Systematic generation and efficient solution of reactor network models

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Abstract: A systematic method to generate reactor network models (RNM) based on the computational fluid dynamics (CFD) results is proposed. Each reactor in the RNM is a perfectly stirred reactor agglomerated from neighboring CFD cells with the residence time determined by the reactor volume and the flux information. The flux between a pair of reactors is the summation of the convection and the turbulent diffusion terms. The accuracy of the RNM is controlled by a user-specified threshold value, and it is shown that the RNM solutions converge to the CFD results as the threshold value decreases. Furthermore, an efficient solver for RNM is developed, with variables in all the reactors being solved simultaneously, rather than using the conventional iterative solvers that solve the reactors one by one in each iteration. Sparse matrix and analytic Jacobian techniques are utilized in the new solver to achieve a computational cost that linearly depends on the number of reactors.

Keywords: reactor network model; computational fluid dynamics; Jacobian matrix; efficient solver; sparse matrix

1. Introduction

Reactor network model (RNM) is an efficient approach to incorporate detailed finite-rate chemistry in complex flow field simulations for prediction of pollutant emissions, such as NO, CO, soot and unburnt hydrocarbons, and semi-quantitative analyses of flame responses to various controls. In the RNM approach, the full domain is segmented into a number of elementary reactors, which can be perfectly stirred reactors (PSR) and plug flow reactors (PFR), which interact with one another through pair-wise mass and energy exchanges. An empirical RNM to approximate the flow field of a gas turbine combustor was performed by Bragg [1], after which various RNMs have been developed to study pollutant formation [2–4] and blowout performance [5–7] in laboratory reactors and gas turbines. Construction of such empirical RNMs was largely based on manual combustor segmentation and estimated inter-reactor fluxes, and the resulting RNM need to be tuned to fit selected global reactor responses [8–10]. Systematic RNM construction was later proposed to automatically generate RNMs based on computational fluid dynamics (CFD) results [11–14], and automated RNM generation has been implemented into various research and commercial CFD codes. While the CFD-based RNM generation can provide significantly more sophisticated networks to approximate complex flow fields, there is a lack of criteria for rigorous flame feature segmentation and cell agglomeration. As a result, tuning is typically still needed for the RNM. Solver accuracy and efficiency is another important issue for RNM. Conventional solvers utilize iterative methods, in which the reactors are typically solved sequentially rather than fully coupled in each iteration, resulting in high computational cost as well as difficulties in convergence.
In the present study, a systematic method to segment different flame features and generate RNM based on CFD is developed. The accuracy of the RNM is controlled by a user-specified threshold error. It is shown that the RNM solutions converge to the CFD results as the threshold decreases. An efficient direct solver is further developed with all the reactors being solved simultaneously. Analytic Jacobian and sparse matrix techniques are utilized in the new solver to achieve a computational cost linearly proportional to the number of reactors.

2. Methodology

2.1 Automated RNM generation

First, chemical explosive mode (CEM) analysis (CEMA) is employed to segment complex flames in the present study. CEMA is a universal and robust flame diagnostic and can rigorously distinguish different flame zones in various turbulent flames [15–17]. The zero-crossing of the CEM eigenvalue ($\lambda_e$) indicates the local premixed reaction fronts, and the positive and negative $\lambda_e$ indicate the pre-ignition and post-ignition mixtures respectively. Figure 1 shows the CEM eigenvalue in a 1-D laminar premixed flame for stoichiometric methane-air under atmospheric pressure with inlet temperature of 300 K calculated using GRI-Mech 1.2 [18], with different colors indicating different flame zones. In the present work, $\lambda_e$ together with local temperature and equivalence ratio are used to identify CFD cells with similar thermodynamic states, which are aggregated, if being spatially adjacent, into a single PSR based on the user-specified threshold error. The residence time of each PSR in the RNM is determined by the volume of the PSR and the agglomerated inter-reactor flow rates, which are attributed to both the convection and the diffusion terms. Note that the diffusion fluxes in different directions induce two-way inter-reactor couplings in the RNM.

