# Reducing the impact of catalyst deactivation in reactive distillation

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Reactive distillation represents a major breakthrough in process intensification, combining reaction and separation into the same physical vessel, with economic and environmental gains. In previous work, authors' developed a framework combining feasible regions and optimization techniques for the design and multi-objective optimization of complex reactive distillation columns. This led to the consideration of reactive distillation columns with distributed feeds, involving the combination of superheated and subcooled feeds that provide a source or a sink of heat at specified trays of the columns, favouring reaction while reducing the total reactive holdup requirements. It was also found that higher conversions could be obtained with the same reactive holdup by using these feed qualities outside the traditional range, which led to the consideration of using this technique to overcome catalyst deactivation during column operation.

**STEP 1**

(GAMS model)

- Design
- Feasibility analysis
- Optimization
- Multiobjective

**STEP 2**

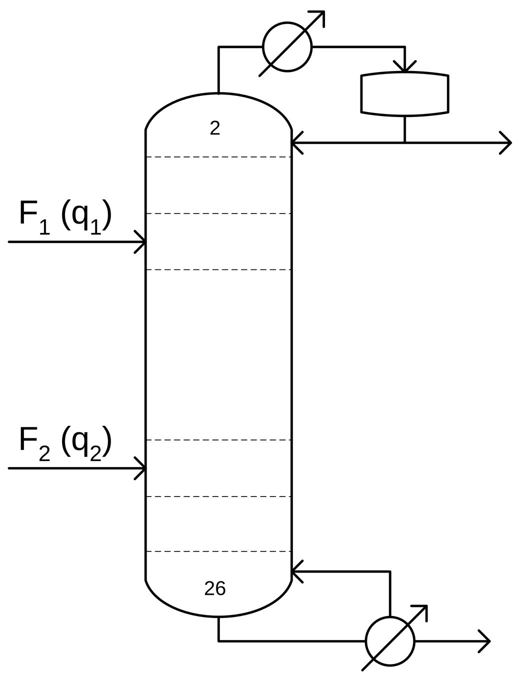
(Aspen Plus model)

- Rigorous modeling
- Steady-state
- Validation
- Sensitivity analysis
- Design simplification

**STEP 3**

(gPROMS model)

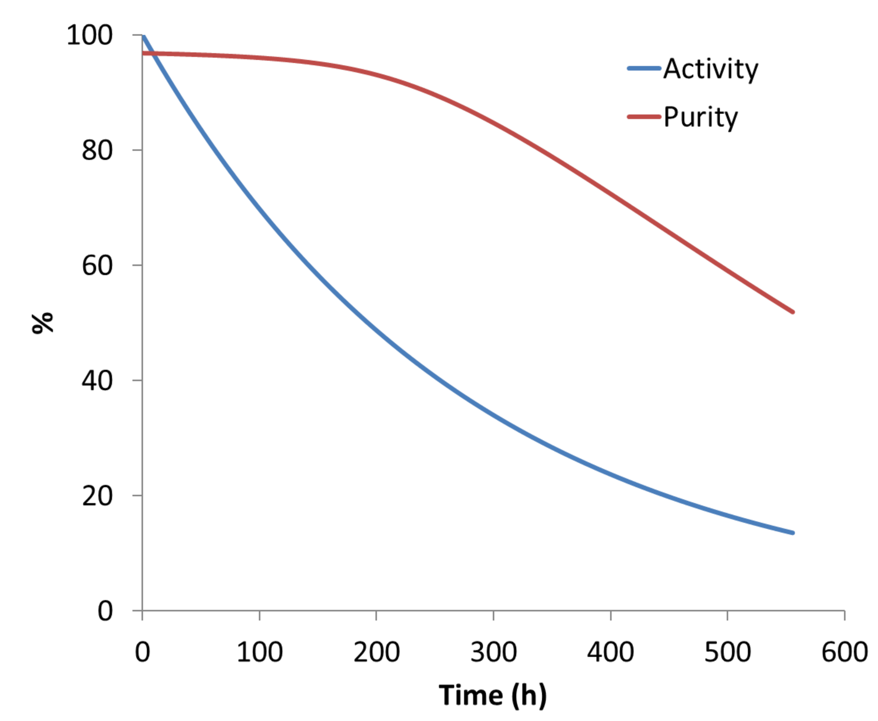
- Rigorous modeling
- Dynamic
- Control
- Catalyst deactivation



