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TRAJECTORY-BASED STUDY AND VISUALIZATION OF COHERENT FLOW STRUCTURES IN CHEMICAL REACTORS

Introduction

Understanding fluid transport and mixing in chemical reactors is crucial to avoid dead zones and control concentration heterogeneities. From a Lagrangian perspective, coherent flow structures are key. Recent computational methods can identify finite-time coherent sets directly from fluid particle trajectories, obtained through numerical simulations or experiments like 4D-PTV or Lagrangian sensors.

In this contribution, we demonstrate the application of different trajectory-based approaches for the identification of coherent flow structures in stirred tank reactors. For this purpose, several recently proposed methods, such as spectral clustering of trajectories [1,2] or single-trajectory diagnostics [3] are used and adapted for these kinds of data.

Trajectory data

For our studies, we use trajectory data from a Lattice-Boltzmann simulation [4] (Fig. 1) and from Lagrangian 4D-PTV measurements (Fig. 2 and Fig. 3), both of a 2.8L stirred tank reactor.

- We assume to be given N tracer trajectories $(x_i(t))$ with $i = 1,\dots,N$, $t \in T$. $x_i(t)$ represents position of i-th tracer at time t.
- Set $T = \{t_0,\dots,t_T\}$ contains all discrete time instances of the simulation or experiment, respectively.
- $t_T - t_0$ corresponds to three stirrer rotations

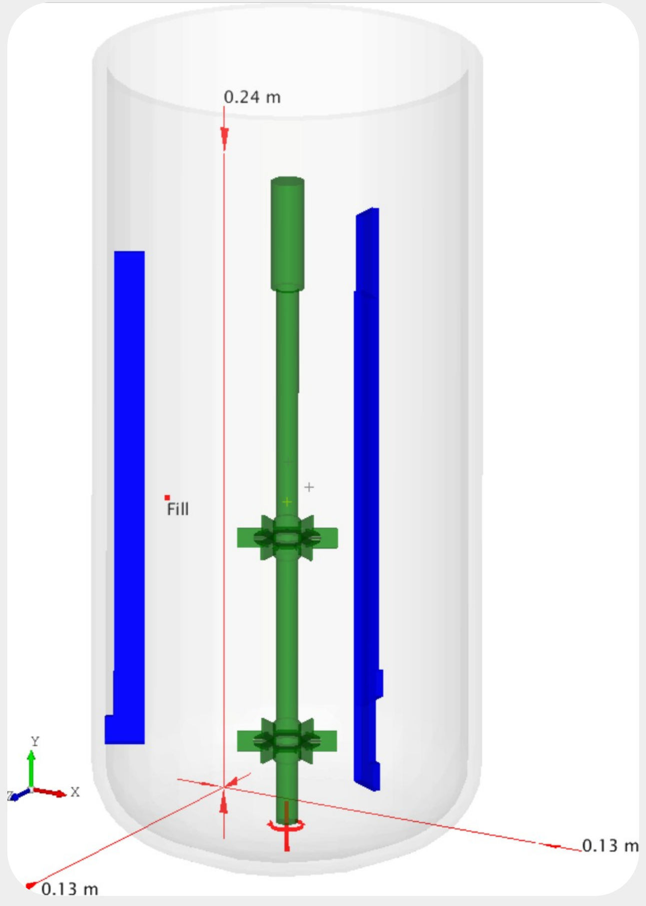

Fig. 1: Geometry of the simulated 2.8L stirred tank reactor with two turbines (green) and three baffles (blue). Fluid: Water 20° Celcius

Fig. 2: Experimental setup for 4D-PTV measurements within 2.8L stirred tank reactor made of acrylic glass. Fluid: Water 20° Celcius

Coherent compartments

Data driven computation of coherent structures, or dynamic regions not mixing well with surrounding fluid, relies on weighted distance matrices [1].

