How predictable are pharmaceutical loads in wastewater treatment plant influents and effluents?

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Introduction & Background

- Geo-referenced simulation **models** can be used to **support chemical exposure assessment** in whole watersheds [1]
- Wastewater treatment plants (WWTPs) are identified as major emission sources for pharmaceuticals and implemented as point sources in such models [2,1]
- Model **outcome** highly relies on the **quality of the input parameters** (i.e. per capita consumption rate, excretion rate, WWTP removal efficiency)

Objectives

1. Quantification of the **prediction accuracy** of pharmaceutical loads in WWTP influents and effluents
2. Analysis of **error span** between predicted and measured loads in WWTP influents and effluents

Data & Methods

1) Data set

- 18 Dutch WWTPs in the Rijn Oost area (9,000 – 200,000 inhabitants)
- Activated sludge technologies, three with sand filtration
- Up to six influent and effluent measurements in each WWTP for winter and summer
- Seven hospitals

2) Loads from measurements

$$L_{meas,i} = C_{diss} \cdot Q \cdot (1 + X_{SS} \cdot K_d) \quad (1)$$

- $L_{meas,i}$ [kg yr^{-1}]: Measured influent/effluent load of measurement i.
- C_{diss} [µg L^{-1}]: Dissolved concentration
- Q [m^3 s^{-1}]: Discharge
- X_{SS} [mg m^{-3}]: Suspended solids concentration
- K_d [kg L^{-1}]: Distribution coefficient

3) Predicted loads

$$L_{in} = (pCC \cdot Inh + pBC \cdot b) \cdot e \quad (2)$$

$$L_{eff} = L_{in} \cdot (1 - RE) \quad (3)$$

- L_{in}, L_{eff} [kg yr^{-1}]: Predicted influent/effluent load
- pCC [kg inh^{-1} yr^{-1}]: Per capita consumption rate
- pBC [kg bed^{-1} yr^{-1}]: Per bed consumption rate
- Inh [inh]: Inhabitants connected to the WWTP
- b [bed]: Beds in hospitals connected to the WWTP
- e [-]: Excretion rate
- RE [-]: Removal efficiency

4) Prediction accuracy

$$\log \Delta_i = \log_{10} \frac{L_{pred}}{L_{meas,i}} \quad (4)$$

$$\zeta = 10^{\text{median}\{|\log \Delta_i|\}} - 1 \quad (5)$$

For a measurement i $\log \Delta$ is a measure for the error, i.e. $\log \Delta = 0$ means that the predicted load L_{pred} is equal to the measurement derived load L_{meas}. The prediction accuracy ζ aggregates all errors for a compound.

Results

Influent loads (Figure 1)

- Larger error spans for compounds with low application frequency (antibiotics AZI, CLA, ERI)
- Tendency to overestimate ($\log \Delta > 0$)
- 90% error span between 0.60 (MTO) and 1.66 (ERY)
- Prediction accuracies ζ between 0.46 (OXA) and 2.12 (N-ASMX), best prediction accuracies (ζ < 0.5) for MTO, MTF and OXA

Effluent loads (Figure 2)

- Wastewater treatment enlarges variability in loads for most compounds (increase in error span)
- Tendency to overestimate remains
- Prediction accuracies ζ between 0.41 (OXA) and 3.61 (VAL), best prediction accuracies (ζ < 0.5) for OXA and AZI
- 90% error span between 0.62 (OXA) and 2.30 (VAL)

