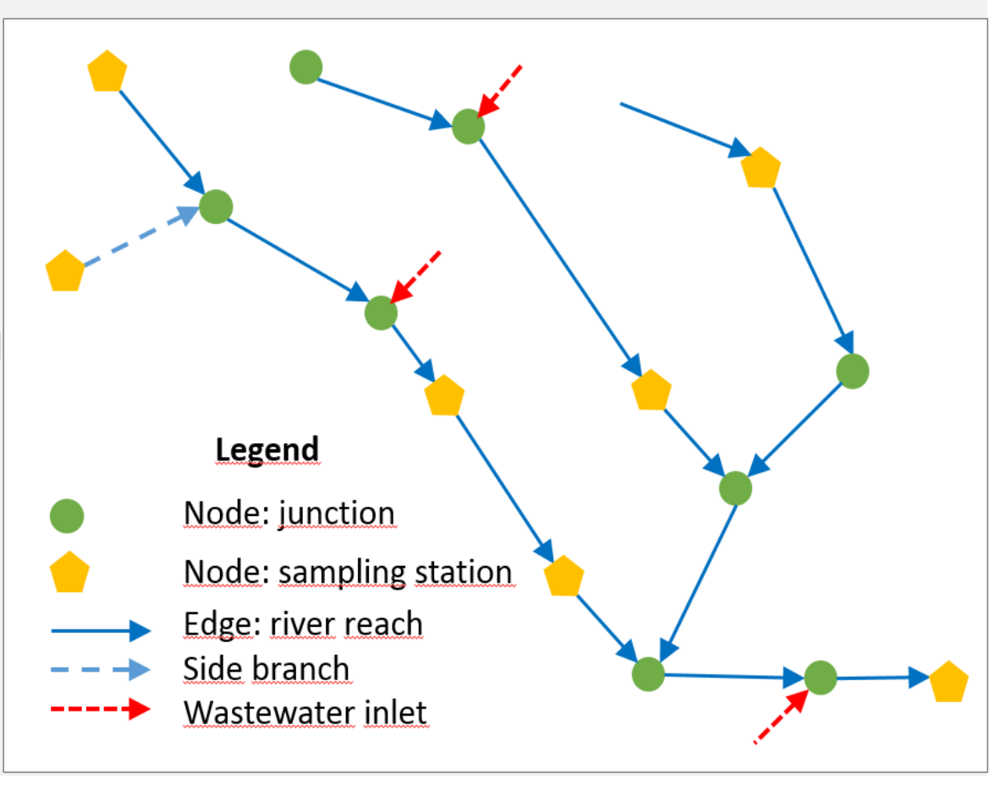


Figure: graph representation of the river network

Approximating the statistics

Edge process (settling):

$$C_1 = C_0 \exp\left(-\frac{v_s}{H}\,t\right)$$

where C_0 and C_1 – upstream and downstream concentration respectively, v_s –settling velocity, H – water depth and t - travel time along the river section.

$$C_1(C_0, Q) = C_0 \exp\left(k\, Q^{-\frac{5}{8}}\right)$$

where k comprises the settling velocity, the roughness and the geometrical properties and is assumed to be constant along an edge (a section of a reach).

Second-order approximation for mean downstream concentration:

$$E(C_1) \approx E(C_0)\exp\left(k\,[E(Q)]^{-\frac{5}{8}}\right) + \frac{1}{2}\left(\frac{\partial^2 C_1}{\partial Q^2}\right)_{E(C_0),E(Q)} \cdot \sigma_H^2 + \left(\frac{\partial^2 C_1}{\partial C_0 \partial Q}\right)_{E(C_0),E(Q)} \cdot \mathrm{cov}(Q, C_0)$$

where E – expected value (mean value) ; σ_Q^2 – variance of water flow and cov(C_0,Q) – covariance between upstream concentration and water flow.

