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TRAJECTORY BASED ANALYSIS AND VISUALIZATION OF COHERENT FLOW STRUCTURES IN STIRRED TANK REACTORS

Introduction

The analysis and quantification of fluid transport and mixing in chemical reactors is of great interest in order to avoid dead zones and to control heterogeneities in concentration distributions. From a Lagrangian perspective, coherent flow structures play a central role in this context. In the past few years, different computational methods have been developed to identify such finite-time coherent sets directly from trajectories of fluid particles. Such type of trajectory data is obtained via numerical simulations or lab experiments (e.g. by time-resolved particle tracking (4D-PTV) or by 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] have been implemented in Python to improve performance and facilitate embedding.

Trajectory data

For our studies, we use trajectory data from a Lattice-Boltzmann simulation of a 2.8L stirred tank reactor [4] (Fig. 1).

In the following, we assume to be given N tracer trajectories $(x_i(t))$ with $i = 1,\dots,N$ and $t \in T$. $x_i(t)$ represents the position of the i-th tracer at time t.

The set $T = \{t_0,\dots,t_T\}$ contains all discrete time instances of the simulation.

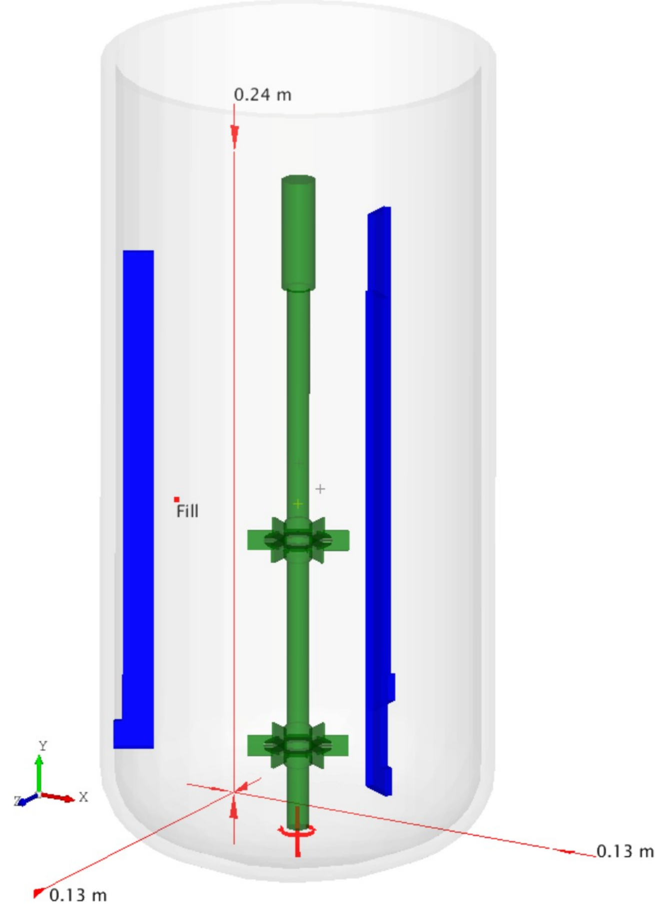

Fig. 1: Geometry of the simulated 2.8L stirred tank reactor with two turbines (green) and three baffles (blue). Fluid: Water 20° Celcius.

Coherent structures

The following trajectory data is based on three rotations of the turbines. The data driven computation of coherent structures, dynamic regions that do not mix well with the surrounding fluid, relies on weighted distance matrices [1]. For each time slice t, we compute the instantaneous kernel matrix $K(t)$ with entries

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

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.

Finally, 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]. The resulting clusters correspond to coherent compartments in the stirred tank reactor (see Fig. 2 for visualization).

Transition probabilities between compartments can be represented in a Markov Chain graph (Fig. 3) to study and quantify an approximate material transfer.

