MANCHESTER 1824
The University of Manchester

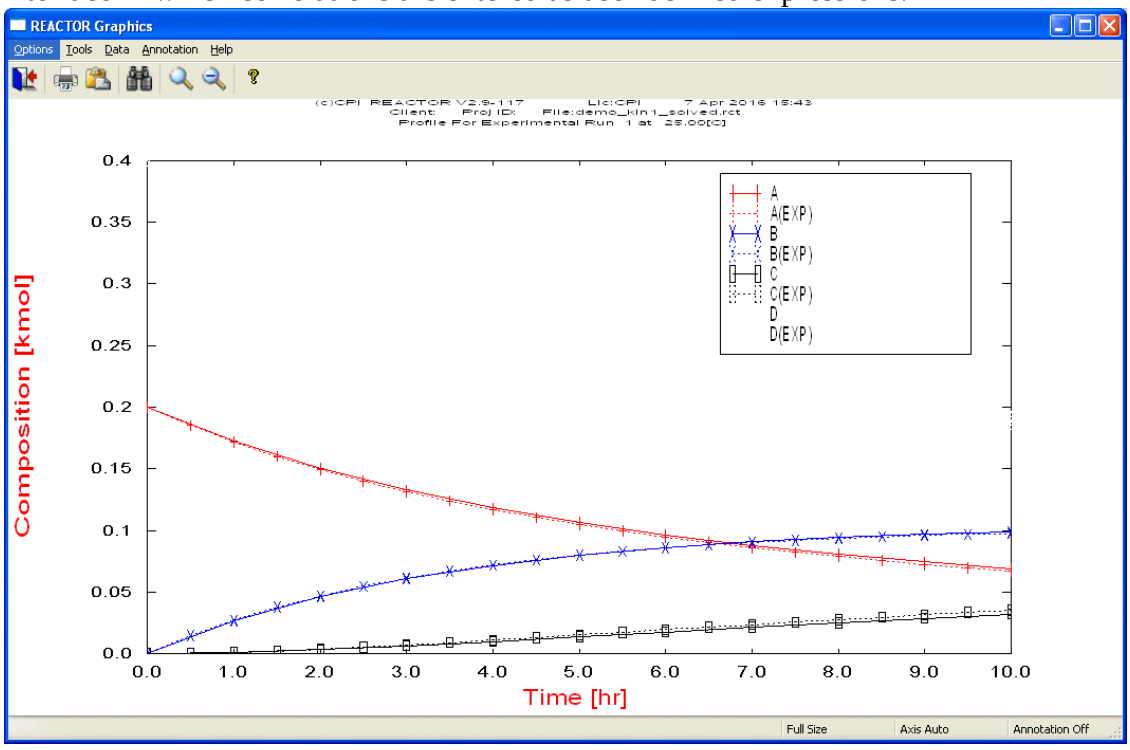
REACTOR Overview

REACTOR is the software package for the design of chemical reactors and reaction-separation systems. Given information on the reaction system stoichiometry and kinetics,
REACTOR provides targets for the maximum selectivity, yield or conversion. Both continuous and batch reactors can be studied. It also provides the mixing patterns, arrangements for feed and recycling and heat transfer arrangements (and cycle time in the case of batch reactors) required to achieve the target reactor performance. Because the analysis is based on fundamental kinetic and mass transfer effects rather than heuristics, novel reactor designs and flowsheets for reaction-separation systems can be identified.

Issues addressed by **REACTOR** include:
• Target for maximum yield, selectivity or conversion
• Single and multi-phase reactors
• Continuous and batch reactors
• Simultaneous mass transfer with chemical reaction
• Ideal mixing pattern to achieve target performance
• Heat transfer arrangements to achieve target performance
• Novel reactor designs
• Design of reaction-separation systems
• Free format input for stoichiometry and kinetic expressions

Reaction and Kinetic Data

Calculations on chemical reactors require stoichiometric and kinetic data. The input of such data can in principle be a problem because there is no general format for such data. **REACTOR** allows stoichiometric and kinetic data to be input via a flexible user interface in which correlations are entered as user-defined expressions.