Second-order approximation for standard deviation of downstream concentration:

$$\sigma^2(C_1) \approx \left[\overline{C_0}\exp\left(const_2\, Q^{-\frac{5}{8}}\right) - \overline{C_1}\right]^2 + \frac{1}{2}\left(\frac{\partial^2 f}{\partial {C_0}^2}\right)_{(\overline{C_0},\bar{Q})} \cdot \sigma^2(C_0) + \frac{1}{2}\left(\frac{\partial^2 f}{\partial Q^2}\right)_{(\bar{Q},\overline{C_0})} \cdot \sigma^2(Q) + \left(\frac{\partial^2 f}{\partial C_0 \partial Q}\right)_{(\overline{C_0},\bar{Q})} \cdot cov(C_0, Q)$$

where $f = \left[C_0 \exp\left(const_2\, Q^{-\frac{5}{8}}\right) - \overline{C_1}\right]^2$.

Second-order approximation for downstream correlation:

$$cov(Q, C_1) \approx \frac{1}{2}\left(\frac{\partial^2 g}{\partial {C_0}^2}\right)_{\bar{Q},\overline{C_0}} \cdot \sigma^2(C_0) + \frac{1}{2}\left(\frac{\partial^2 g}{\partial Q^2}\right)_{\bar{Q},\overline{C_0}} \cdot \sigma^2(Q) + \left(\frac{\partial^2 g}{\partial C_0\, \partial Q}\right)_{\bar{Q},\overline{C_0}} \cdot cov(Q, C_0)$$

where $g = \left(C_0 \exp\left(const_2\, Q^{-\frac{5}{8}}\right) - \overline{C_1}\right)(Q - \bar{Q})$.

Node process (instant complete stirring):

$$C = \frac{Q_1\, C_1 + Q_2\, C_2}{Q_1 + Q_2} = h(Q_1, C_1, Q_2, C_2)$$

Mean of node outflow concentration:

$$\begin{aligned} E(C) = {} & \frac{\overline{Q_1}\,\overline{C_1} + \overline{Q_2}\,\overline{C_2}}{\overline{Q_1} + \overline{Q_2}} + \frac{\overline{C_1} - \overline{C_2}}{\left(\overline{Q_1} + \overline{Q_2}\right)^3}\left(\overline{Q_1}\,\sigma_{Q2}^2 - \overline{Q_2}\,\sigma_{Q1}^2\right) + \\ & + \frac{\left(\overline{C_1} - \overline{C_2}\right)\left(\overline{Q_1} - \overline{Q_2}\right)}{\left(\overline{Q_1} + \overline{Q_2}\right)^3} cov(Q_1, Q_2) + \frac{\overline{Q_2}}{\left(\overline{Q_1} + \overline{Q_2}\right)^2} cov(Q_1, C_1) + \\ & + \frac{\overline{Q_1}}{\left(\overline{Q_1} + \overline{Q_2}\right)^2} cov(Q_2, C_2) - \frac{\overline{Q_2}}{\left(\overline{Q_1} + \overline{Q_2}\right)^2} cov(Q_1, C_2) - \frac{\overline{Q_1}}{\left(\overline{Q_1} + \overline{Q_2}\right)^2} cov(Q_2, C_1) \end{aligned}$$

Variance of node outflow concentration:

$$\begin{aligned} \sigma^2(C) = {} & \left(\frac{\overline{Q_1}\,\overline{C_1} + \overline{Q_2}\,\overline{C_2}}{\overline{Q_1} + \overline{Q_2}} - \bar{C}\right)^2 + \left(\frac{\partial^2 h}{\partial {Q_1}^2}\right)_{\overline{C_1},\overline{C_2},\overline{Q_1},\overline{Q_2}} \sigma_{Q1}^2 + \\ & + \left(\frac{\partial^2 h}{\partial {Q_2}^2}\right)_{\overline{C_1},\overline{C_2},\overline{Q_1},\overline{Q_2}} \sigma_{Q2}^2 + \left(\frac{\partial^2 h}{\partial {C_1}^2}\right)_{\overline{C_1},\overline{C_2},\overline{Q_1},\overline{Q_2}} \sigma_{C1}^2 + \left(\frac{\partial^2 h}{\partial {C_2}^2}\right)_{\overline{C_1},\overline{C_2},\overline{Q_1},\overline{Q_2}} \sigma_{C2}^2 \end{aligned}$$

