CFD Reactor Modelling and Improvement

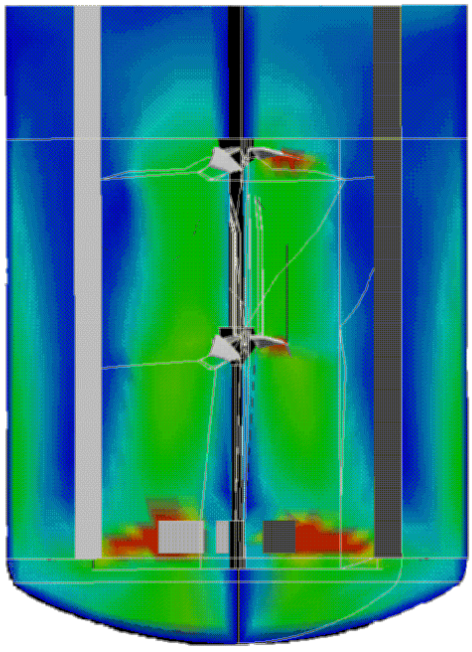
Case Study

Reactor design limitations were identified and cost-effective recommendations made for improved design

The Problem

An acetic acid reactor had a large temperature profile resulting from a hot recycle stream fed back to the cooler bulk, creating:

- Temperature differential up to 80ºC
- Low yield
- Poor product quality
- Difficult thermal control
- Low productivity



Liquid speed contours predicted by CFD model for client's original design

The Need

Faster and more uniform blending to reduce temperature gradients

The Solution

Desk assessment followed by CFD modelling to evaluate and optimise suggested reactor modifications

The Benefits

Design modifications reduce blend time by 33% with:

- Significantly reduced temperature profile
- Increased yield
- Improved productivity
- Safer reactor operation

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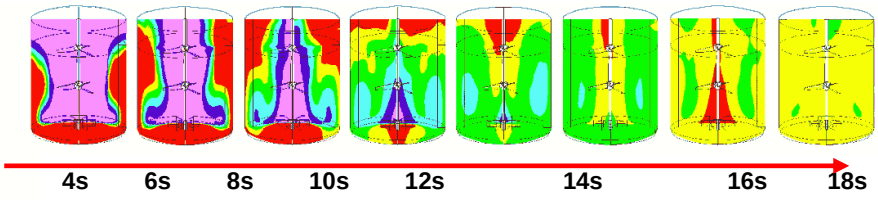
Methodology

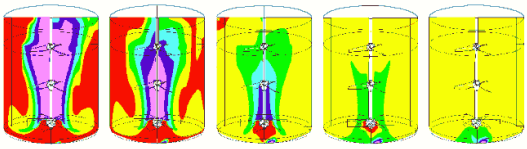
- Assessment of existing reactor assessed gas dispersion, liquid blending performance and potential for hot spots in the reactor
- CFD model study, backed by LDA validation data and 20 years practical work on stirred tanks reactors
- Examination of concentration profiles and investigation of effects of modifications to agitation equipment on homogenisation
- CFD studies identified a flow loop in the upper part of the vessel and a strong circulation loop between the bottom impeller and vessel base, producing significant reactor temperature gradients.

Results

Original Design



Modified Design



Normalised tracer concentration versus time, introduced from the inlet for both original and modified design, on a longitudinal plane between two baffles

- Agitation and feed details varied, systematically to identify optimum configuration for blending performance
- Increased rate of fluid transport around reactor reduced blend time by 33% and increased heat transfer through higher liquid velocity at reactor wall.

BHR Group's work on Reactor Design and Improvement

BHR Group is an international centre of fluid mixing expertise and knowhow in the design, optimisation and scale-up of chemical reactors for single-phase, two-phase and multiphase processes. Expertise in CFD modelling, chemical engineering and chemistry is backed by unrivalled pilot and production-scale experimental facilities for model validation.

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