Modeling Reacting Flow with Uncertainty Quantification[1]

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Introduction and Background

Uncertainty quantification (UQ) in computational predictions is useful from an engineering point of view, where confidence intervals on predicted system behavior are necessary for design optimization. It is also useful from a scientific point of view, where model validation with respect to experimental measurements requires careful measures of uncertainty in both experimental data and computational predictions. In general, uncertainty in computational results can be due to both model and parametric uncertainty. The present work deals with the latter. We investigate the propagation of uncertainty from parameters to model outputs in the context of low Mach number reacting flow. The goal is to arrive at uncertainty "error-bars" on model outputs based on those of the parameters.

Earlier studies have addressed this issue from various angles. To begin with, Monte Carlo (MC) techniques can be used in conjunction with parametric variations. However, this approach has significant computational requirements, and does not provide sensitivity information as regards the contributions of individual parameters to the output uncertainties—except by allowing one uncertain parameter at a time and losing the nonlinear coupling between parameters. Alternatively, sensitivity analysis [1, 2, 3] has been used to provide a measure of the dependence of model outputs on individual parameters, and as a basis for error-analysis [4] and variance-propagation [5, 1, 6, 7, 8] techniques. These techniques provide the variance in model outputs resulting from known variances in the parameters using rules of propagation of errors. However, this approach does not model higher-order non-linear couplings among parameter uncertainties. Perturbation techniques have also been used, based on Taylor series, with the typical limitations of small perturbations. Another approach, based on expanding the inverse of the stochastic operator in a Neumann series [9] is also limited to small perturbations.

Recent UQ developments have been based on the use of Polynomial Chaos (PC) for stochastic representation of uncertainty. Polynomial chaos [10, 11, 12, 13, 14, 15, 16] is a member of the set of homogeneous chaos, first defined by Wiener [10]. Ghanem and Spanos [16] implemented a spectral PC expansion in terms of Hermite polynomials of gaussian basis functions with a finite element method for UQ. This was applied in the modeling of transport in porous media [17], solid mechanics [18, 19] and

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structural [20] applications. The utility of the Hermite-Gaussian PC for modeling non-gaussian processes was also investigated in [21, 22]. Le Maître *et al.* [23, 24] extended the application of these techniques to thermo-fluid applications in the context of low Mach number flow. Xiu *et al.* [25] used generalized PC [26] for stochastic UQ in the modeling of flow-structure interactions, and for diffusion problems [27]. Debusschere *et al.* [28, 29] used PC for UQ in the context of electrochemical flow in microfluidic systems. In general, these implementations of spectral PC expansions for stochastic UQ involve (1) the introduction of a new stochastic dimension for each uncertain parameter in the problem, (2) the expansion of parameters and field quantities using PC in terms of these stochastic dimensions, (3) the substitution of these expansions in the governing equations and their reformulation using a Galerkin projection procedure into equations for the stochastic mode strengths, and (4) the solution of this larger system of equations and the reconstruction of the field quantities of the solution based on their PC expansions in terms of the now known stochastic modes. These approaches are "intrusive" in the sense of requiring a reformulation of the governing equations.

Non-intrusive PC UQ techniques have also been developed, involving the use of MC sampling coupled with PC processing of the statistics. Given MC sampling of the stochastic parameters, the corresponding solutions of the deterministic system are evaluated and projected onto the PC basis to compute the spectral mode coefficients. These coefficients are then used to construct probability density functions (PDFs) of the solution, to infer sensitivity to various model parameters, and to highlight the dominant sources of uncertainty. This "non-intrusive" spectral projection (NISP) approach, which is based on [20], has the advantage of being applicable to legacy codes, which are run with varying parameters to compute the statistics and spectral mode values. NISP has been used for UQ in low Mach number H_2-O_2 flames [30].