Tests

Test 1: synthetycally generated data

Input value	Range	Step	Units
Riverbank slope (φ)	15 … 45	15	deg
Riverbed slope (S)	10^{-5} … 10^{-4}	4.5	-
Manning's coefficient (k_{st})	10 … 40	10	$m^{1/3}\ s^{-1}$
Settling velocity (v_s)	0.1 … 10	*10	$m\ d^{-1}$
Mean discharge ($E(Q)$)	0.1 … 2000	-	$m^3\ s^{-1}$
Coefficient of variation for discharge ($\sigma(Q)/E(Q)$)	0.2 … 1.5	-	-
Mean upstream concentration ($E(C_0)$)	10.0 … 400	-	$g\ m^{-3}$
Coefficient of variation for concentration ($\sigma(C_0)/E(C_0)$)	0.5 … 3.0	-	-
Discharge: parameter μ of logN random variables	-1 … 7	1	$\ln(m^3\ s^{-1})$
Discharge: parameter σ of logN random variables	0.2 … 1	0.2	$\ln(m^3\ s^{-1})$
Concentration: parameter μ of logN rand variables	2 … 5	1	$\ln(g\ m^{-3})$
Concentration: parameter σ of logN rand variables	0.5 … 1.5	0.5	$\ln(g\ m^{-3})$
Correlation coefficient r(Q,C_0)	-0.2 … 0.8	0.2	-

Test 2: Measured upstream versus calculated downstream data

- 35-years long series of water flow and total suspended solids (TSS), measured daily on the Zala river at Zalaapáti between 1978 – 2012.
- 350 randomly selected, one-year long sections of measured discharge-concentration data pairs were selected.
- Settling velocity and river geometry were determined randomly in the same range as in Test 1

Input value	Range	Units
Reach length (L)	100	km
Riverbank slope (φ)	26.5	deg
Riverbed slope (S)	10^{-6}	-
Manning's coefficient (k_{st})	40	$m^{1/3}\ s^{-1}$
Settling velocity (v_s)	1	$m\ d^{-1}$

Test 3: Measured upstream and downstream data

- upstream and downstream of Kis-Balaton Water Protection System
- 1998 – 2006

Input value	Value / Range	Units
Riverbank slope (φ)	11.3	deg
Riverbed slope (S)	10^{-6}	-
Manning's coefficient (k_{st})	40	$m^{1/3}\ s^{-1}$
Settling velocity (v_s)	0.4 – 3.7	$m\ d^{-1}$
Mean discharge ($E(Q)$)	2.0 – 5.8	$m^3\ s^{-1}$
Coefficient of variation (CV) of discharge ($\sigma(Q)/E(Q)$)	0.3 – 1.1	-
Mean upstream concentration ($E(C_0)$)	11 – 65	$g\ m^{-3}$
CV of concentration $\sigma(C_0)/E(C_0)$	0.9 – 3.0	-
Correlation coefficient r(Q,C_0)	-0.25 – 0.52	-
Observed mean downstream (ds) concentration ($E(C_1)$)	2.9 – 7.8	$g\ m^{-3}$
Observed ds CV of concentration ($\sigma(C_1)/E(C_1)$)	0.6 – 1.3	-

