# REACTOR SCALE-UP FROM ISOTHERMAL BENCH-SCALE TO ADIABATIC TRICKLE BED REACTORS

Katherine E. Nies*, Daniel A. Hickman, and David C. Molzahn
The Dow Chemical Company

*Summary*

Direct scale-up from isothermal, bench-scale kinetic models to adiabatic trickle bed reactors is viewed as risky. Errors may be introduced into kinetic models derived from isothermal experiments due to insufficient instrument accuracy, relative insensitivity to inaccurate models, and the absence of the enthalpy balance necessary for modeling adiabatic reactors. Consequently, validation of the kinetic model on non-isothermal reactors is encouraged in the literature prior to scale-up. The current report, however, discusses a highly successful scale-up from isothermal, bench scale reactors directly to pilot plant scale adiabatic trickle bed reactors, with a scale-up factor of 50,000. Five kinetic models, in LHHW form, were proposed, varying in overall reaction order and number of estimated parameters. Results using the best fit model demonstrated the agreement of the predicted and pilot plant conversion data, successfully demonstrating that kinetic models generated from isothermal reactors can be used for direct scale-up to adiabatic trickle bed reactors without additional non-isothermal lab scale validation. In addition, this work utilizes several measures of the goodness of fit for model discrimination, including the Posterior Probability Share, the Akaike Information Criterion, and the Bayesian Information Criterion, showing the benefit of using all three of these measures.

*Keywords*

Multiphase and particulate reactors

## Introduction

Very few successful reactor scale-ups from isothermal, bench-scale reactor to adiabatic, pilot plant reactors are documented in the literature. In general, industrial reaction engineers encounter resistance when proposing scale-up of multiphase reactors over several orders of magnitude. However, a team from The Dow Chemical Company has developed a kinetic model based on upflow, isothermal fixed bed reactors with cocurrent flow of gas and liquid and demonstrated its accuracy in a pilot plant consisting of a series of adiabatic trickle bed reactors. Thus, model-based scale-up by a factor of 50,000 was demonstrated.

## Experimental

Isothermal experiments were conducted with two continuous fixed bed reactors, each made from 0.5 inch O.D. Hastelloy C with a bed length of only a few inches. The small diameter reactor, combined with a relatively small heat of reaction, provided sufficient heat transfer to validate the isothermal assumption. The reactors were packed with 5 to 20 grams of 1/8" diameter catalyst pellets as well as silicon carbide fines (100 mesh). The inert fines were included to minimize back-mixing and enhance gas-liquid contacting in the upflow reactors, validating the plug flow assumption.

The feed flow rate and jacket temperature of the reactors were controlled to vary the conversion, providing concentration data as a function of reactor space velocity. These data were used for parameter estimation and model discrimination for the various postulated kinetic models.

## Kinetic Model

Five alternate LHHW-type rate expressions were coded in Athena Visual Studio version 11 in order to estimate the kinetic parameters and perform model discrimination, predicting the conversion and selectivities as a function of flow rate and temperature. Each of the models was subjected to model discrimination based on Posterior Probability Share (PPS), Akaike Information Criterion (AIC), and Bayesian Information Criterion (BIC). All three measures discriminate among the proposed models based on the lowest residual sum of squares, but the BIC weights the number of parameters heavier than the AIC when the number of experiments is greater than seven, placing a higher penalty on adding parameters to obtain a better fit. All three measures were used in conjunction to choose the best model.

* To whom all correspondence should be addressed

## Pilot Plant Results

Kinetic models were developed for two different generations of catalyst. The model based on the first generation catalyst was used to design the pilot plant reactor system. A system with three adiabatic beds in series was chosen, with interstage heat exchange between the beds. By the time the pilot plant was operational, a second generation catalyst was available and loaded. The performance of this catalyst was compared to model predictions based on the kinetic model for the second generation catalyst. A very good agreement between the predicted temperature profiles and reactor yields validated both the modeling work and the scale-up methodology.

## References

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