Supporting Information

Title: In Situ Monitoring of Groundwater Contamination Using the Kalman Filter

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6 pages, 1 text, 3 figures

Text S1

The Kalman filter is a recursive two-step process consisting of a state prediction step and an update step, as graphically shown in Figure S3. A detailed derivation is available in Reid (2011).[1] The goal is to estimate the state vector $\boldsymbol{x}_t$ as $\hat{\boldsymbol{x}}_t$ and its error covariance $\boldsymbol{P}_t$ at each time step t. The prediction step describes the temporal evolution of the state vector $\boldsymbol{x}_t$ from the previous step. The state-transition equation (Equation 5) is used to predict the expected value of the state vector as $\hat{\boldsymbol{x}}_{t|t-1}$ based on the estimate at the previous time step $\hat{\boldsymbol{x}}_{t-1}$:

$$\hat{\boldsymbol{x}}_{t|t-1} = \boldsymbol{F}\,\hat{\boldsymbol{x}}_{t-1}$$

Similarly, the error covariance $\boldsymbol{P}_t$ is predicted as $\boldsymbol{P}_{t|t-1}$ based on the covariance at the previous step $\boldsymbol{P}_{t-1}$:

$$\boldsymbol{P}_{t|t-1} = \boldsymbol{F}\,\boldsymbol{P}_{t-1}\,\boldsymbol{F}^T + \boldsymbol{Q}$$

The update step improves the estimate of the state vector by including observations $\boldsymbol{z}_t$ through the data correlation model. Based on the state-observation equation (Equation 7), the estimate $\hat{\boldsymbol{x}}_t$ is determined by:

$$\hat{\boldsymbol{x}}_t = \hat{\boldsymbol{x}}_{t|t-1} + \boldsymbol{K}_t[\boldsymbol{z}_t - (\boldsymbol{H}\,\hat{\boldsymbol{x}}_{t|t-1} + \boldsymbol{u})]\,,$$

where the Kalman gain $\boldsymbol{K}_t$ is determined by:

$$\boldsymbol{K}_t = \boldsymbol{P}_{t|t-1}\,\boldsymbol{H}^T[\boldsymbol{H}\,\boldsymbol{P}_{t|t-1}\,\boldsymbol{H}^T + \boldsymbol{R}]^{-1}\,.$$

The error covariance is updated as:

$$\boldsymbol{P}_t = (\boldsymbol{I} - \boldsymbol{K}_t\,\boldsymbol{H})\boldsymbol{P}_{t|t-1}(\boldsymbol{I} - \boldsymbol{K}_t\,\boldsymbol{H})^T + \boldsymbol{K}_t\,\boldsymbol{R}\,\boldsymbol{K}_t^T\,,$$

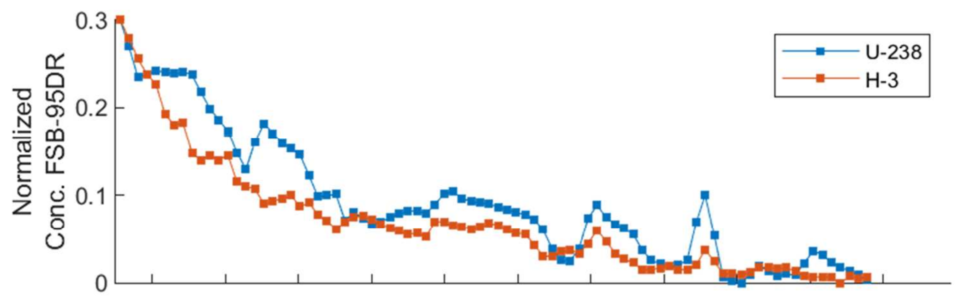
where $\boldsymbol{I}$ is the identity matrix.

