

Abstract Submitted  
for the DFD17 Meeting of  
The American Physical Society

**Inference of missing data and chemical model parameters using experimental statistics.**<sup>1</sup> TIERNAN CASEY, HABIB NAJM, Sandia National Laboratories — A method for determining the joint parameter density of Arrhenius rate expressions through the inference of missing experimental data is presented. This approach proposes noisy hypothetical data sets from target experiments and accepts those which agree with the reported statistics, in the form of nominal parameter values and their associated uncertainties. The data exploration procedure is formalized using Bayesian inference, employing maximum entropy and approximate Bayesian computation methods to arrive at a joint density on data and parameters. The method is demonstrated in the context of reactions in the H<sub>2</sub>-O<sub>2</sub> system for predictive modeling of combustion systems of interest.

<sup>1</sup>Work supported by the US DOE BES CSGB. Sandia National Labs is a multimission lab managed and operated by Nat. Technology and Eng'g Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell Intl, for the US DOE NCSA under contract DE-NA-0003525.

Habib Najm  
Sandia Natl Labs

Date submitted: 28 Jul 2017

Electronic form version 1.4