Fluid Dynamics Seminar

Date: Wednesday, December, 6, 2017 at 13:00
Location: ZARM, Room 1730

Direct numerical simulation of the mixing process underlying liquid antisolvent precipitation

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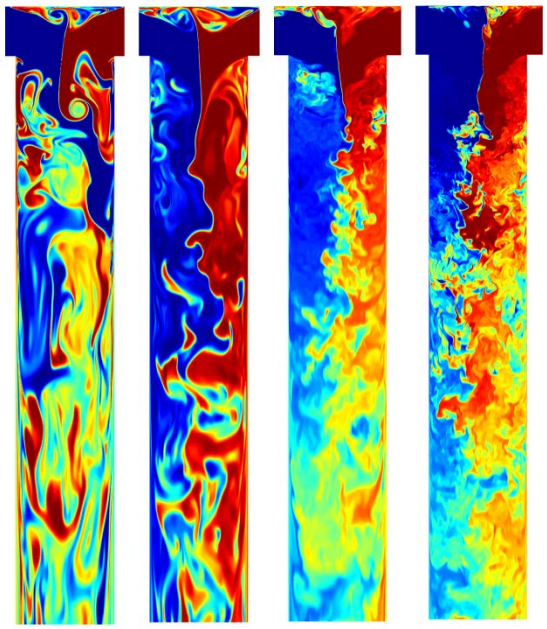

Recent estimates indicate that up to 40% of newly developed drugs are poorly water soluble, and the trend is steadily increasing. An old and fundamental, but not well understood, manufacturing process has attracted the attention of pharmaceutical industry in the recent years, namely liquid antisolvent precipitation. The drug is initially dissolved in a solvent like ethanol, which is then mixed with an antisolvent like water. In the mixing region, a thermodynamic imbalance (supersaturation) arises as water and ethanol tend to mix but the dissolved drug with water not which causes the drug to precipitate forming nanoparticles. The specific surface area of the nanoparticles determines the bioavailability of the drug in the human body, and hence the pharmaceutical industry aims to produce monodisperse particle distributions of the smallest possible sizes. The size of the nanoparticles is determined by the local supersaturation level, which in turn depends strongly on the local mixing efficiency. Hence a detailed understanding of the flow phenomena is required to control and improve the particle nucleation and formation. A promising approach to understand the fundamentals of the mixing of water-ethanol flows is direct numerical simulation.

In this seminar, I will discuss the ongoing mixing phenomena induced by inherent flow structures in a T-mixer. The Reynolds number regime considered spans from Re=100 up to real operating condition (at about 4000). This state is achieved when the mean particle size reaches an almost asymptotic value with an increasing energy input. Similarities and differences between water-water and water-ethanol mixtures will be addressed. A theoretical perspective on the arising turbulence beyond Re>600 will be given. Not forgetting to draw a comparison to experimental outcome.