Reference:

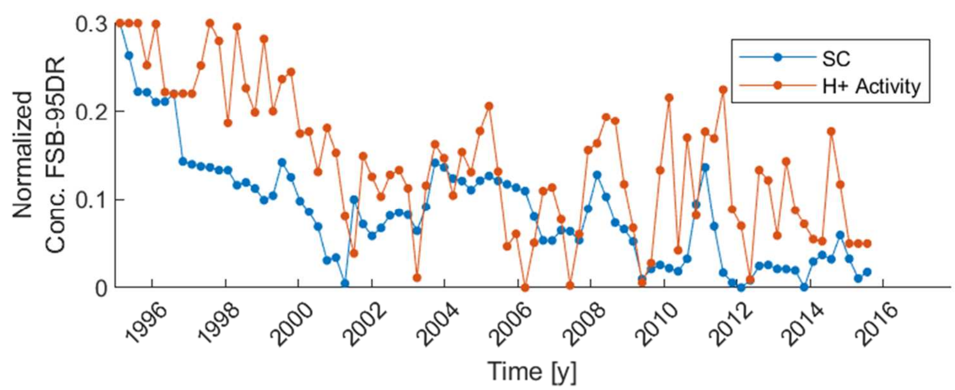
(1) Reid, I. Estimation II http://www.robots.ox.ac.uk/~ian/Teaching/Estimation/LectureNotes2.pdf (accessed Jan 1, 2017).

Figure S1

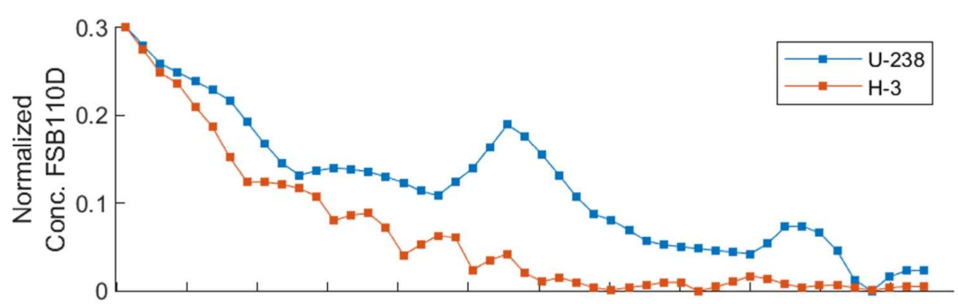
a)



b)



c)



d)

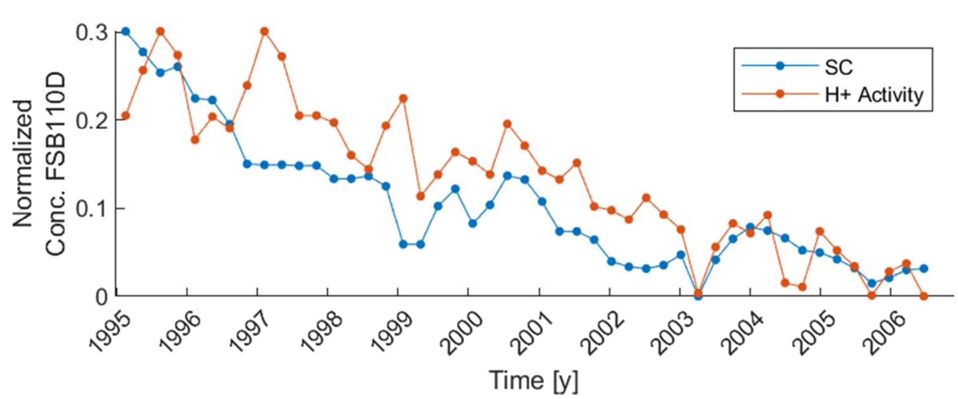


Figure S1

Figure S 1 – a) Interpolated log-normalized (see Methodology) time series of the contaminants U-238 and H-3, as well as b) the groundwater quality variables SC and H^+ for samples taken between 1995 and 2016 at well FSB-95DR. c), d) The same variables for samples taken between 1995 and 2007 at well FSB-110D.