For each time slice t, we compute the instantaneous kernel matrix $K(t)$ with entries

$$k_{ij}(t) = k_\epsilon(\mathbf{x}_i(t),\mathbf{x}_j(t)) = e^{\frac{-\|\mathbf{x}_i(t)-\mathbf{x}_j(t)\|_2^2}{\epsilon^2}}$$

$$\text{with} \quad \|\mathbf{x}_i(t)-\mathbf{x}_j(t)\|_2^2 \le r_\epsilon$$

where r_ϵ is a cut-off and ε is a scaling parameter. The stochastic transition matrix $P(t)$ is obtained from $K(t)$ by row-normalization. We form the time averaged matrix

$$Q_T = \frac{1}{|T|}\sum_{t\in T} P(t),$$

which encodes the spatiotemporal distances between tracer trajectories. Q_T serves as an input for a standard spectral clustering method [5], combined with classification based on a sparse eigenbasis approach (SEBA) [2].

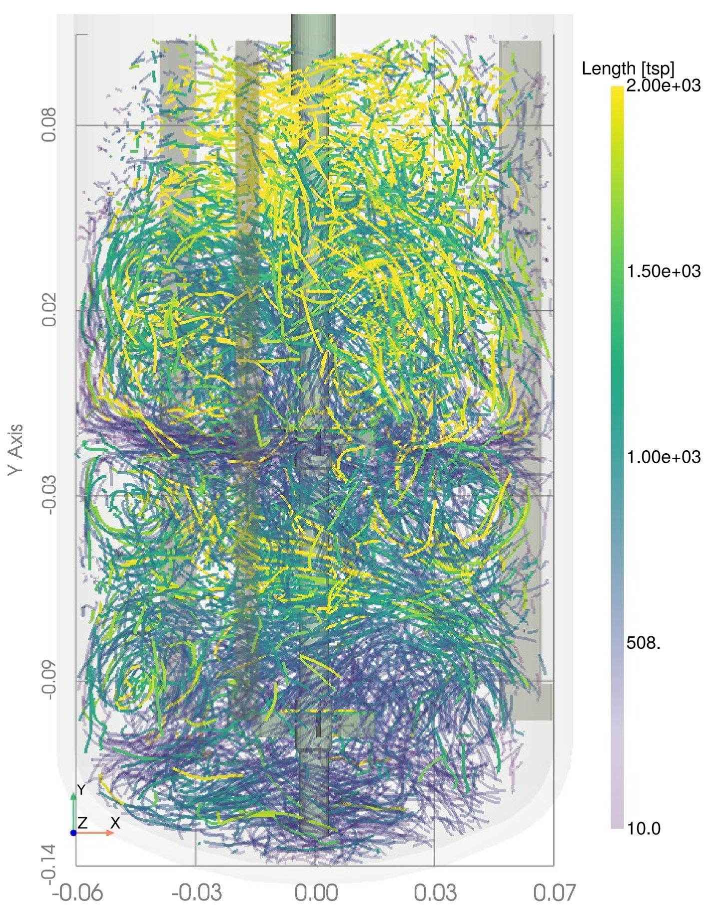

Fig. 3: Experimental trajectory data colored by track length

Resulting clusters correspond to coherent compartments in the stirred tank reactor, both from simulated and experimental data (Fig. 4).

