Summary of the doctoral dissertation

The presented work deals with the issues of co-simulation of multi-physical CFD models in order to calibrate the NCM-9924 microcalorimeter model and to combine multi-phase models of the population balance of the oxidation of sewage sludge flocs in a tank reactor with a stirrer. Co-simulation with models described by FEM (Finite Element Method) or FVM (Finite Volume Method) is extremely rare, due to the complexity and complexity of CFD models described by different types of PDE (partial differential equations) and constantly developed tools "Software" for working with those models in co-simulation mode, which have their limitations. Often, these models require simplifications, but in numerical fluid mechanics, the modeled simplified phenomena are a source of uncertainty. This requires elimination of simplifications, which significantly increases the resources and the time of performing calculations in this type of simulation. Current "software" tools for co-simulating multi-physical CFD models, such as Simplorer, have their limitations and underdevelopment.

In the work, the multi-physical CFD model of the NCM-9924 microcalorimeter was calibrated using the sensitive parameter, which was the membrane thickness, based on experimental measurement data, using step input. The validation of the model was carried out for a calorimeter with a drop of distilled water and a drop of glycol, where these data showed good agreement with the experimental data. Based on CFD simulations using ANSYS Fluent it was also possible to analyze the sensitivity of the microcalorimeter. The liquid drop on the membrane also influenced the dynamic properties of the microcalorimeter setup in the initial time steps, where this information is critical in analyzing thermal rapid biochemical reactions. Each mounting of the aluminum can generated a different thickness of the silicone paste layer, unavailable for measurement, affecting the result of the experimental measurement. In this case, the model was extended and calibrated with the uncertain parameter of the thickness of the silicone layer for the sine signal using co-simulation. This type of calibration allowed for a wider range of model operation using the uncertain parameter. The cosimulation allowed to determine the appropriate thickness of an uncertain parameter, which is the thickness of the silicone layer, which cannot be measured experimentally. The possibility of combining CFD models with high computational cost and time with Simplorer allows for modeling phenomena that are not measurable in real time, supporting the work of the experimenter. The second multi-physical CFD model in which co-simulation was used is a stirred tank reactor, which used co-simulation to multiphase combining multi-physical models of the population balance of solid and gas phases. This allowed to study the influence of the interaction of both phases, where these phenomena are simplified in the literature, and also have an impact on the hydrodynamics of multiphysical phenomena or the efficiency of the process taking place.

The innovative method of co-simulation of multi-physical CFD models presented in the paper allows for an effective way of calibrating multi-physical models, combining population balance models, extending the multi-physics of phenomena in multi-phase systems, contributing to the minimization of the scope of laboratory tests necessary for process design. The work carried out allows to confirm the thesis about the possibility of co-simulating models with distributed parameters with the use of complicated software implementing the co-simulation process in the scope of software boundary conditions. The analysis and design of complex control systems requires the use of both cosimulation and efficient computer simulation software environments. The considered directions include the search for both testing and integration of new structures of co-simulation models using simulation environments for models with distributed parameters extended with new multi-physical phenomena.