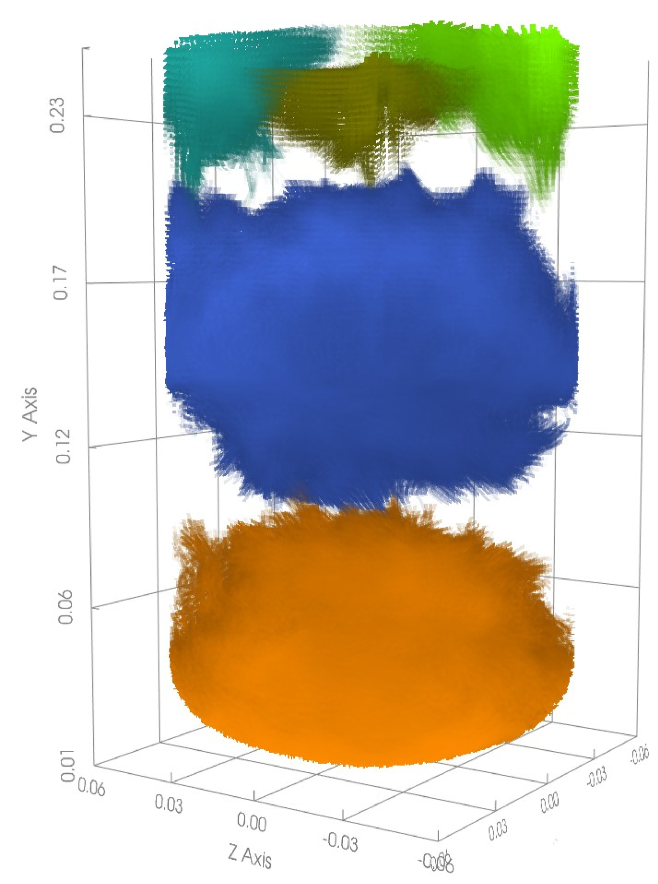

Fig. 2: Five compartments are determined via spectral clustering, which are colored accordingly.