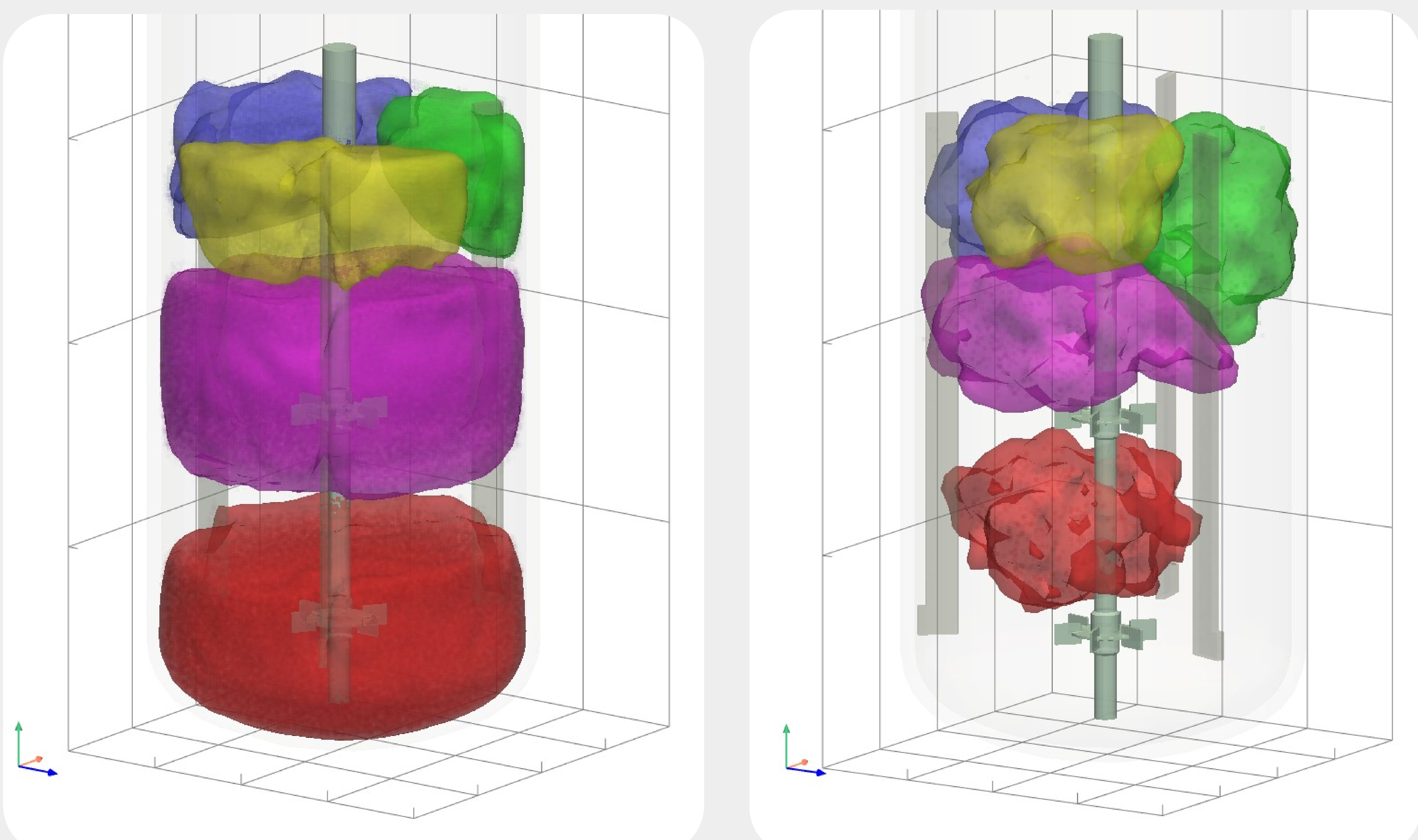

Fig. 4: Five compartments determined via spectral clustering (colored accordingly), from simulated data (left) and experimental data (right)

Vortical structures

To study and visualize smaller flow structures, we apply recently proposed single trajectory diagnostics.

We approximate instantaneous velocities via

$$\dot{x}_i(t_k) \approx \frac{x_i(t_{k+1}) - x_i(t_k)}{t_{k+1} - t_k}$$

The total rotation angle (TRA) [3] is defined as:

$$\overline{TRA}_{t_0}^{t_T}(\mathbf{x}_i) = \frac{1}{t_T - t_0}\sum_{k=0}^{T-1} \cos^{-1}\frac{\langle \dot{\mathbf{x}}_i(t_k), \dot{\mathbf{x}}_i(t_{k+1})\rangle}{|\dot{\mathbf{x}}_i(t_k)|\,|\dot{\mathbf{x}}_i(t_{k+1})|}$$

Trajectories with large TRA can be related to vortical structures (Fig. 5 and Fig. 6).

