Numerical analyses of fertiliser industrial-scale unit operations: ammonia synthesis, ammonia oxidation and droplet removal using computational fluid dynamics modelling with detailed reaction kinetics

Abstract

Despite the world's economy's constant growth, many fundamental problems remain unresolved. Undernourishment and food insecurity, now also intensified by global political instabilities and environmental issues, cause pressure on the fertiliser industry to increase its efficiency as much as possible. Existing industrial technologies have excellent potential for improvements since, due to their large-scale character, even minor upgrades can significantly benefit efficiency and reduce operational costs. Furthermore, modifying existing technologies is cheaper and faster than developing new ones, which is incredibly challenging for large-scale production lines. Computational fluid dynamics (CFD) have an excellent potential for supporting experimental work and design processes. Computing Navier-Stokes equations with proper turbulence models using the finite element method allows for simulating the flow field inside the investigated apparatus, which can be extended by adding energy and species transport models and implementing the reaction kinetics.

This thesis is focused on creating and applying CFD models of primary fertiliser industrial-scale unit operations: ammonia synthesis using the Haber-Bosch method and ammonia oxidation in the Ostwald process. The last section is dedicated to droplet removal through wave-plate mist eliminators, a vastly applied supporting process in many industries, including fertilisers. Every analysis contains detailed information about methodology, including geometry, computational setup, boundary conditions, process parameters and applied models such as porous zone or discrete phase modelling. The results include critical parameter fields and functions, including those unavailable to obtain through experimental methods such as reaction rates or particle deposition areas. Novel approaches to the CFD model applications, such as studying the influence of catalyst particle size within the catalytic bed or trajectories and deposition tracking of entrained catalyst particles due to the catalyst gauze degradation phenomenon, were used. The obtained CFD models were the basis of the proposed novel improvements of the considered systems, such as alternative geometries of catalyst beds, catalyst gauze and drainage channels.

The significant contribution of this work was made in cooperation with the Yara Technology and Projects – Technology (Yara International ASA) located in Porsgrunn, Norway, which granted access to geometrical and experimental data of the actual pilot plat ammonia synthesis converter, allowing to fully recreate this apparatus and process in the form of the CFD model including the modification the reaction kinetics to obtain a model with excellent accuracy. The obtained model was validated using two independent experimental runs, and it gave detailed insight into the process and further experimental research support, providing more control of the converter's geometry and process parameters. The company also offered overall support for the substantive correctness of this dissertation's research regarding ammonia synthesis and oxidation processes.

Keywords: ammonia synthesis, Haber-Bosch Process, ammonia oxidation, Ostwald Process, chemical reactor, wave-plate mist eliminators, droplet removal, computational fluid dynamics, catalyst gauze degradation, heterogeneous catalysis, catalytic bed, multiphase flows