Results

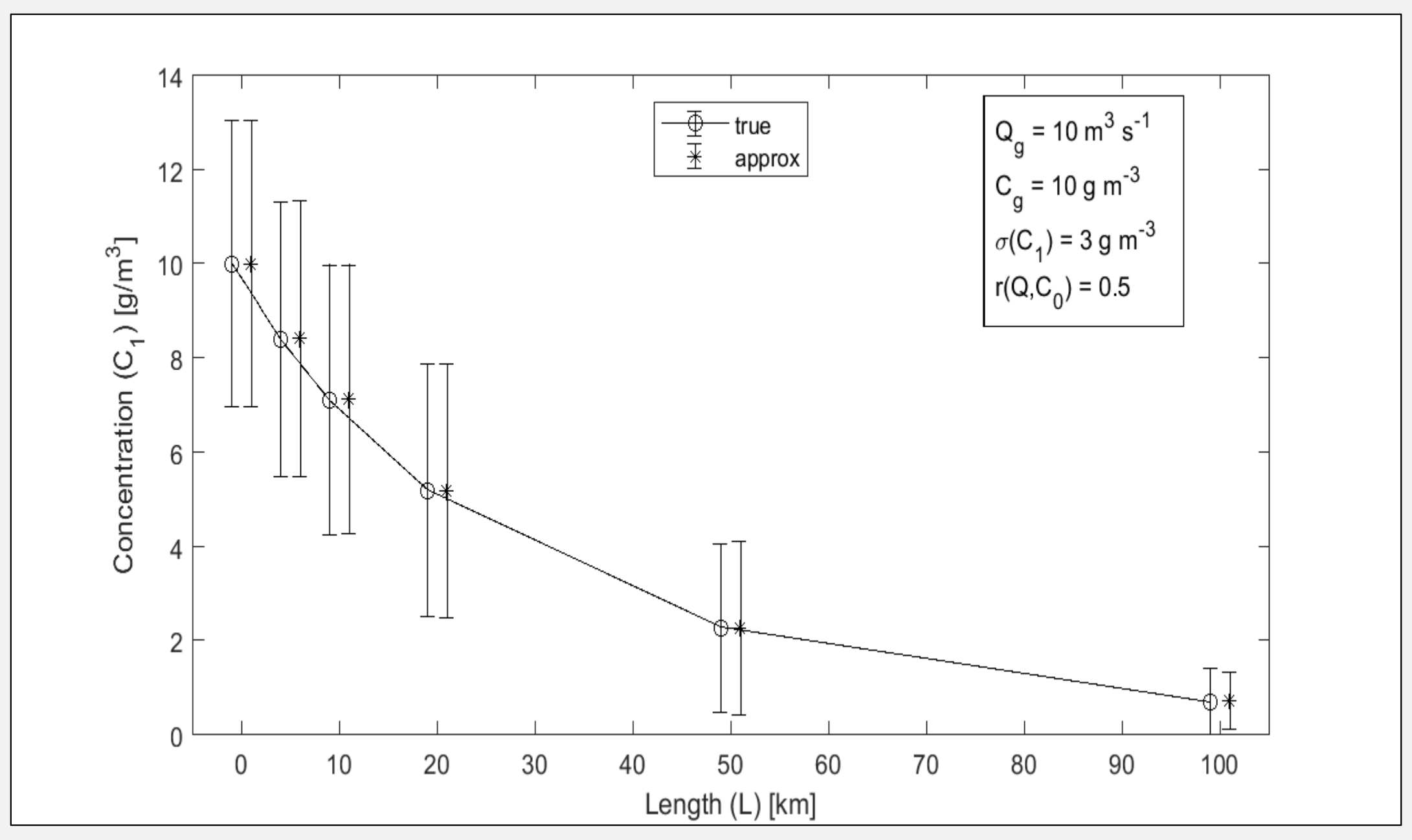


Figure: Longitudinal section of a unique test

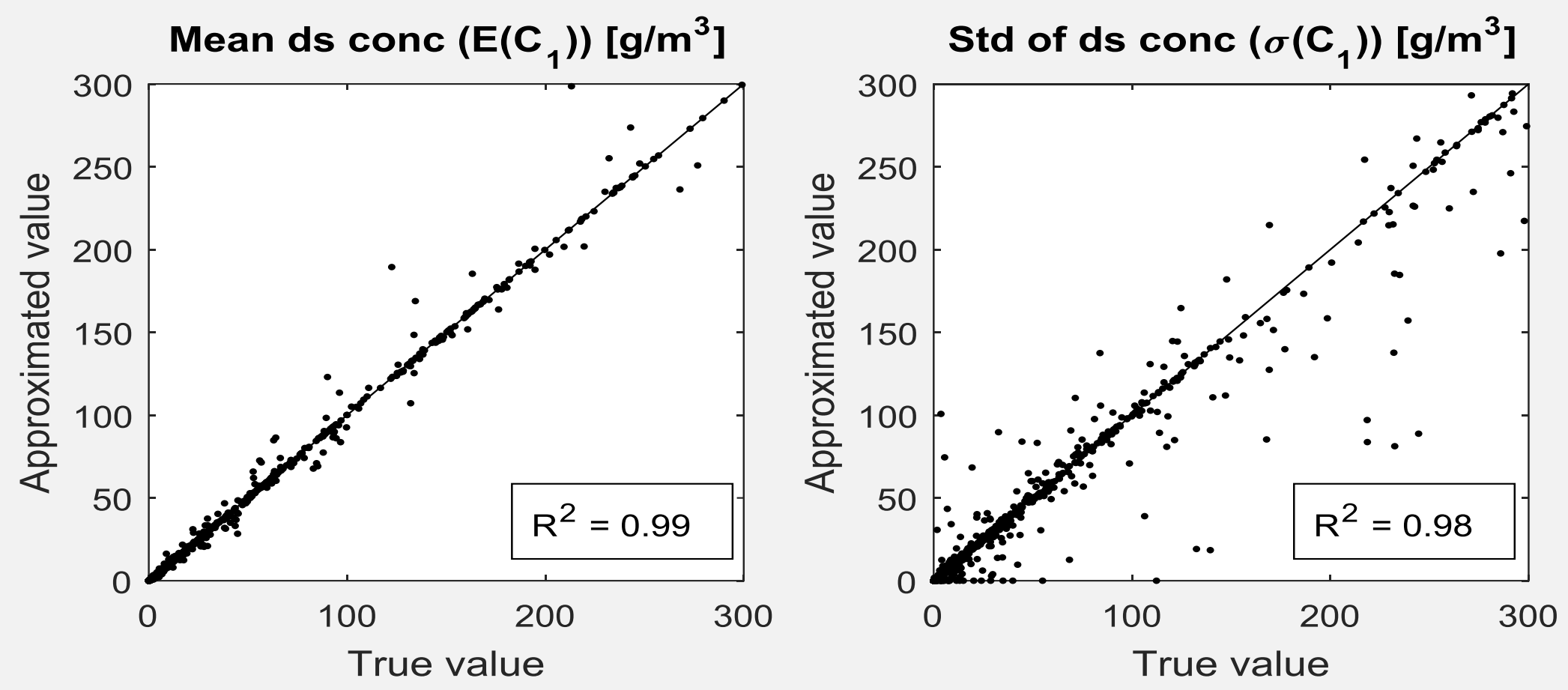


Figure: Approximated vs. true values

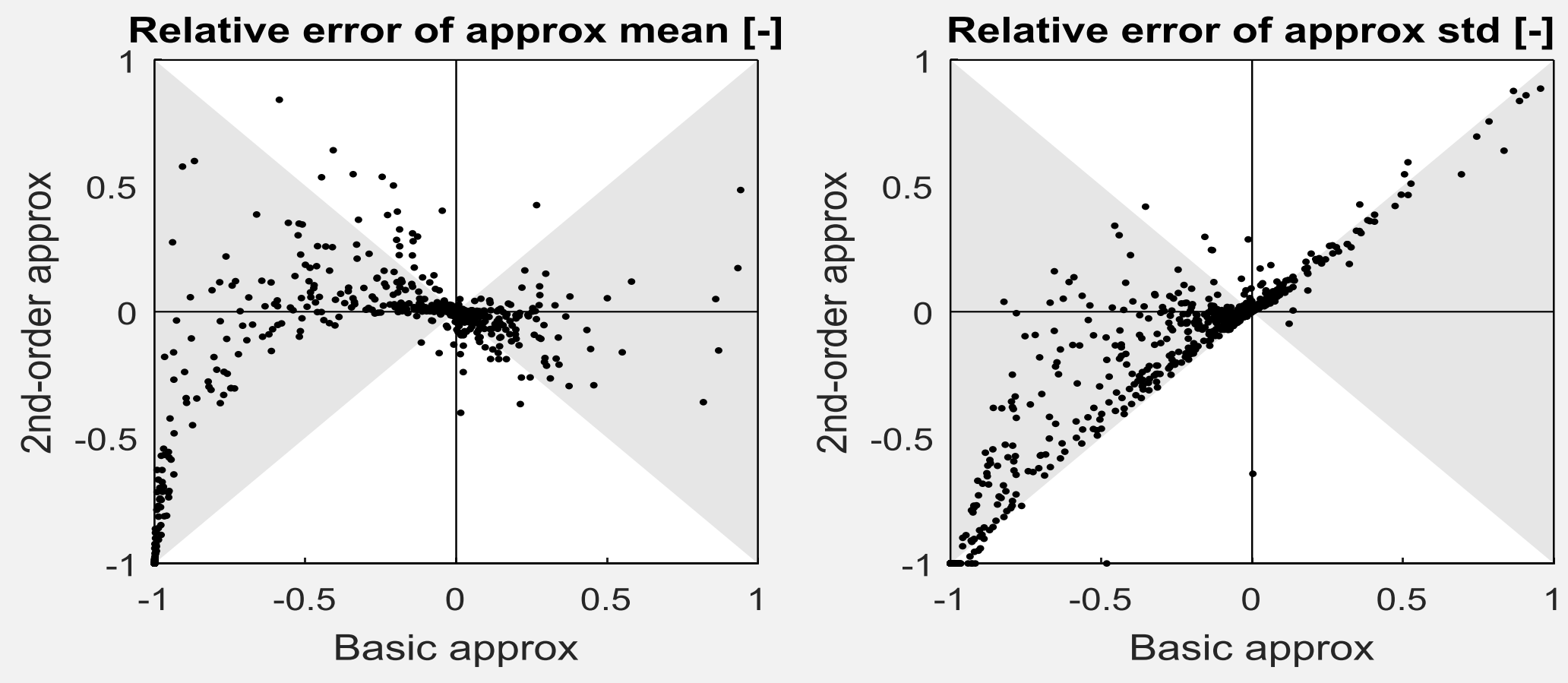


Figure: Errors of second-order approximations vs. errors of basic apx.

Results of Test 3:

	Std of downstream concentration					Correlation between conc & disch				
year	Obs [g/m³]	Bapx [g/m³]	Rerr of bapx	Apx2 [g/m³]	Rerr of apx2	Obs ds [-]	Us [-]	Err of us	Apx2 ds [-]	Err of apx2
1998	8	12	51%	12	56%	0.11	0.23	0.11	0.72	0.61
1999	6	19	243%	11	98%	-0.04	0.28	0.33	0.56	0.60
2000	4	4	-13%	5	7%	-0.09	0.12	0.21	0.51	0.60
2001	8	6	-14%	7	-9%	0.08	0.52	0.43	0.64	0.56