These vortices might be partly responsible for faster mass transfer between compartments.

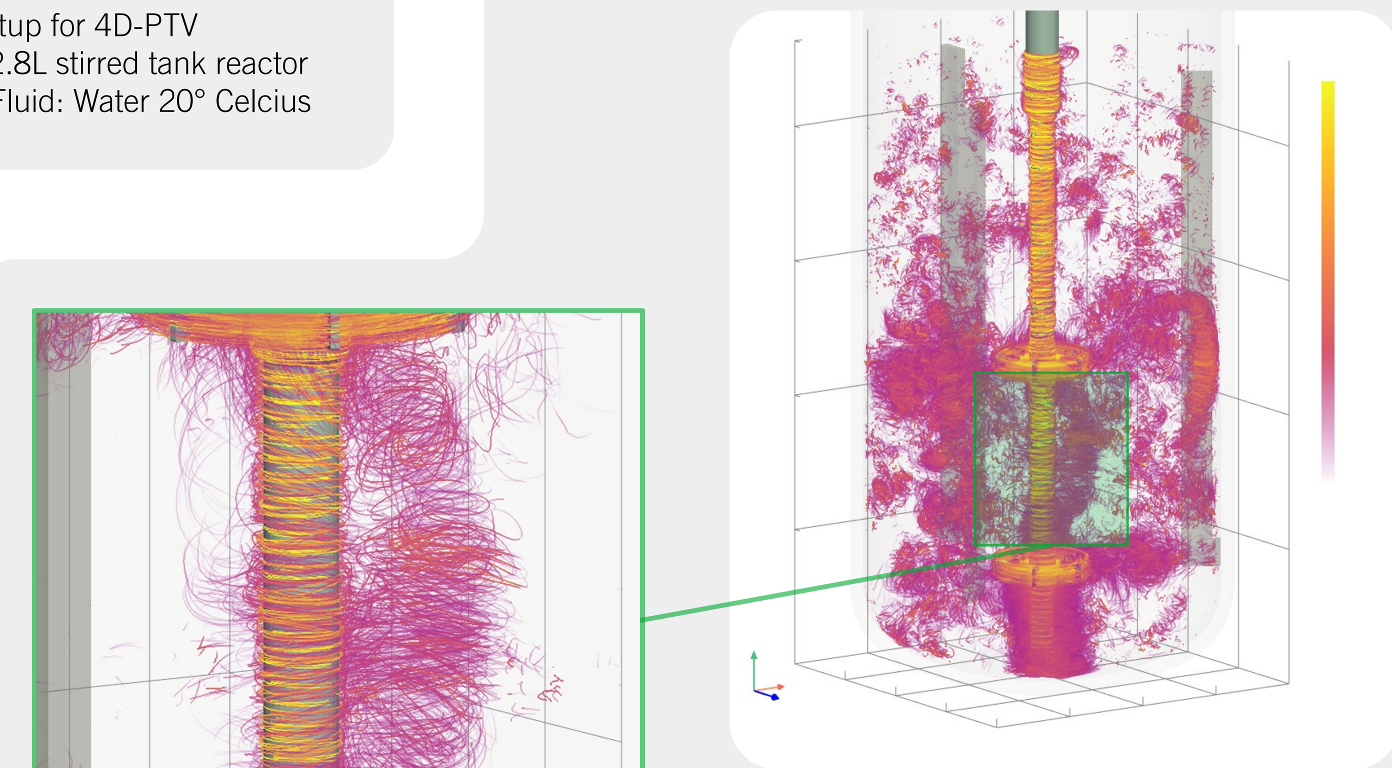

Fig. 5: Simulated trajectories with large TRA

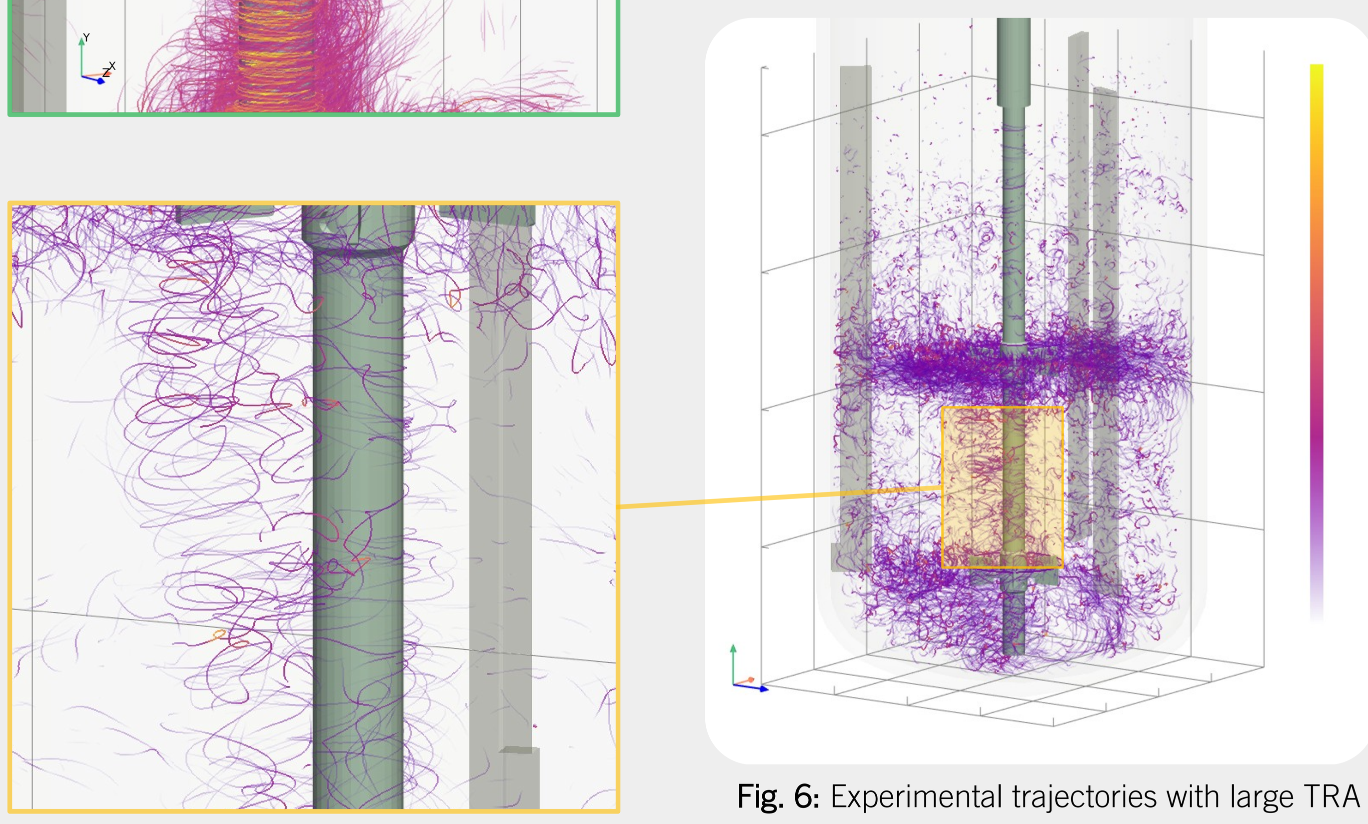

Fig. 6: Experimental trajectories with large TRA

Conclusion and outlook

Numerical simulations usually provide complete and clean data, but experimental data are often subject to perturbations and missing records.

Still we found good correspondence between flow structures in simulations and experiments. Further analysis and quantification of transport and mixing is subject to ongoing research.

As an outlook, to fill the gaps of incomplete data appropriately, methods such as fitting interpolations or machine learning need to be further explored and utilized.

Our overarching goal is to identify coherent structures in real time from sparse observations in chemical reactors.

Acknowledgment

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