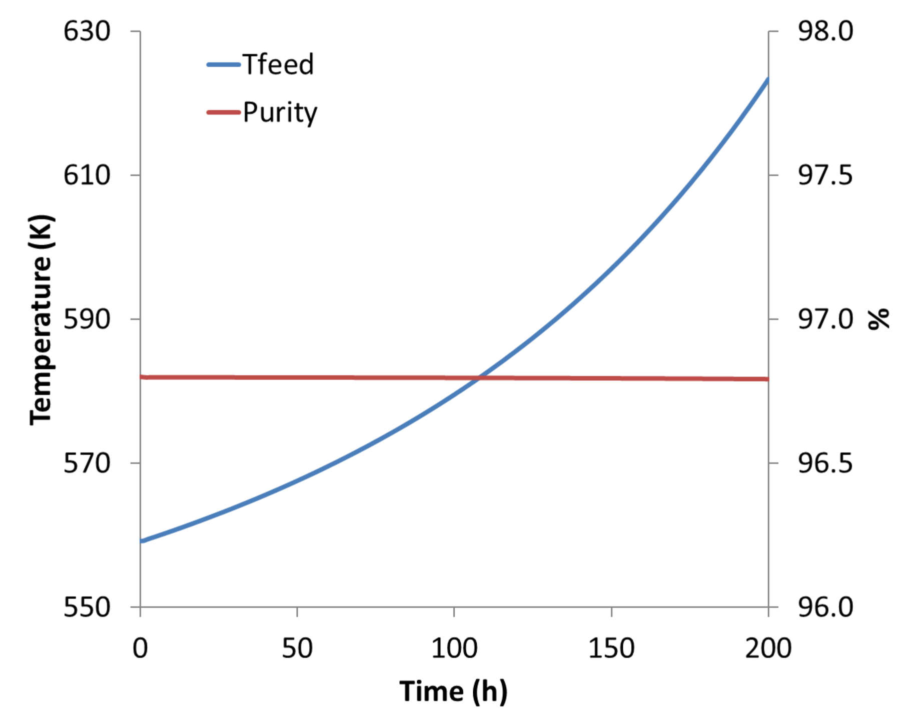

This work addresses the effects of catalyst deactivation in reactive distillation columns and investigates methods to reduce their impact on column performance. A rigorous dynamic model developed in gPROMS and applied to an illustrative example, the olefin metathesis system, wherein 2-pentene reacts to form 2-butene and 3-hexene, is used to investigate how the feed quality manipulation can maintain product purity while the catalyst deactivates. Besides identifying column behaviour under situations of reduced reaction conversion, strategies to overcome catalyst deactivation are also addressed, namely through manipulation of the feed temperature. This procedure extends the operating time of the column without having to interrupt production and replace the catalyst load. The effectiveness of these actions is largely dependent on column design, but satisfactory results are obtained with the proposed strategies to handle situations where catalyst activity is decreased down to 50%, at the expense of increased energy consumption.

## Dynamic model in gPROMS

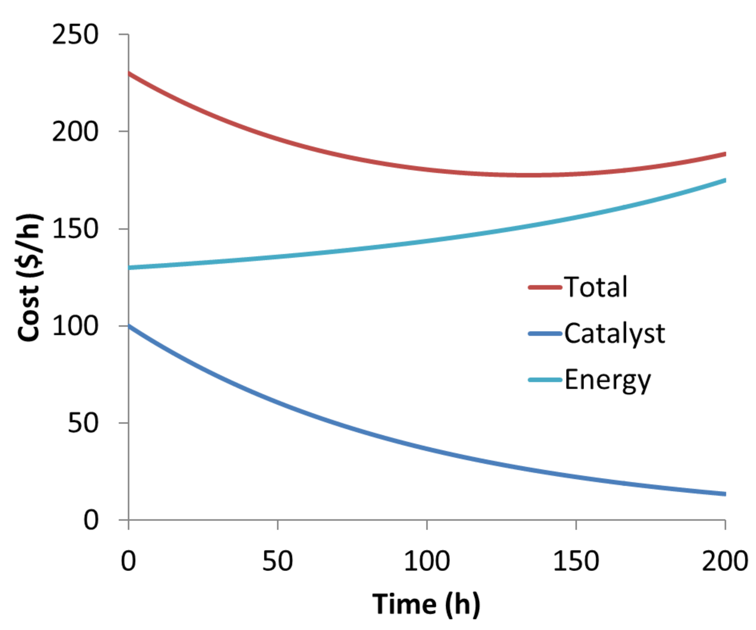
- Modular (tray, reboiler, condenser,…)
- MESH equations
  - Mass, Equilibrium, Summation, Heat (enthalpy)
- Variable number
  - Stages, Feeds and Reactive stages
- IPPFO ideal property model (coefficients obtained by regression using Aspen Plus data)
- Reactive holdup specified for each tray
- Reaction in the liquid phase