Other non-intrusive PC UQ methods are available, and for certain problems may have efficiency advantages. The determinisitic equivalent modeling method (DEMM) [31], is a probabilistic collocation method that generates a PC expansion of model outputs for systems with well-behaved response functions. It limits sampling to a subset of the roots of the next-higher order Hermite polynomial. The stochastic response surface method (SRSM) [32] expands sampling by using regression to generate coefficients from a complete set of higher-order roots. Both of these methods fit the probabilistic response function to a set of PC coefficients. However, it is not clear that limiting sampling to the partial or full set of polynomial roots can adequately sample the necessary range of stochastic space.

Description of the Present Work

In the present work, we focus on the implementation of intrusive PC UQ in the context of low Mach number reacting flow, and on the comparison of the results with NISP H_2-O_2 data.

We consider a one-dimensional N_2-diluted H_2-O_2 flame under atmospheric pressure, which we model using a low Mach number reacting flow model with a 9-species 19-step chemical mechanism [33]. We allow for the uncertainties in Arrhenius rate constants and enthalpies of formation, neglecting for the

time being uncertainties in the entropy [34]. The governing equations are reformulated using a pseudo-spectral PC approach that allows for code modularity and increased computational efficiency. This approach is particularly advantageous for algebraic handling of the propagation of PC expansions in complex non-linear chemical source terms, thus avoiding the need for MC simulations imbedded in the intrusive computation.

We illustrate the implementation of the spectral approach in a projection-scheme solution of the low Mach number momentum equations, which leads to a set of *decoupled* poisson solutions for each of the spectral modes of the pressure field. This Stochastic Projection Method (SPM) [23] is then coupled to an operator-split implicit-explicit time integration of the detailed energy and species governing equations. The reformulated stochastic chemical source term is integrated implicitly using a stiff ODE-integration code (DVODE [35]), while the diffusion and convection operators are integrated explicitly in a symmetric Strang-splitting using Runge-Kutta-2 and Adams-Bashforth-2 time integration.

Discrete satisfaction of the stochastic poisson equation solvability constraint and overall robustness of non-polynomial operations, e.g. $1/\rho$, $\ln(T)$, $\exp(-E/T)$, lead to the requirement of a specialized treatment that avoids Taylor series polynomial expansion approximations of these operators. We will describe both direct matrix solution approaches for the inversion operations, and more general integration approaches for other non-polynomial operations [29].

We investigate the efficacy of the PC approach in modeling uncertainty propagation in the H_2-O_2 system, particularly with regard to the handling of random variables and fields with extremely skewed probability density functions (PDFs), and with regard to ignition-like behaviour where positive eigenvalues lead to the fast growth of field variances, necessitating high-order PC expansions to avoid significant non-physical (negative concentration, temperature, etc) PDF tails and consequent stability problems.

We present results from both the intrusive PC and NISP approaches. The 1D planar premixed H_2-O_2 flame solution is computed in time from a deterministic initial condition, and allowed to relax towards a steady-state. Uncertainties in flow quantities are observed to grow in space, particularly in the primary flame region where positive eigenvalues are prevalent. We find particularly large uncertainty in the computed H_2O_2 concentration field. In fact, allowing for the actual uncertainty in reaction rate constants and thermodynamic properties leads to a 1-σ variation that is on the order of 100% of the mean of H_2O_2. The results indicate clearly the parameter with largest influence on this H_2O_2 variability, namely the rate constant of the reaction (H_2O_2+OH=H_2O+HO_2). Evidently, the present model lacks sufficient robustness for prediction of H_2O_2 in this flame under the prevalent parametric uncertainties. The identification of the particular rate constant with dominant role in the large H_2O_2 variability serves as a guide for future experimental investigations of the above reaction in order to reduce the effective uncertainty in its rate constant and improve confidence in model predictions.

Uncertainty quantification should be included by default in reacting flow computations in order to provide meaningful predictive capabilities and allow for rational model validation. While this is a signifi-

cant challenge, the present work shows a potential route towards this goal with promising results. Much optimization and refinement of the intrusive PC procedures is still necessary to deal efficiently with the strong non-linearities prevalent in chemical systems. This is a matter of continuing work.

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