## A Framework for Chemical Plant Safety Assessment under Uncertainty

## Xiaoyan Zeng, Mihai Anițescu\*,

Mathematics and Computer Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Building 221, Argonne, IL 60439-4844, U.S.A Email: anitescu@mcs.anl.gov

## Candido Pereira and Monica Regalbuto

Chemical Sciences and Engineering Division, Argonne National Laboratory,

9700 South Cass Avenue, Building 205,

Argonne, IL 60439-4837, U.S.A

## \*Mihai Anițescu dedicates his work on this article to the 60th birthday of Dr. Neculai Andrei. Neculai, thanks for your extraordinary work for the benefit of the numerical optimization community in Romania and everywhere.

**Abstract:** We construct a framework for assessing the risk that the uncertainty in the plant feed and physical parameters may mask the loss of a reaction product. To model the plant, we use a nonlinear, quasi-steady-state model with stochastic input and parameters. We compute the probability that more than a certain product amount is diverted, given the statistics of the uncertainty in the plant feed, in the values of the chemical parameters, and in the output measurement. The uncertainty in the physical parameters is based on the one provided by the recently developed concept of thermochemical tables. We use Monte Carlo methods to compute the probabilities, based on a Cauchy-theorem-like approach to avoid making anything but the safest asymptotic assumptions, as well as to avoid the excessive noise in the region of low-probability events.

Keywords: Safety Assessment, Uncertainty, Chemical Process, Stream Methane Reforming, Active Thermochemical Tables, Monte Carlo Methods