Abstract Submitted
for the DPP12 Meeting of
The American Physical Society

Python framework for kinetic modeling of electronically excited reaction pathways[1] JOHN VERBONCOEUR, GUY PARSEY, YAMAN GUCLU, ANDREW CHRISTLIEB, Michigan State University — The use of plasma energy to enhance and control the chemical reactions during combustion, a technology referred to as "plasma assisted combustion" (PAC), can result in a variety of beneficial effects: e.g. stable lean operation, pollution reduction, and wider range of p-T operating conditions. While experimental evidence abounds, theoretical understanding of PAC is at best incomplete, and numerical tools still lack in reliable predictive capabilities. In the context of a joint experimental-numerical effort at Michigan State University, we present here an open-source modular Python framework dedicated to the dynamic optimization of non-equilibrium PAC systems. Multiple sources of experimental reaction data, e.g. reaction rates, cross-sections and oscillator strengths, are used in order to quantify the effect of data uncertainty and limiting assumptions. A collisional-radiative model (CRM) is implemented to organize reactions by importance and as a potential means of measuring a non-Maxwellian electron energy distribution function (EEDF), when coupled to optical emission spectroscopy data. Finally, we explore scaling laws in PAC parameter space using a kinetic global model (KGM) accelerated with CRM optimized reaction sequences and sparse stiff integrators.

[1]Supported by AFOSR and a Michigan State University Strategic Partnership Grant.

John Verboncoeur
Michigan State University

Date submitted: 19 Jul 2012 Electronic form version 1.4