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Data Required for Predicting Reactive Chemical Pathways

**Dr. Sam Mannan and Dr. Ken Hall
Department of Chemical Engineering
Texas A&M University
College Station, Texas 77843-3122**

**Dr. Harry West
Shawnee Engineers
1415 N Loop W, Suite 1150
Houston, Texas 77008**

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ABSTRACT

Extensive reactivity data for a particular mixture of chemicals at the potential operating conditions of a process under consideration are rarely available. The impact of vessel size, catalytic contaminants, and other potential reactivity parameters must be extrapolated from available data. The high cost of obtaining laboratory data on all possible combinations forces consideration of predictive techniques.

The focus of this presentation is the available reactive chemical predictive techniques and the basic thermodynamic and physical properties needed by these fundamental predictive

methods.

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