Figure S1

Figure S2

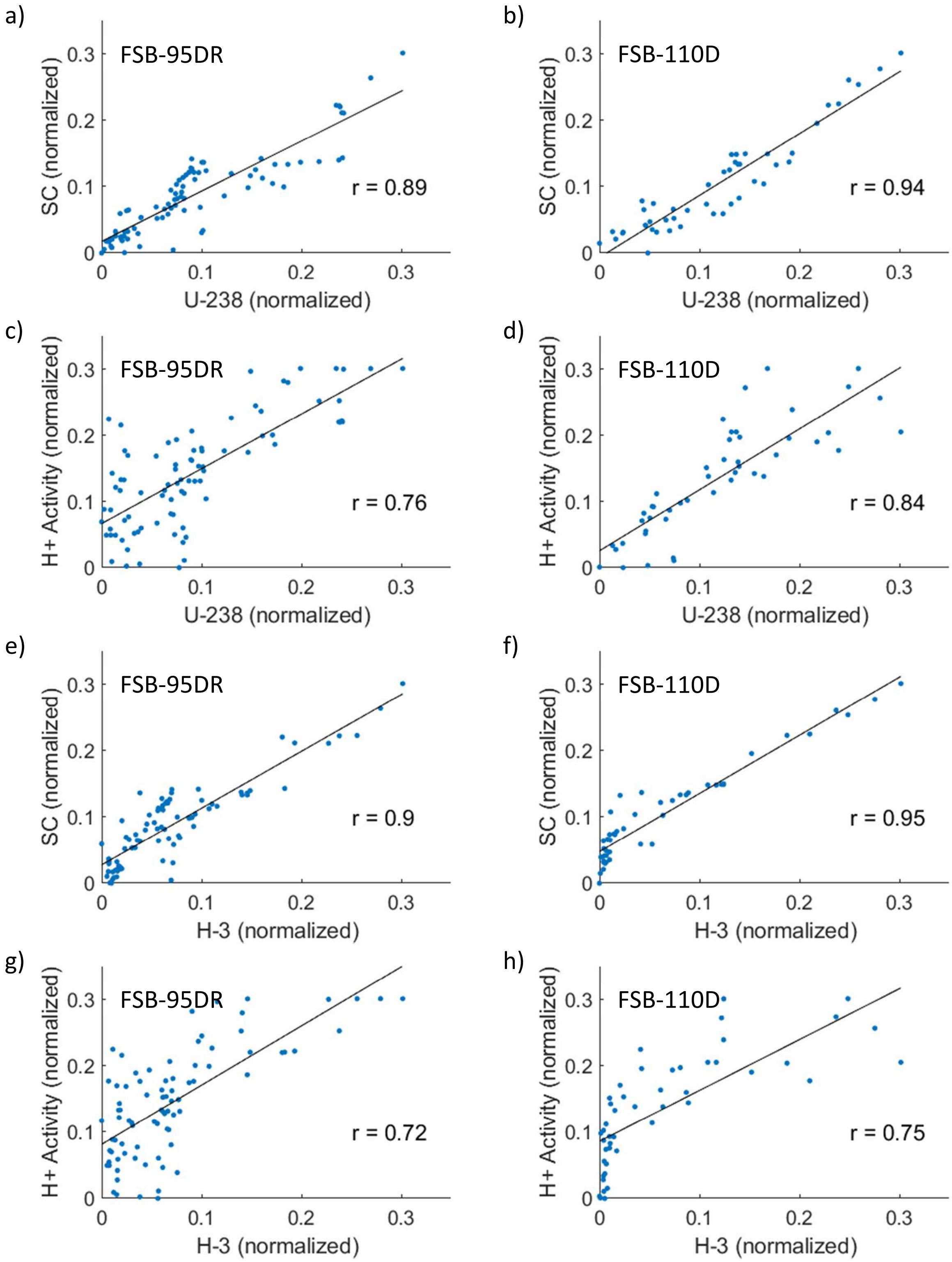


Figure S 2 – a) Scatterplots for the entire time series with first order fitted trend lines and Pearson's r for a) the SC and c) H^+ vs. U-238 at well FSB-95DR and well FSB-110D (b) and d), respectively). e) – h) The same plots with H-3 as the contaminant.

