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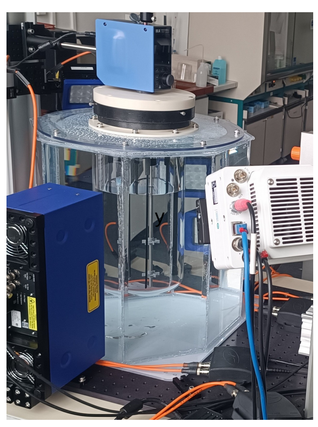
TRAJECTORY-BASED STUDY AND VISUALIZATION OF COHERENT FLOW STRUCTURES IN CHEMICAL REACTORS

Introduction and motivation

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, experiments like 4D-PTV, or Lagrangian sensors.

In this contribution, we demonstrate the application of a trajectory-based approaches for identifying coherent flow structures in a stirred tank reactor from simulation and experiment. For this purpose, recently proposed methods, such as spectral clustering of trajectories [1] are used and adapted for these kinds of data.



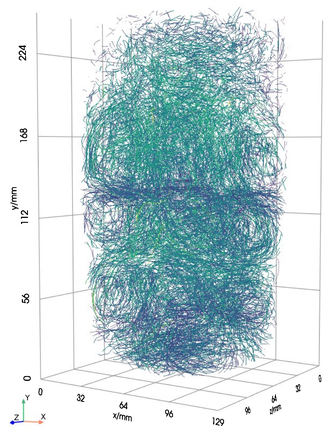


Fig. 1: Trajectory data extracted from experimental 4D-PTV measurements (left), experimental setup for 4D-PTV measurements within 2.8L stirred tank reactor made of acrylic glass (right). Fluid: Water 20° Celsius

Data in use

For our studies, we use trajectory data from two different sources but with the same setup for comparison. The stirrer rotation speed is set to 252 rpm in both cases.

Experimental data (Fig. 1)

- Lagrangian 4D-PTV measurements
- Time span ~ 4.0 sec or 2000 frames (120 frames per rotation)
- 290.000+ tracks with 7518 ± 6 particles per frame

Simulated data [4] (Fig. 2)

- Lattice-Boltzmann simulations
- Time span ~ 2.4 sec or 239 frames (24 frames per rotation)
- 355.000+ (usable) particles per frame

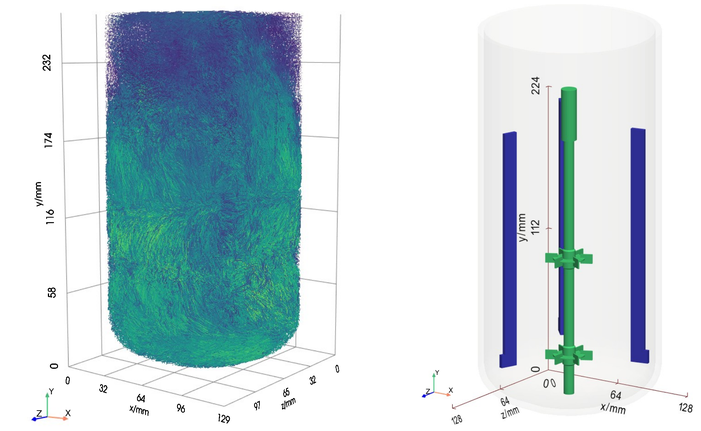


Fig. 2: Trajectory data extracted from Lattice-Boltzmann simulation (left), geometric setup for Lattice-Boltzmann simulation within 2.8L stirred tank reactor (right). Fluid: Water 20° Celsius

Data settings

For our studies, we use the following trajectory data extracted from Lattice-Boltzmann simulations and from Lagrangian 4D-PTV measurements

- N Lagrangian tracer trajectories
  $x_i(t) \in \mathbb{R}^3$ with $t \in T$, $i = 1,\ldots,N$
- $x_i(t)$ represents position of i-th tracer at time t
- Set $T = \{t_0,\ldots,t_T\}$ contains all discrete time instances of the simulation or experiment, respectively
- $t_T - t_0$ corresponds to one single stirrer rotation

Coherent compartments from network method

Data driven computation of coherent structures, or dynamic regions not mixing well with surrounding fluid, relies on weighted distance matrices [2].

We set up a network with trajectories corresponding to nodes and links weighted according to trajectory closeness or similarity.

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

$$k_{ij}(t) = k_\epsilon(x_i(t), x_j(t)) = \exp\left(-\frac{\|x_i(t) - x_j(t)\|_2^2}{\epsilon}\right)$$

with ε as scaling parameter. Here, only a certain number of nearest neighbors are considered for each $x_i(t)$ to ensure sparsity.

A transition matrix $P(t)$ is obtained from $K(t)$ by symmetric normalization

$$P(t) = D(t)^{-1/2} K(t) D(t)^{-1/2} \quad \text{where} \quad d_i(t) = \sum_{j=1}^{n} k_{ij}(t)$$

and the degree matrix $D(t)$ is a diagonal matrix with $d_1,\ldots,d_n$ on the diagonal. This defines a Markov process for that time slice.

$P(t)$ is then summed over T and row-normalized.

$$Q_T = \hat{D}^{-1} \hat{Q}_T \quad \text{with} \quad \hat{Q}_T = \sum_{t \in T} P(t) \quad \text{and} \quad \hat{d}_i(t) = \sum_{j=1}^{n} \hat{q}_{ij}(t)$$

The degree matrix $\hat{D}(t)$ is the diagonal matrix with $\hat{d}_1,\ldots,\hat{d}_n$ on the diagonal. Q_T encodes the spatio-temporal closeness of tracer trajectories over T and then serves as an input for a standard spectral clustering method [4], followed by a classification based on Sparse EigenBasis Approximation (SEBA) [3].

