LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125, 9052 Gent, Belgium

Coach	**Supervisor(s)**	**Funding**
Ir. Klaus Jacobs	Prof. Dr. Ir. Joris Thybaut Dr. Ir. Soroush Zareghorbaei	e-CODUCT

Numerical strategies for modelling gas phase hydrodynamics in turbulent fluidized bed reactors

Aim

Modelling of gas velocity and species concentration axial profiles for a turbulent fluidized reactor considering variable gas velocity.

Justification

Fluidized bed reactors are widely used in industry due to their excellent performance in good fluid mixing, high heat transfer rates and low pressure drop. Typical applications range from fuel production (Fluid catalytic cracking) over polymerization (Ethylene and propylene) to solid material processing (Graphite purification). Reactions occurring in the gas phase, whether catalysed or not can induce a volume change (expansion or contraction) due to the change in the total number of moles involved as reactant and product, hence, affecting the hydrodynamic behaviour in the bed. If the volumetric flow changes across the bed, the linear gas velocity profile inside the bed also changes affecting residence times, influencing conversion and selectivity as well as the hydrodynamic stability of the bed as de-fluidization or solid entrainment could occur.
The most widely used reactor model for turbulent fluidized bed reactors is the Axially Dispersed Plug Flow Rector (ADPFR). Assuming constant gas velocity, the reactor model is shown in Eq.1. where C_i is the species concentration, t is the temporal dimension, z is the spatial dimension, D is the axial dispersion coefficient and R_i is the production rate of the species.

$$\frac{dC_i}{dt} = D\frac{d^2C_i}{dz^2} - u\frac{dC_i}{dz} + R_i \qquad (1)$$

At steady state operation, such a reactor model can be solved using the function *scipy.integrate.solve_bvp* in python or in dynamic operation using the *pdepe* tool in matlab. When the gas velocity is not constant Eq.1 should be replaced by Eq.2 and, as a result, the reactor model can no longer be solved by such routines. To the best of our knowledge, no easily accessible routine is available to solve such a reactor model. Consequently, manual numerical differentiation becomes a necessity.

$$\frac{dC_i}{dt} = D\frac{d^2C_i}{dz^2} - u\frac{dC_i}{dz} - C_i\frac{du}{dz} + R_i \qquad (2)$$

Numerical strategies reported in the literature for such a situation have focused mostly on a specific reaction and, as a result, they are difficult to be generalized. Due to the reasons mentioned above a thorough investigation of the possible numerical strategies as well as the solution of the numerical model for a system with multiple reactions for Eq. 2 will be done for the cases where the reactor is in steady and unsteady state operation and there volume change due to reaction.

Program

1. Literature review on fluidized bed modeling as well as numerical differentiation
2. Solution of Eq 1 using the available tools in the programming language of your choosing
3. Numerical discretization and solution of Eq 2. in the programming language of your choosing
4. Analysis of the solutions given by Eq. 1 and Eq 2.