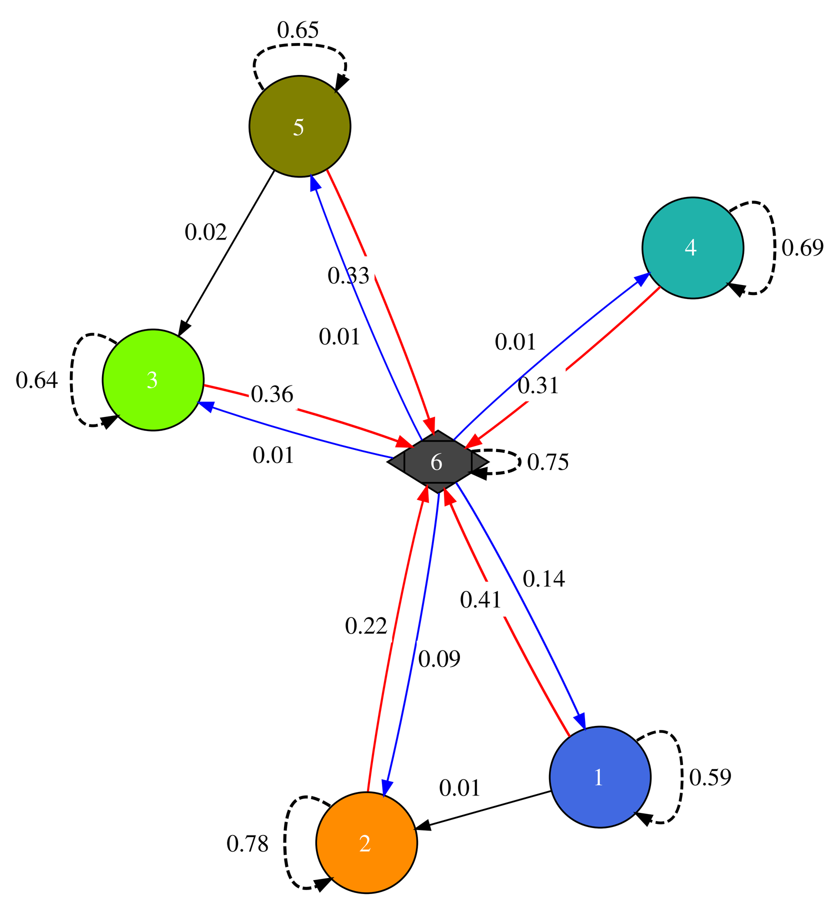

Fig. 3: A Markov Chain representation of the compartments in Fig.2. The 6th compartment corresponds to the incoherent background.

Visual discoveries within trajectory data

Visualization is crucial to gain a better understanding of the flow behavior.

By highlighting trajectories with particularly large modulus of the velocities

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

we already observe vortex-like structures, which appear to connect coherent compartments (Fig. 4). This becomes even more clear when considering the absolute acceleration (Fig. 5).

Finally, we use a recently proposed single trajectory diagnostics, the total rotation angle (TRA) [3] (Fig. 6):