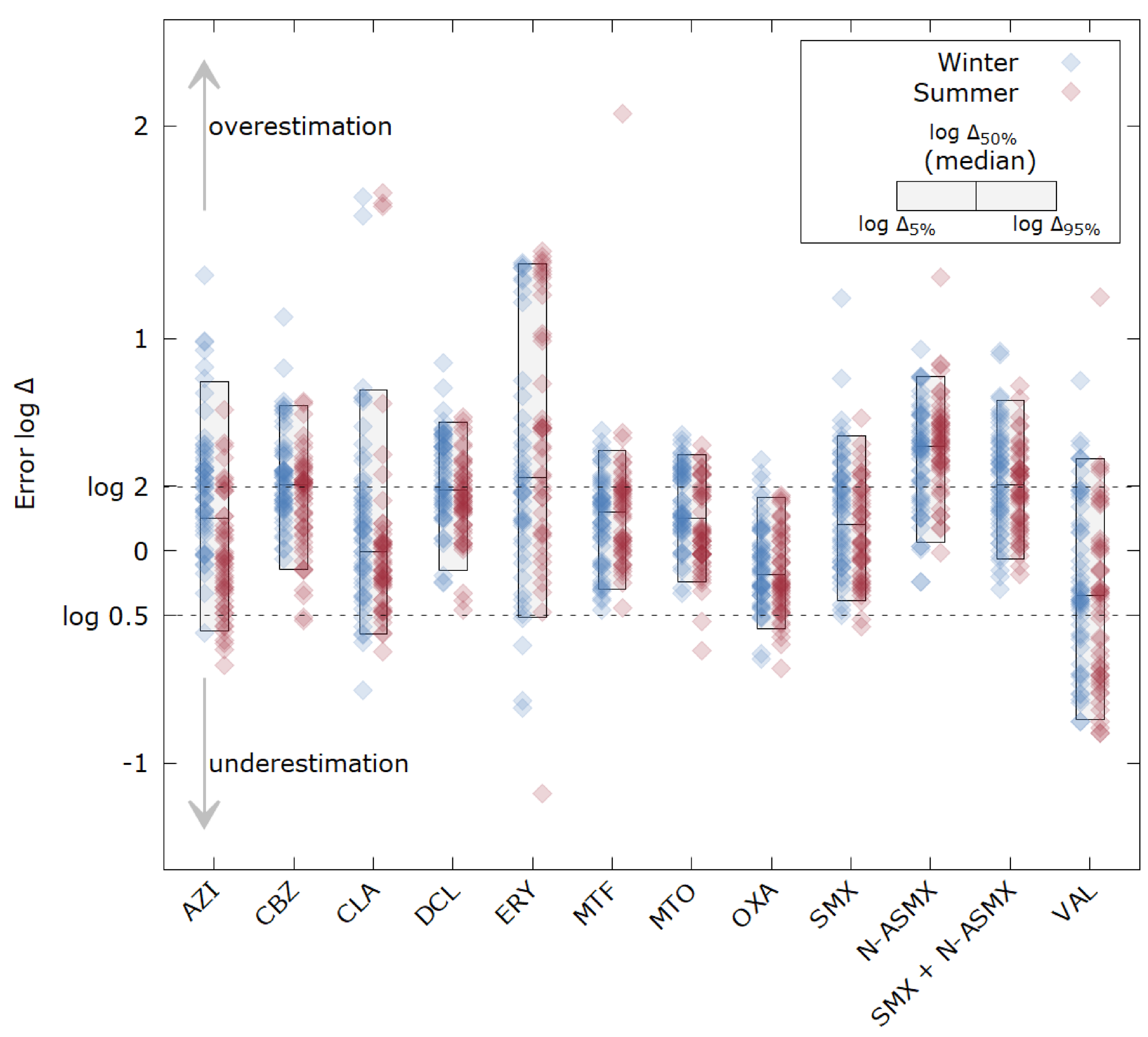

Figure 1: Error log Δ for winter and summer influent loads. Number (n) of data points for all compounds is 105 fexcept for ERY (n=88). 90% error span is marked by gray boxes.