With eigengap heuristic [6], five clusters were chosen in this study. To obtain transport and mixing statistics for particles within each cluster, evolutionary clustering [1] over three stirrer rotations was conducted.

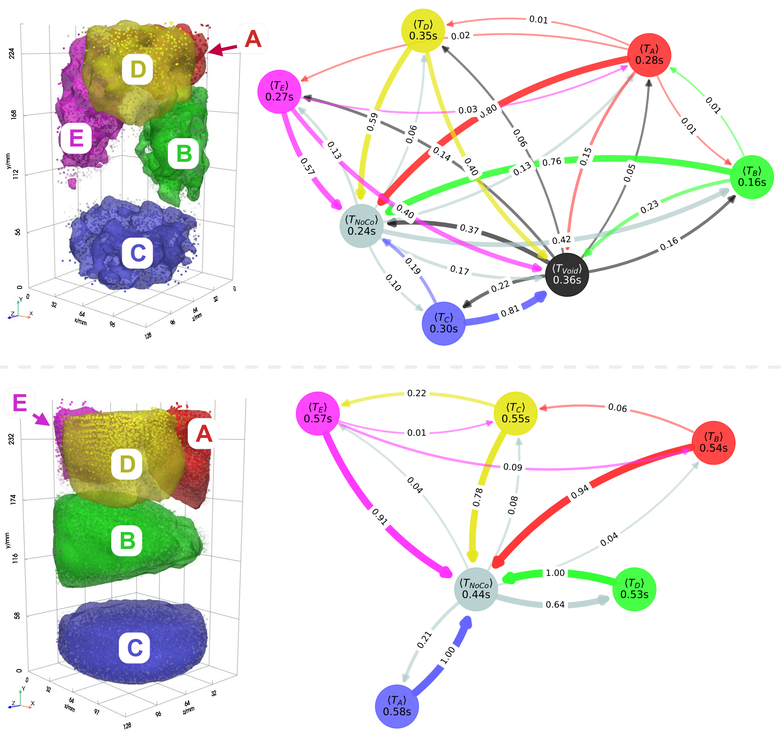


Fig. 3: Five compartments determined via spectral clustering (colored accordingly), from experimental data (left), corresponding graph network representing transport and holding times for three stirrer rotations (0.72s) (right)

Fig. 4: Five compartments determined via spectral clustering (colored accordingly), from simulated data (left), corresponding graph network representing transport and holding times for three stirrer rotations (0.72s) (right)

Results

Fig. 3 shows the position of each of the five compartments within the experimental STR, denoted with letters A to E. Similarly, **Fig. 4** also shows the extracted compartments, but from simulated data.

Furthermore, the corresponding graphs show the probability of transition of material between compartments on the edges. Each node is labeled with the average holding time, which is the time each particle spends within the corresponding cluster. In both cases for three stirrer rotations (0.72s).

Void in experimental data indicates particles completely absent in that time.

To show that those compartments can mitigate transport and mixing, we modeled advective-diffusive mixing from experimental particle tracks in silico [2,7]. Every particle has an initial value $c \in [0,1]$, representing coloring or scalar quantity.

The color vector is propagated in time, using the matrices P(t) and plotted at the respective particle positions.

Here, we focus on the relative coverage during the mixing process, where any value larger than zero counts as colored. As expected, mixing is slower if initial coloring is mostly in coherent structure areas (**Fig. 5** & **Fig. 6**).

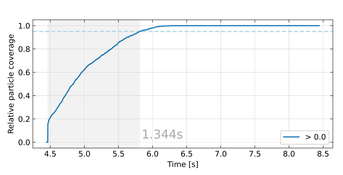
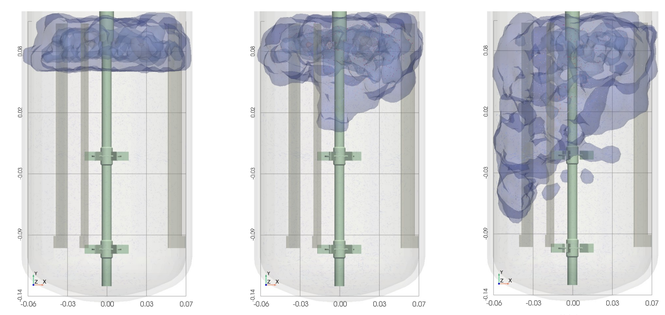


Fig. 5: Mixing of scalar field, initialized at relative height of 0.85 to 1.0 of reactor height. Distribution at 4.5s, 6.5s and 8.5s (right), relative particle coverage over time (above)



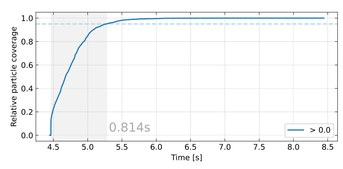
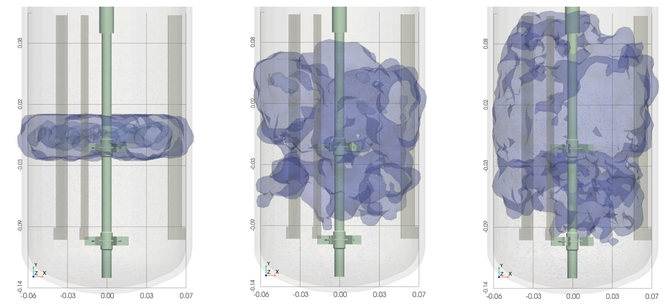


Fig. 6: Mixing of scalar field, initialized at relative height of 0.5 to 0.6 of reactor height. Distribution at 4.5s, 6.5s and 8.5s (right), relative particle coverage over time (above)



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.

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