Simulations and pre-experiment uncertainty analyses for a hydrogen diffusion experiment using a “two side purged membrane” setup

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Background and Objective
An experiment “Q-PETE” representative for the situation in the Helium Cooled Pebble Bed breeding zone and suitable for validation of relevant tritium transport codes is planned. In a temperature controlled setup a hydrogen loaded feed gas is directed over a steel membrane into which it can permeate. On the other side of the membrane a sweep gas flow collects the permeated hydrogen and transports it to a gas analysis (QMS) for quantitative time resolved detection.

Methods to handle time resolved permeation experiments with sweep gas, considering the residence time distribution of the sweep gas are introduced.

Issue
- The time resolved permeate flux signal over the membrane \( j_{Q}^{MS} (t) \) is of interest for code validation and material parameter (Diffusivity D, Sieverts constant \( K_{S} \)) determination
- The purge flow residence time distribution in the permeate chamber (PSC) and the piping effects a lag and a dispersion in the measurable concentration signal \( x_{QMS} (t) = j_{Q}^{MS} (t) / j_{SG} \)
- The difference between \( j_{Q}^{M} (t) \) and \( x_{QMS} (t) \) must be described!

Simulation methodology
- System response \( j_{Q}^{MS} (t) = j_{Q}^{M} (t) * g (t) = \int_{u=0}^{u=\infty} s (u) * g (t-u) du \)
- Impulse response function \( g (t) \) is residence time distribution
- Convolution integral \( j_{Q}^{M} (t) * g (t) \) is numerically solved
- Further model for QMS sampling and noise applied

Complete system signal simulation (prediction) implemented.

Uncertainty estimation
- As figure of merit, propagated uncertainties to D and \( K_{S} \) are estimated for a simplified analytic evaluation method.
  \[ (1) \; D \approx 0.16877 \cdot \frac{w_{M}^{2}}{\Delta \tau}, \quad (2) \; \phi = D \; K_{S} = \frac{2 \; w_{M}^{2}}{\lambda_{M}} \cdot \frac{x_{QMS} (t=t_{0})}{j_{SG}} \]
- Experimental setpoints can be optimized. For example: large flow rate and/or large membrane thickness: good time resolution but low signal level (and vice versa).

The residence time distribution in the permeation setup volume before the analysis station has significant effect and can be predicted by appropriate methods.

Experimental uncertainties of ~ 15% for the derived Sieverts constant for breeder zone typical conditions are expected for the Q-PETE purged permeation experiments.