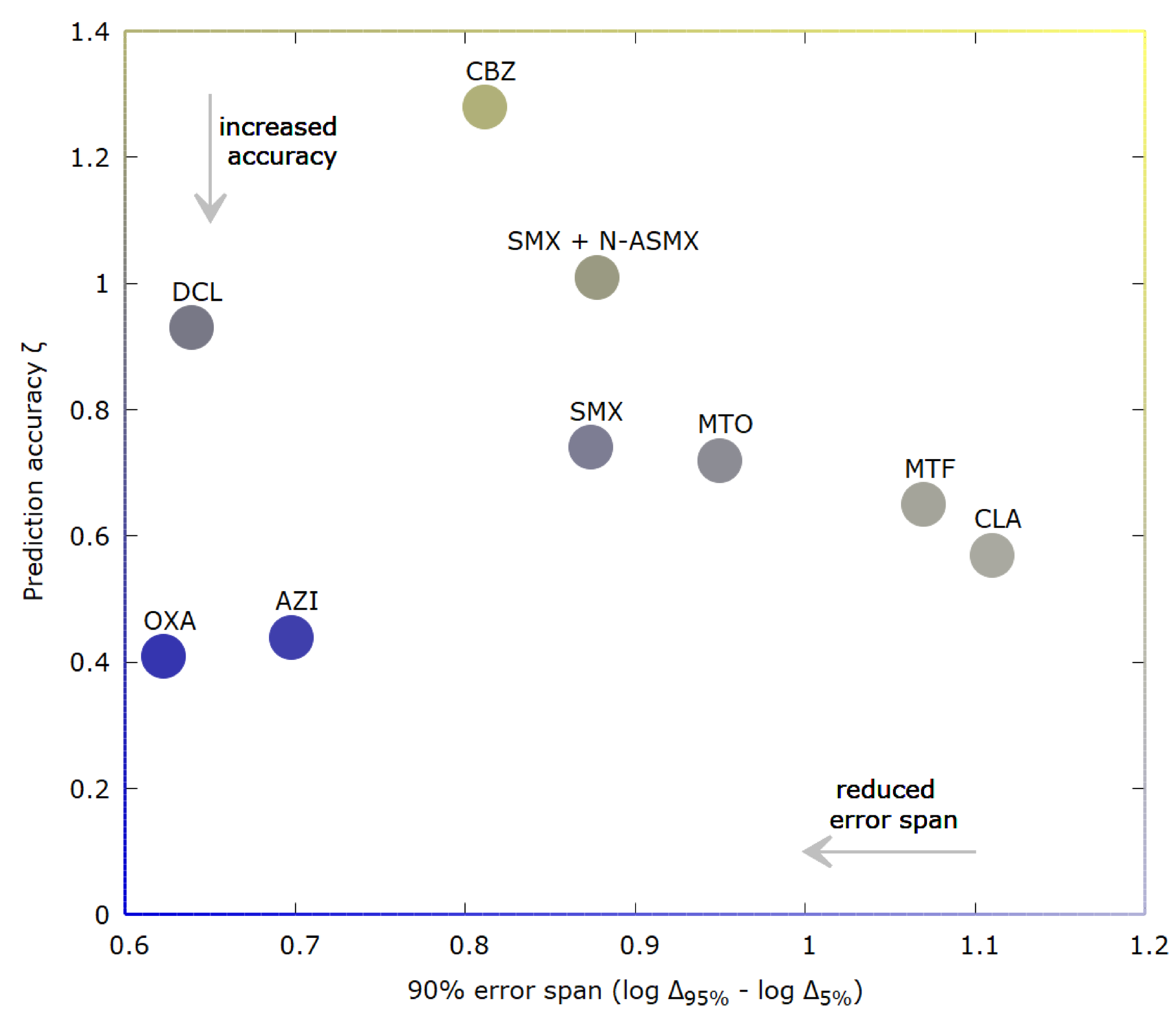

Figure 2: Prediction accuracy and error span of final treated effluent. Missing ompounds: N-ASMX (1.48,1.30), ERY (1.96,2.20), VAL (2.30,3.61).

Pharmaceuticals: azithromycin (AZI), carbamazepine (CBZ), clarithromycin (CLA), diclofenac (DCL), erythromycin (ERY), metformin (MTF), metoprolol (MTO), oxazepam (OXA), sulfamethoxazole (SMX), SMX metabolite N4-acetylsulfamethoxazole (N-ASMX)

Conclusion

- Two measures were applied to evaluate the prediction quality of pharmaceutical loads in WWTP influents and effluents
- The approach of constant WWTP emissions is applicable for OXA and AZI, for the other compounds further evaluation needs to be done

Next Steps

- Calibration of predicted to measurement derived loads
- Stochastic predictions, parameters expressed as distributions

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References

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