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

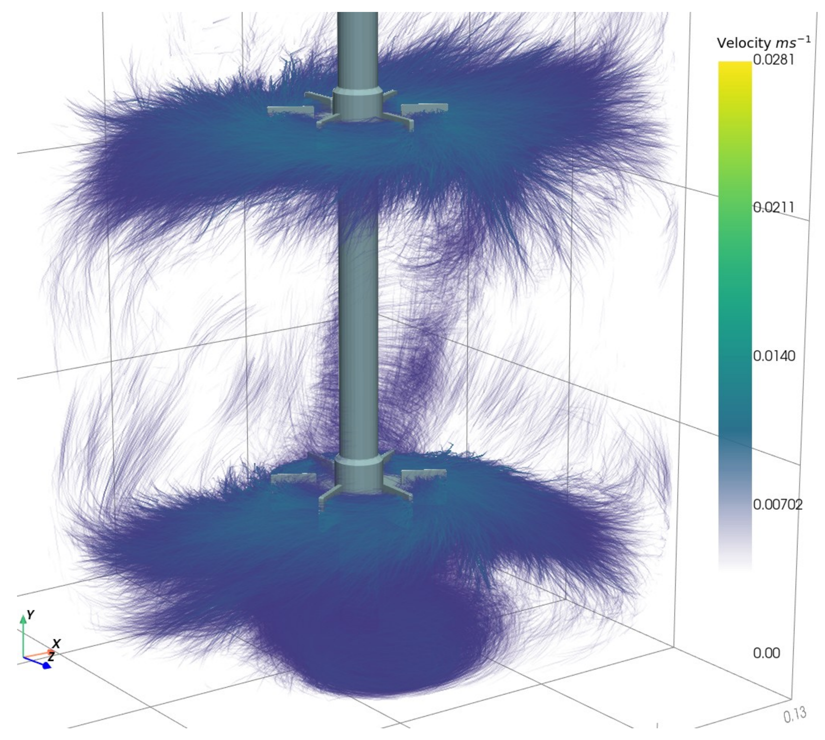

Fig. 4: Velocity visualized in trajectory data

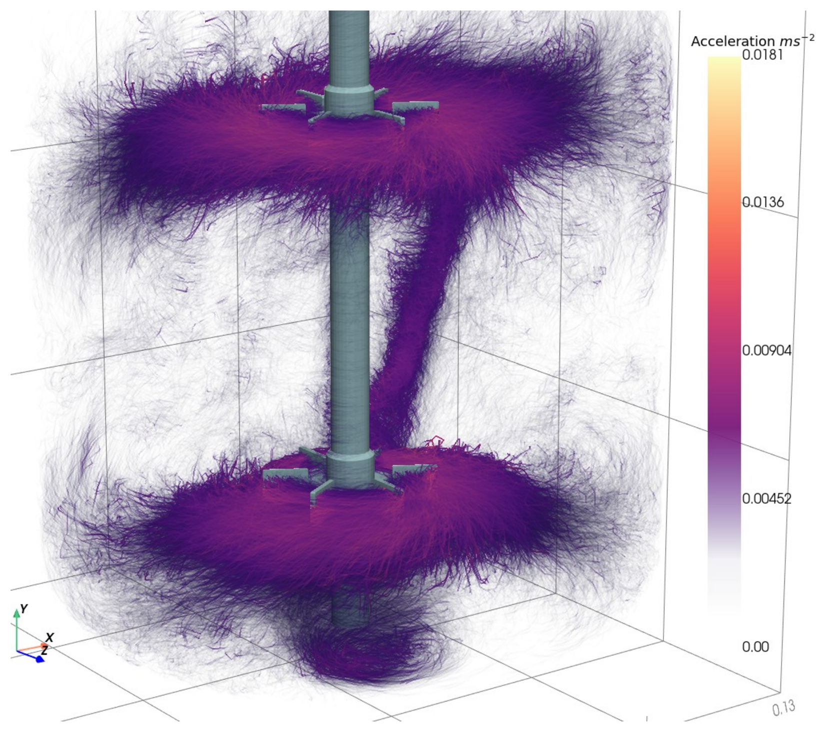

Fig. 5: Acceleration visualized in trajectory data.

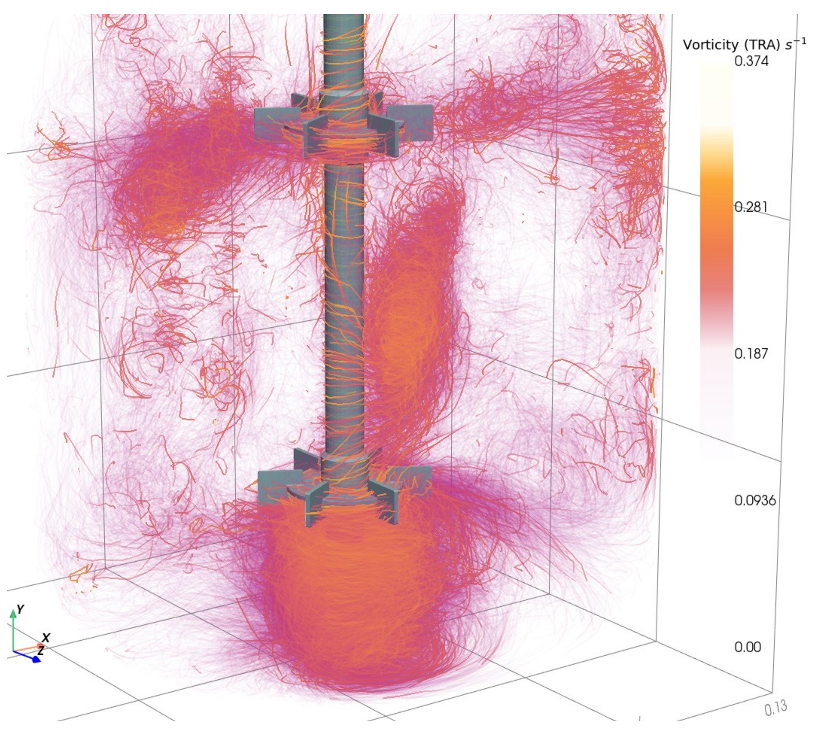

Fig. 6: Angular velocity visualized in trajectory data.

We assume that these vortices might be partly responsible for a faster mass transfer between compartments. They might also influence the shape-changing behavior of all the compartments. This is subject to ongoing research.

Outlook

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

In case of optical recordings, shadows or suboptimal lightning can result in missing and thus sparse trajectory data.

As an outlook, to fill the gaps of missing trajectories 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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