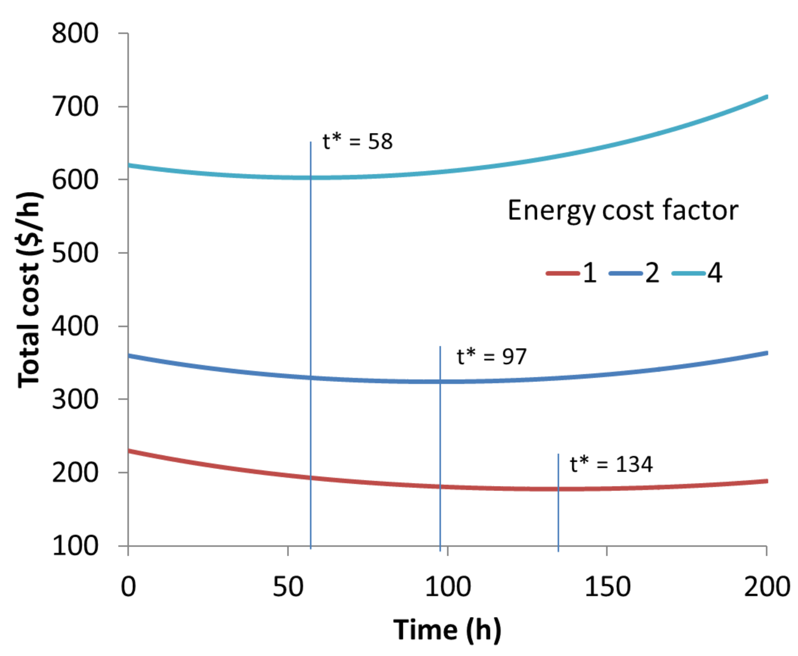

Catalyst activity decay and the effect in product purity.



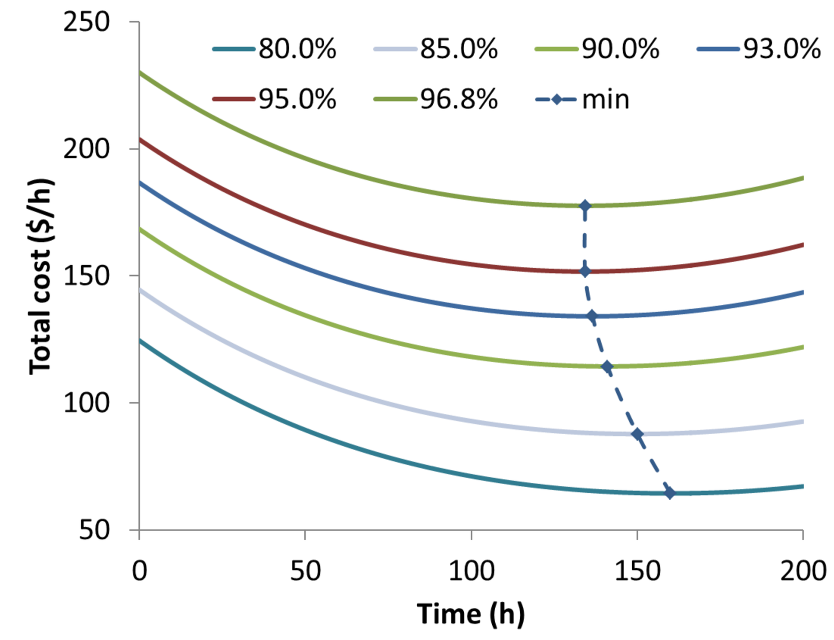

Feed temperature variation with catalyst activity decay. Product purity is kept constant by increasing the energy supplied through the feed stream.




Effect of energy and catalyst related costs (catalyst, shut-down, replacement, start-up) on total operating cost. The optimal cycle time (operating period before catalyst replacement) is 134 h.




Effect of the energy cost on total operating costs. When different cost factors are applied, as the energy cost increases the optimal cycle time t* is reduced.




Effect of product purity. When lower specifications are used for product purity the cost decreases and the cycle time increases. The dotted line shows the evolution of the cycle time for the different scenarios.

Reactive distillation columns operational schedule should be preceded by a economic evaluation accounting for the incurred extra energy costs and the savings associated to the extended life-cycle of the catalyst and reduced number of column shut-down and start-up operations. The trade-off between the cost of increasing energy supply and replacing the catalyst is investigated aiming at the determination of the ideal time for column operation interruption and catalyst replacement. Different scenarios are used to assess how the total operating costs can be minimized, while maintaining the required product specifications.