2.2 Efficient RNM solver

The governing equations of the RNM can be formulated as:

$$0 = \omega^i(\phi^i) + s(\phi^i) + \sum_{i=1,i\neq j}^{N} A^{i,j} m(\phi^i, \phi^j), j = 1, 2, ..., N$$

(1)

where $\omega$ indicates the reaction term, $s$ indicates the mixing term from the inlet, $m$ indicates the mixing term from other PSRs. $\phi$ is the vector of variables including temperature and species mass fraction. Superscript $i$ and $j$ indicate the $i^{th}$ and $j^{th}$ PSR, respectively, and $N$ is the total number of PSRs in the RNM. $A^{i,j}$ is the flow splitting factor, which represents the contribution of the $i^{th}$ PSR to the total mass flow into the $j^{th}$ PSR. $K$ is the number of species in the mechanism and thus total there are $(K + 1) \times N$ variables in total. The time complexity of the direct solvers based on numerical and dense Jacobian matrix is $O(N^3 + K^3)$ in the large limit of $N$, and can become prohibitive when $N$ reaches more than a few hundreds. If iterative solvers are used, convergence typically slows down as the number of reactors increases.

In the present study, a new direct solver is developed to take advantage of the sparse coupling in the RNM as demonstrated in Figure 2, which shows the pattern of nontrivial entries in the Jacobian of a 93-reactor RNM that will be elaborated in section 3.1. The Jacobian can be clearly seen to be highly sparse, and thus sparse matrix techniques can significantly improve the computational efficiency. Analytic and optimized Jacobian evaluation is further employed to minimize the computational cost [19].
Figure 1. Temperature profile of a 1-D laminar premixed flame for stoichiometric methane–air, with $\lambda_e$ indicated by the face color of the symbols.

Figure 2. Pattern of the nontrivial entries (black pixels) in the Jacobian of the 93-reactor RNM constructed in section 3.1.

Figure 3. Temperature isocontours for Sandia Flame D, calculated by RNMs of different sizes in comparison with the CFD solution.

3. **Results and Discussion**

3.1 **RNM generation and validation**

The RNMs are constructed based on the RANS of the Sandia Flame D [20], simulated by using OpenFOAM with a 16-species skeletal mechanism [21]. RNMs with 92 to 3325 PSRs are constructed from the CFD result by using various threshold values. Figure 3 compares the temperature distribution between selected RNMs with the CFD results, showing that the RNM converges to CFD as the threshold value decreases (or the number of reactors increases). Figure 4 further shows the average error in temperature as a function of the RNM size. The average error in temperature is defined as $\frac{\sum_i V_i |T_i^{RNM} - T_i^{CFD}|}{\sum_i V_i}$, where $V$ indicates the cell volume. It is seen that as the error reaches a plateau when the number of PSRs reaches about 500. Note that the error of
around 2 K in the plateau is attributed to the unity Lewis number assumption in the RNM, and vanishes when the CFD employs the same treatment. The 748-PSR RNM is further compared with the CFD results in Fig. 5 for OH and H profiles.

![Figure 4](image1.png)

**Figure 4.** Average error in temperature, as a function of the number of reactors in the RNM.

![Figure 5](image2.png)

**Figure 5.** OH and H mass fraction from the 748-PSR RNM (left panels) in comparison with CFD (right panels).

![Figure 6](image3.png)

**Figure 6.** Computational costs for the direct and iterative solvers as functions of the RNM size.

![Figure 7](image4.png)

**Figure 7.** Computational costs of the different components in the direct solver as functions of the RNM size.

3.2 Scaling of computational cost

The computational cost of the direct solver is then measured and compared with the conventional iterative solver for different sizes of RNM as shown in Fig. 6. In the calculation, the initial guesses of the variables are the average values from the CFD data in each reactor. Significant speedup and an overall linear scaling were achieved by using the direct solver. Computational costs of different components in the direct solver, including the function evaluation, Jacobian evaluation, Jacobian...
factorization and solving linear system, are further shown in Fig. 7, showing that the computational cost of each component scales linearly with the RNM size.

4. Conclusions
An automated RNM construction method based on CFD is developed. Spatially adjacent CFD cells with similar temperature, equivalence ratio, and CEM eigenvalue are aggregated into a single PSR based on a user-specified threshold value. The mass flow rates between the PSRs are evaluated as the summations of convection and diffusive fluxes between the CFD cells. The RNM results converges to the CFD results as the user-specified threshold value decreases. Furthermore, an efficient direct solver is developed by solving all the variables in the RNM simultaneously, using the TWOPNT newton solver with pseudo time stepping, analytic and optimized Jacobian evaluations, and sparse matrix techniques. Significant speedup is achieved compared with the conventional iterative solver, and a linear scaling in computational cost is achieved as a function of the number of reactors.

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6. References