Fast Solution of Quasi-Steady State Species by Combination of Fixed-Point Iteration and Matrix Inversion

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Introduction

Development of predictive chemical kinetics has become increasingly important in various applications of combustion engineering. A computationally affordable method for the integration of chemical kinetics is often necessary to enable simulations of realistic geometry in the context of RANS or Large Eddy Simulation (LES). The concept of Quasi-Steady State Approximation (QSSA) has been widely used in construction of conventional reduced chemistry.

The basics of QSSA

Species selected for QSS do not appear in the set of Ordinary Differential Equations (ODEs) describing the chemical system. However, their concentrations are needed to evaluate the source terms for the set of ODEs.

\[ \frac{\partial S_j}{\partial t} = \omega_{i,p} - \omega_{i',p} = f(S_i, S_j) \quad i \notin \Omega_{\text{QSSA}} \]

The concentration of QSS species is a solution to the following non-linear algebraic equations:

\[ S_i = \sum_{j=1, j \neq i}^{M} a_{i,j} S_j - b_j \]

where \( a_{i,j} \) are functions of QSS species making the system non-linear and computationally expensive to solve.

Fixed Point and Newton iterations

The non-linear system of QSS species is usually solved with Fixed Point Iteration (FPI) or Newton Iteration (NI) methods. Each method has drawbacks:

(a) FPI shows low convergence for complex chemistry with strongly coupled isomers

(b) NI's computational cost scales \( \propto N^3 \) with the number of QSS species plus precluding usage with large mechanisms.

\[
\begin{vmatrix}
1 & 10^{-5} & \epsilon \\
-\epsilon & 1 & 10^{-10} \\
\end{vmatrix}
\]

The solution to the system above via FPI displays slow convergence as \( \epsilon \rightarrow 1 \)

FPI with Matrix Inversion

Methodology

1. Identify the groups of QSS species that are strongly coupled.
2. Gather all remaining uncoupled QSS species.
3. At each iteration, solve for the uncoupled species via FPI and for each group of coupled species via direct inversion of the linear system (e.g. LU decomposition).

First an undirected graph for the QSS species is constructed based on the following:

\[ E_{i,j} = 1, \quad \text{if} \quad C_{i,j} = \alpha_{i,j} \geq \epsilon, \quad i \neq j = 0, \quad \text{otherwise} \]

A Depth-First Search algorithm is used to identify the QSS species in closely connected groups. Coupling between species \( i \) and \( j \) is determined by the threshold \( \epsilon \).

Assessment of FPI-MI

Three reduced mechanisms are used in auto-ignition numerical tests:

- 18-species methane with 17 QSS from 900 K, 1 and 60 atm (\( \Phi = 0.7, 1.6 \))
- 63-species isoctane with 152 QSS from 700 K, 10 and 60 atm (\( \Phi = 0.3 \))
- 101-species Primary Reference Fuel (PRF) with 251 QSS from 875 K, 10 and 60 atm (\( \Phi = 0.3 \))

Conclusions

We developed an efficient algorithm that combines Fixed Point Iteration (FPI) with Matrix Inversion (MI) for solving the non-linear system of QSS in reduced chemistry. The new method offers substantial advantages in terms of computing time for reduced chemistry with strong coupling among species. It is found that for PRF chemistry the time savings the greatest, while for small sets of QSS (such as methane/air), little is gained.

Figure 1. A group of QSS species is formed after performing a DFS starting from vertex 1 (species 1) with an undirected graph of E(1,2) except E(1,2) = E(2,5) = 1. Vertices with thick circles are those explored by during DFS. Groups can be formed at each chemical states during the simulation or prior to the simulation using chemical states representative of the intended regime.

Figure 2. Total number of coupled species versus coupling threshold for methane-air auto-ignition at different initial compositions (ambient air and pressure).

Figure 3. Evolution of species of different coupling groups as the threshold parameter is tightened (top to bottom) for methan-air auto-ignition. For the smallest threshold, 16 species are coupled in a single group.

Figure 4. Number of iterations required for convergence versus temperature for auto-ignition of PRF/air charge. The Newton Iteration (NI) method converges in the least number of iterations, while Fixed Point Iteration (FPI) takes the most.

Figure 5. Total CPU time normalized by fixed-point iteration versus coupling threshold for the three reduced mechanisms with a different number of QSS species (17, 152 and 251). Labels indicate the number of coupled QSS species. The greatest CPU savings are obtained for the PRF/air auto-ignition.

Figure 6. CPU time per non-linear system solution iteration normalized by the time taken for a fixed-point iteration versus maximum number of coupled species. For a large number of coupled species, the CPU time scales as the third power of N. Note that FIP is computationally most convenient on a per iteration basis.