

Following profiles in subcritical water: the deconvolution work-around

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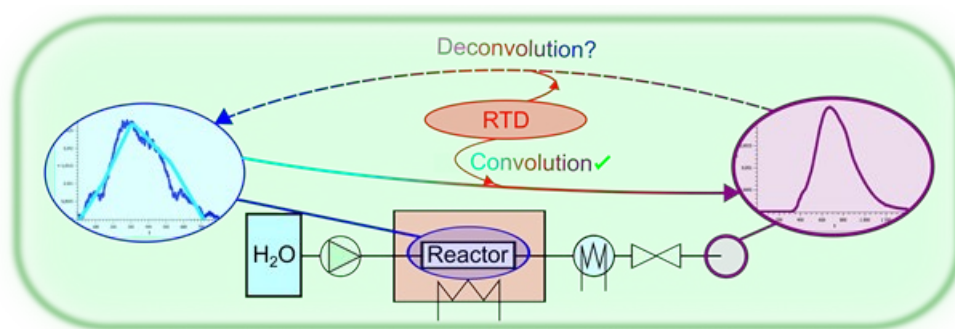


Figure 1: Prediction of a concentration profile in a subcritical reactor from end-of-pipe measurements by deconvolution.

Monitoring a process, especially a reaction's progress, is rarely an easy task in high-pressure vessels, even more so in subcritical water. The hydrothermal environment limits the range of applicable optical analytic methods, while the highly laminar nature of the flow in a micro-flow reactor renders most kinds of probe-based measurement methods unreliable, due to the high level of inhomogeneity in the reactor volume. It is an option to measure the flow at the end of piping, however, relating the results to the conditions in the reactor is not trivial. While it is relatively

simple to calculate end-of-pipe profiles of concentration from known reactor profiles with convolution when the retention-time distribution (RTD) is known, reversing this operation is rather difficult. The inverse, deconvolution, does not even have a direct mathematical definition[1], much less a well-established optimal algorithm of computation, although some algorithms exist for special applications.

In our work, we propose a deconvolution algorithm based on simulated annealing, implemented in Python utilizing solely open-source packages. To test the method's predictive capabilities, we conducted measurements on a reactor system used primarily for semi-continuous hydrothermal liquefaction experiments. The reactor system is operated with subcritical water at 265-285°C at 10 MPa, to simulate typical conditions for hydrothermal processes. Multiple reaction profiles were emulated by introducing NaCl as a tracer at the inlet of the reactor, and conductivity was measured at the pipe outlet at ambient conditions. After obtaining the RTD of the system at the operating conditions by deconvolution, experiments to assess predictive capabilities were conducted, the graphical summary of which is represented in Fig. 1. New, known profiles were introduced (light blue), and the end-of-pipe conductivity profile (purple) was recorded. After sufficient data transformation (normalization, smoothing), the proposed algorithm was used to approximate the profile in the reactor using the previously determined RTD (the result represented by the dark blue graph). The evaluation of predictive power was assessed by comparison with the known reactor profile.

The results suggest that the algorithm, while computationally moderately expensive, provided a reasonable estimation of the reactor profile, even in a subcritical system, where the effect of multiple segments, mixing of flows and high temperature and density gradients complicate system dynamics, and introduce significant non-linearity. Additionally, using box-like finite-length disturbance to obtain experimental RTD improves predictive power significantly compared to calculating with RTD obtained by impulse-like disturbance. This work was supported by the ÚNKP-23-2-I-BME-256 New National Excellence Program of the Ministry for Culture and Innovation from the source of the National Research, Development and Innovation Fund.

References

- [1] S. M. Riad, *Proc. IEEE* **1986**, 74, DOI: 10.1109/PROC.1986.13407



**20th European Meeting on
Supercritical Fluids**
Maribor, Slovenia, May 26 - 29, 2024

To the Attention of
Mihály Hegyi
University of Budapest
Hungary

May 29, 2024

Subject: certificate of attendance

Dear Mihály Hegyi,

I am pleased to confirm that you attended the **20th European Meeting on Supercritical Fluids (EMS F 2024)** **joint event with High Pressure Working Party** from 26th to 29th to May 2024, in Maribor, Slovenia, and presented a poster entitled:

“Following profiles in subcritical water: the deconvolution work-around“

This meeting was chaired by Željko Knez and co-organized with ISASF (International Society for the Advancement of Supercritical Fluids) and Working party High-Pressure Process Technology. The objective of the meeting was to gather all the members of the supercritical fluid community and to give the opportunity to academic researchers and industrial practitioners to provide a complete and critical update on all the current technologies using Supercritical Fluids, their different applications as well as the latest innovations being developed.

Yours sincerely,

Željko Knez

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