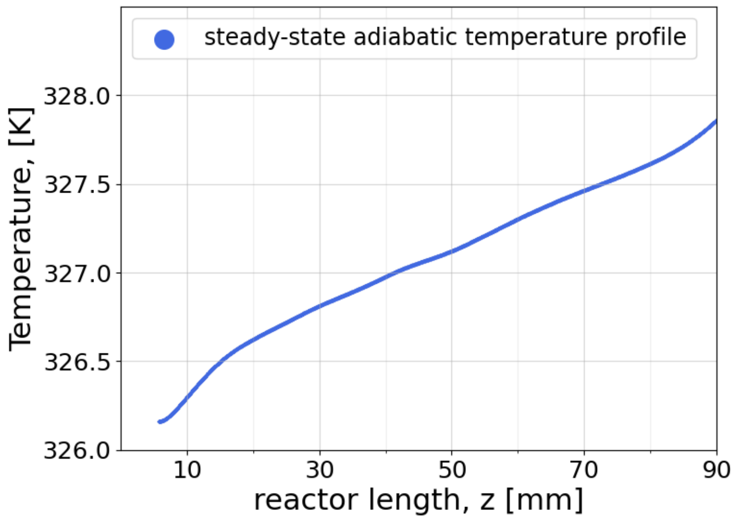
Flow Calorimetry: A Methodology for Determining Kinetics of Exothermic Reactions

Zeynep Gulsoy Serif[1], Mimi Hii[2], Dominik Ohlig[3], Markus Goedde[3], Klaus Hellgardt[1]
1 Department of Chemical Engineering, Imperial College London, London, UK
2 Department of Chemistry, Imperial College London, London, UK
3 BASF SE, Ludwigshafen am Rhein, Germany

The kinetics of exothermic reactions are an important aspect of chemical engineering, as they determine the rate at which heat is released during the reaction. Industrial processes should always prioritise safety, particularly for fast and highly exothermic reactions containing toxic reactants as these pose significant risks. Hence, accurately measuring the kinetics and heat release can play a vital role in understanding and controlling the risks involved, whilst also leading to improved process efficiency.

Due to a number of unique features of continuous flow reactors, flow calorimetry can provide an intrinsically safer way to study the kinetics of exothermic reactions, particularly when spatial temperature distributions are measured under steady-state conditions. By monitoring the temperature as a function of reactor length, and fitting the data to appropriate kinetic models, kinetic information like the activation energy, pre-exponential factor, and rate constant of the reaction can be determined. Furthermore, real-time monitoring of process conditions and control of potential hotspots via time-dependent spatially resolved temperature profile is another significant strength of flow calorimetry.

In this work, an optical isoperibolic flow calorimeter, designed and built at Imperial College London, was used to validate the methodology for kinetic studies. Hydrolysis of acetic anhydride reaction was performed as a model reaction in flow calorimetry and the collected data was evaluated by kinetic modelling to extract the activation energy and pre-exponential factor. The graph below displays an experimental adiabatic temperature profile as a function of reactor length. After the heat loss to the environment was corrected, steady=state adiabatic temperature profiles this graph was obtained. Steady-state adiabatic temperature profiles were then evaluated using kinetic models. In this presentation, we will explain our setup and how we conducted the case study, along with the comparison of our results with literature.



steady-state adiabatic temperature profile
328.0
327.5
327.0
326.5
326.0
Temperature, [K]
10
30
50
70
90
reactor length, z [mm]