

## **HEAT TRANSFER IN A PLAIN JACKET OF A PILOT SCALE STIRRED TANK REACTOR**

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### **ABSTRACT**

Recent literature on thermal runaway reaction research in vessels, such as that conducted by Rudniak et al. [2011], still assumes a constant jacket temperature. In this investigation, three-dimensional steady state CFD simulations are performed for the plain jacket of a pilot scale vessel, which predict that the jacket temperature can vary by tens of degrees Celsius across different parts of the jacket even in reactors under a third of a metre in diameter, and that the distribution of heat transfer coefficients is strongly dependent on the flow path. The CFD output values are compared with experimental data of temperature measurements and with the use of correlations to predict heat transfer coefficients from the experimental data.

The commercial code Ansys CFX Version 15 has been used to simulate the flow of the commercial heat transfer oil “DW-Therm” through a plain jacket of a pilot scale stirred tank reactor that is boiling water inside the vessel, to approximate a constant process temperature.

Industrially used correlations for overall heat transfer coefficients overlook large non-uniformity in the distribution of heat transfer coefficients in jackets that use a liquid heat transfer medium. Westerterp and Molga [2006] gathered sources estimating that about 30% to 45% of runaway reaction incidents have been attributed to either inadequate understanding of reaction kinetics and thermodynamics or inadequate temperature control.

Correlations for heat transfer in the jacket side, based on experimental work, were developed for laminar flow by Chen et al. [1946], and for turbulent flow a correlation found in Perry and Chilton [1973]. Bondy and Lippa [1983] and Dream [1999] use these equations as the basis of their correlations.

In this simulation of a jacket, correlations for boiling water on the process side use the Cooper [1984] method. Correlations for heat loss through the external wall use general formulae for natural convection in air, combined with an overall radiation coefficient for the external surface. These are combined with conduction through the glass walls (constructed from the material “borosilicate glass 3.3”) these external correlations provide the wall boundary conditions. The mass rate of the DW-Therm and its inlet and outlet temperature were measured during the experiment, providing information about the total heat transferred by the medium and the remaining boundary conditions for

the simulation. The CFX simulation produced values of total heat transferred by the jacket within 10% of the experimental results. These simulations use the  $k-\omega$  SST model [Menter, 1994] performed on a manual mesh constructed in ICEM using data on the geometry of the experimental reactor. Grid independence tests were conducted initially to ensure consistency with the results of finer meshes. The experiments and CFD simulations have been performed using a range of DW-Therm inlet temperatures.

The default configuration of the jacket, from the experiment, uses a tangential inlet pipe at the bottom and a radial outlet pipe at the top. The flow was very non-uniform, following the path of the inlet flow and spreading out over the cylindrical part of the jacket in one revolution.

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