Targeting Selectivity, Yield and Conversion

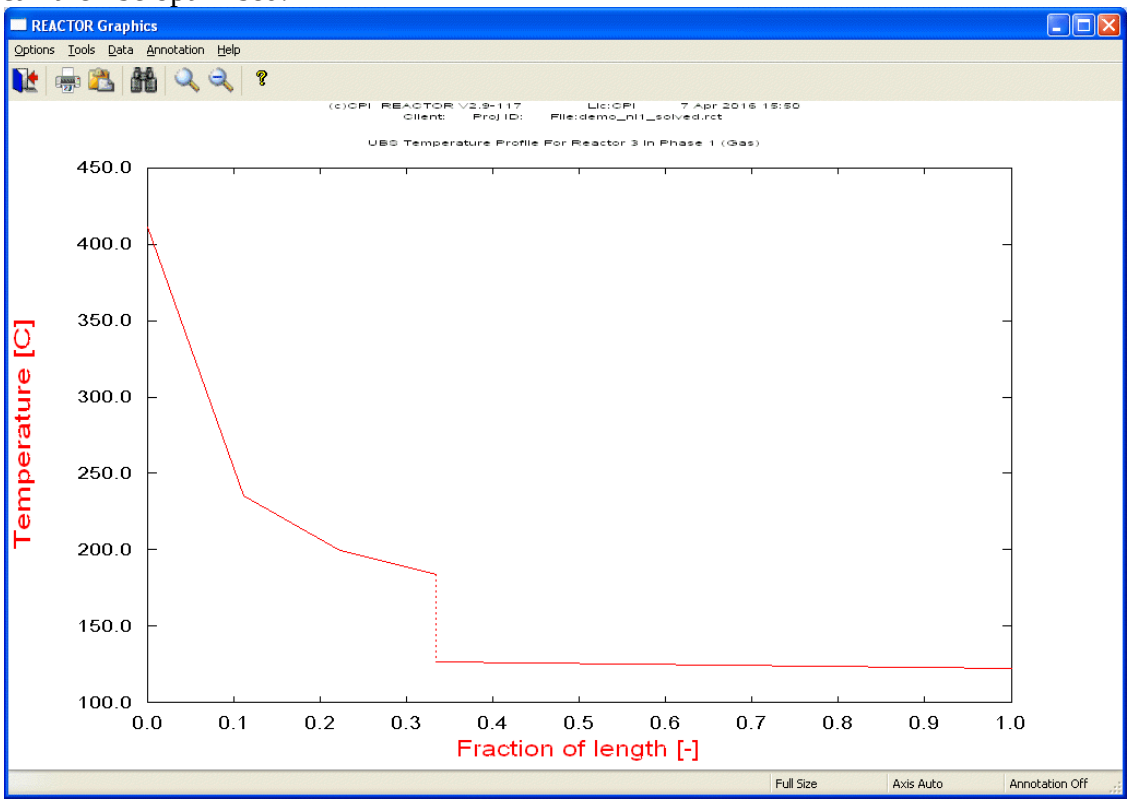
REACTOR uses a methodology for the systematic design of chemical reactors which sets performance targets, predicting the maximum selectivity, yield or conversion for a given reaction system with its catalyst. In addition to the pre-programmed optimisation objectives, user-defined objectives can be specified. Single and Multiphase Systems Even the most complex systems can be analysed, including multiple phases. Mass transfer and chemical reaction are considered simultaneously. Different mass transfer correlations are used depending on the mixing arrangement being analysed.

Continuous and Batch Reactors

Both continuous and batch reactors can be optimised. Mixing Patterns **REACTOR** also identifies the mixing pattern to achieve the predicted target performance. This provides the designer with the ideal mixing pattern to be emulated in the design. If computational fluid dynamics is to be used to simulate the performance of the reactor then the mixing pattern provided by **REACTOR** gives the designer unique insights into the ideal design, removing trial and error.

Heat Transfer

Non-isothermal reactor design can be explored in two ways. In the first approach, the ideal temperature profile through the reactor can be optimised. Control over the complexity of the temperature profiles is maintained to avoid impractical designs being suggested. In the second approach, adiabatic beds are assumed in the reactor. Heat transfer between the beds, intermediate feed injection, recycling and splitting of flows can then be optimised.



Novel Designs

The application of the technology leads to the development of novel reactor schemes that would be virtually impossible to derive using an approach based on trial and error.

Reaction-Separation Systems

The traditional approach to process design is to carry out the design of the reactor and separation system independently and then to connect them together with recycle

streams. **REACTOR** allows a different approach, in which the reaction and separation system (including the separation tasks and task order) are designed simultaneously.