2002	7	18	155%	19	182%	-0.47	-0.26	0.21	-0.19	0.27
2003	5	9	70%	11	110%	-0.19	-0.20	-0.01	0.06	0.25
2004	5	12	118%	9	66%	0.27	0.31	0.04	0.67	0.40
2005	2	8	259%	5	121%	0.03	0.20	0.17	0.62	0.59
2006	2	8	401%	3	97%	0.13	0.20	0.07	0.82	0.69

Conclusions

- The method can be considered as satisfactory in estimating downstream mean and variance.
- In almost all cases, relative error of the second-order approximation of mean downstream concentration remained very low.
- It performed well on both generated lognormal and measured data, compared to „basic" approximations.
- The approximated amounts were close to „true" values.
- Significant improvement in approximation of the mean downstream concentration
- In most cases, relative error of the second-order approximation of standard deviation of downstream concentration remained below 10%.
- Relative errors associated with smaller standard deviations sometimes remained high
- Approximation was unsatisfactory compared to downstream measurements, which indicates the need for more detailed description of the in-stream processes.

Next steps

- More detailed description of the in-stream process.
- Test on other WQ components
- Investigation of second-momentum approximations of formulas more capable to describe complex in-steam processes
- Further ivestigation needed for
  - node processes
  - resuspension
  - diffuse pollution and/or continuos discharge-increment