Process Engineering

Bubble column reactors, Separation in hydrocyclones, Surface reaction in catalytic pollutant converters, Nanoparticles precipitation in impinging jet reactors
Process Engineering

Flow processes in chemical and process engineering are target application areas of our engineers. The modelling framework employed is packaged in the form of a tractable workflow concept for chemically-reacting, multiphase flow processes, based on TransAT’s extended modelling capabilities for multiphase flows involving complex rheology, with fast or infinite chemical reactions.

Chemical Vapor Deposition (CVD) Reactors

CVD is a chemical process used to produce high quality, high-performance, solid materials. The process is often used in the semiconductor industry to produce thin films. In typical CVD, the wafer (substrate) is exposed to one or more volatile precursors, which react and/or decompose on the surface to produce the desired deposit. CMFD coupled with the appropriate chemical reaction models is used to model various CVD processes.

Fluidized Bed Process Intensification (FBPI)

Practical objectives of FBPI include improving heat and mass transfer between gas & solids, fluidize smaller particles, increase gas-solid slip velocity, reduce gas-solid contact time, and increase ratio freeboard surface to bed height. CMFD simulations help assess the selected intensification mechanisms, thus adding value to the design of increased fluidization gas flow rate, increased flexibility with respect to cooling or heating, increased gas-solid heat and mass transfer coefficients, and improved particle bed temperature uniformity.

Flow partition in Gas-liquid Reactors

Accurate modelling of transient two-phase flow with chemical reaction and mass transfer at gas-liquid interfaces is a critical step in the design of chemical reactors. TransAT solutions can help quantifying flow and residence time in reactors, which is critical for reactor model up-scaling. The practical outcome of simulation includes process optimization, evaluation of different operating parameters, and define the optimal dimensioning of the reactor for plant scaling.

Polymerization Reactors

Polymerization reactions are strongly influenced by temperature variations and non-uniform residence time. Flow properties may change dramatically due to polymerization and thus process parameters (mixing, heat transfer). Polymerization processes are calculated and scaled up by assuming plug flow conditions in tubular reactors and ideally mixed conditions in batch reactors or by using simplified reactor cascade models. CMFD can be used for evaluating the effect of non-ideal reaction conditions in polymerization processes and scale-up.
Bubble Column Reactors

The most recurrent multiphase flow apparatus in process engineering is Bubble Column Reactors (BCR), where flow transients and multiplicity of the scales dictate the reactor performance. TransAT Suite offers a pallet of predictive models to help obtaining better, economically viable technologies for process intensification and optimization. The overall workflow built around TransAT offers technical valuable terms of operating parameters, working to replace empiricism-based trial-and-error by detailed flow hydrodynamics.

Surface Reaction in Catalytic Pollutant Converters (CPC)

Advanced CPC in automotive applications combine efficient pollutant conversion with a low pressure drop. Pore scale simulations in ceramics-foams CPC have been used to characterize pressure drop, heat and mass transfer. Combining the strength of IST/BMR meshing with advanced models, TransAT Multiphysics is capable of modelling catalytic reactors with micro-kinetics considering coupled heat and mass transfer.

Separation of Dispersed Fluid Systems in Hydrocyclones

Hydrocyclones provide an efficient way of removing solid particles from various slurries (sands out of water). Hydrocyclones can also be used to separate dispersed oil-water systems in the petrochemical industry, and as such they involve droplet-droplet interaction mechanisms. TransAT provides coupled solutions involving population balance* for the droplets cloud including droplet breakup and coalescence*, describing the impact on separation processes.

Nanoparticles precipitation in Impinging Jet Reactors

Micromixers are employed in pharmaceutics, cosmetics, and other processes like dyes and pesticides. Impinging jet reactors employed for precipitation processes of micro- and nano-particles. Active principles and the polymer are dissolved in an organic solvent and then mixed with an anti-solvent. The faster the mixing process, the smaller and monodisperse the particles will be. TransAT simulations helped quantify the effects on mixing of inlet conditions.
EXCELLENCE IN MULTIPHASE FLOW SIMULATION

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