Figure S3

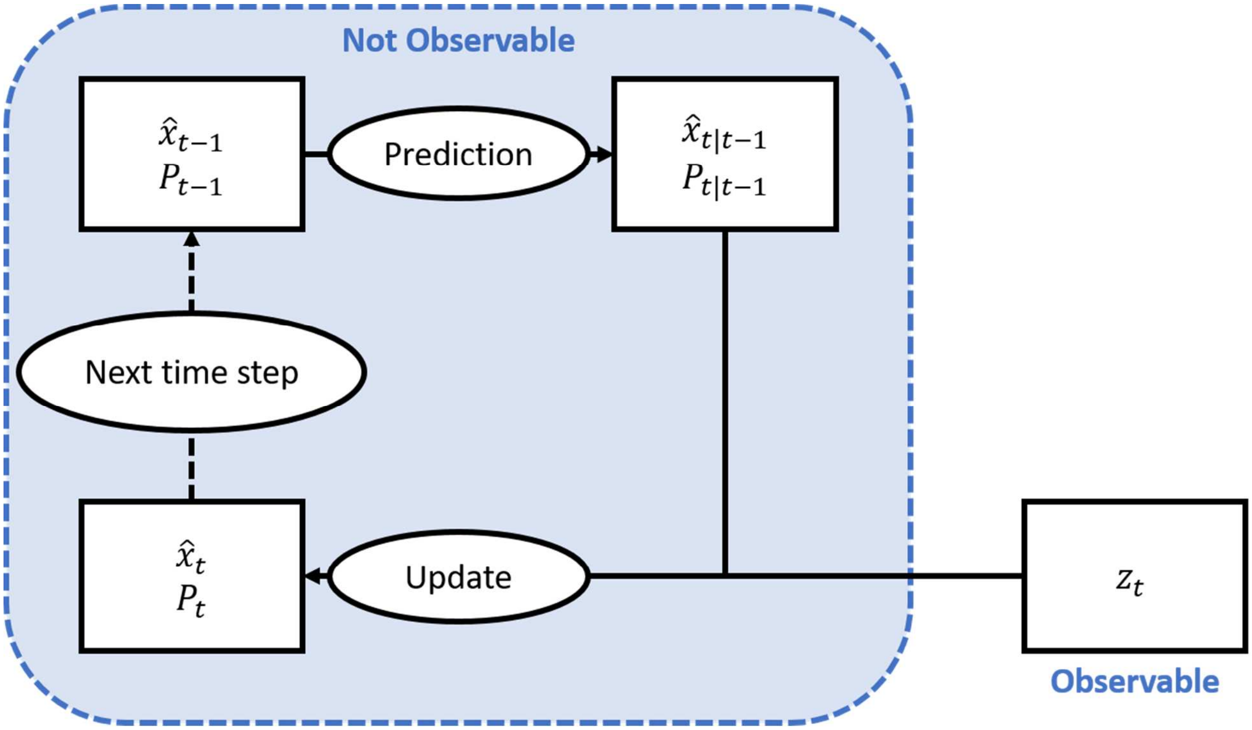


Figure S 3 – Kalman filter overview. The filter is recursive and repeats two steps: the prediction and the update step. It predicts the system state $\hat{x}_{t|t-1}$ based on the previous time step at $t-1$ and via the temporal evolution model. The predicted value is then updated based on external observations z_t. The resulting estimate is used as the basis for the next prediction.