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Original Paper

Reduced Chemical Kinetic Models of DME Based on Variance Filtering Method

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Abstract

Based on the variance value of each species concentration during the combustion process, a new chemical mechanism reduction method is proposed. The data sets which are the molar concentration of each species are generated based on numerical results of zero-dimensional homogeneous ignition process using detailed chemical kinetic mechanisms under various operating conditions. By calculating and analyzing the variance value of each species concentration during the combustion process to determine the contribution of each species to the combustion process, and by selecting a suitable threshold value to determine whether the species and elementary reactions are removed or not. The skeletal mechanisms of DME generated by using the present VFM method are compared to those generated by the path flux analysis (PFA) method and the detailed mechanism. The comparisons of the temperature and the concentration of important species showed that with either the same or significantly smaller number of species, the skeletal mechanisms generated by the present VFM method are more accurate than that of PFA in a broad range of initial pressures, temperatures and equivalence ratios. In addition, the reduction speed of VFM is one orders of magnitude faster than that of PFA.

Keywords

mechanism reduction, variance filtering, chemical kinetic mechanism, DME

1. Introduction

Numerical simulation of combustion reaction flows has become one of the most important tools for the development and design of high-performance burners and new alternative fuels (Hawkes, Sankaran, Sutherland, & Chen, 2005), whereas it is often difficult to reproduce the kinetic processes and flow characteristics of fuel combustion quickly and economically using detailed chemical kinetic mechanisms. Therefore, many types of mechanism reduction methods have emerged. The commonly used methods of reducing combustion dynamic mechanism contain sensitivity analysis (SA) (Turányi, 1990; Kramer, Calo, Rabitz, & Kee, 1982), principal species analysis (PCA) (Vajda, Valko, & Turanyi, 1985), direct relational graph (DRG) (Lu & Law,, 2005) and its derivative methods, including the direct relational graph based on error propagation (DRGASA) (Niemeyer, Sung, & Raju,, 2010), the modified direct relational graph (DRGEP) (Pepiot-Desjardins & Pitsch, 2008), path flux analysis PFA (Sun, Chen, Gou, & Ju, 2010), path flux analysis with multi generations MPFA (Gou, Wang, Gui, & Shi, 2012; Xiao-Long, Wei, & Ying, 2014). In addition, the mapping/storage method is also widely used, and the main representative algorithms are the dynamic adaptive list (ISAT) method (Pope, 1997), the piecewise reusable implementation of solution mapping (PRISM) (Tonse, Moriarty, Frenklach, & Brown, 2003) and the random sample high dimensional model representation (RS-HDMR) (Rabitz, Ali, Shorter, & Shim, 1999). Even though the above-mentioned mechanism reduction methods have been made in significant progress, there are still many shortcomings. Such as DRG and PFA, they all face the problem of unbearable computational time when reducing large and complex detailed reaction mechanisms. However, as an effective feature selection method in the data-driven technology, the variance filtering method (VFM) is mainly based on the variance value of the features to determine their importance in the whole system, so the VFM only needs to calculate the variance value of the features during the working period, which has a very clear physical meaning and this method is still computationally efficient for chemical kinetic mechanisms.

In this paper, we propose a chemical kinetic mechanism reduction method based on variance filtering method (VFM) and verify it based on the DME mechanism with improved model reduction accuracy compared to PFA method with the same or smaller size of a reduced mechanism.

In the following, at first, the reduction mechanism principle of the VFM method is presented and analyzed. Secondly, the computation accuracy of the VFM method is demonstrated through the comparisons with PFA reduction method from the simulations of auto-ignition of DME. Finally, the last section is a summary of the conclusions.

2. A Chemical Kinetic Mechanism Reduction Method with Variance Filtering Method

As a dimensionality reduction technique, the purpose of feature selection is to select a small set of the most representative and important features from the original features by removing redundant features. The variance filtering is a feature selection technique by selecting features based on their variance. The basic idea of this method is to determine the importance of features by calculating the variance value of each feature. If the value of the feature varies more within a certain range, it means that the feature contributes more to the whole system. For a combustion system, the molar concentration of species i can represent its importance to the whole combustion process. If the molar concentration of species i fluctuates considerably, this indicates that the species i is more actively involved in the combustion process. Therefore, it can be considered as an important species and retained.

For a system $X = \left[x_1, x_2, ..., x_n\right]^T \in R^{n \times d}$, where y_n is the molar fraction of species *i*, *n* is the number of data sets and *d* is the dimension of the samples, specifically, the number of species.

It's worth pointing out that to eliminate order of magnitude differences between the different features. The data sets need to be normalized in advance. In this paper, the max-min normalization method is selected to map the data linearly between 0 and 1. The specific expression is as follows:

$$x_{i,normalized} = \frac{x_i - x_{i,\min}}{x_{i,\max} - x_{i,\min}} \quad (1)$$

For species *i*, the mean value of the molar fraction is

$$\overline{x}_{i,normalized} = \frac{1}{n}\sum_{j=0}^{n} x_{i,normalized} \quad (2)$$

Then the variance value of the molar fraction about species *i* can be expressed as:

$$\sigma_{i,g} = \frac{1}{n}\sum_{j=0}^{n}\left(x_{i,normalized} - \overline{x}_{i,normalized}\right)^2 \quad (3)$$

In order to fully consider the effects of volatility in species concentrations, the local variance is defined, i.e.

$$\sigma_{i,l} = \max\left(x_{i,normalised} - \overline{x}_{i,normalized}\right)^2 \quad (4)$$

Therefore, the variance selected in this paper is the sum of the global and local variances, i.e.

$$\sigma_{i,c} = \sigma_{i,g} + \sigma_{i,l} \quad (5)$$

The Eq. (5) represents the degree of contribution of species *i* to the overall combustion process.

By Calculating Eq. (5) to obtain an order of importance value for each species, and judge whether to retain or discard species by selecting an appropriate threshold value ε.

3. Results and Discussion

3.1 Reduced Chemical Kinetic Model of DME at High Temperature

Dimethyl ether (DME) is an ideal alternative fuel for compression-ignition engines and its combustion mechanism is receiving increasing attention. Therefore, in this paper, the detailed mechanism of DME containing 79 species and 351 primitive reactions (Curran, Fischer, & Dryer, 2000; Fischer, Dryer, & Curran, 2000) is reduced. To verify the reliability of the VFM method, the simulation results with the skeletal mechanisms obtained by VFM are compared by those obtained by PFA and the detailed mechanism under a wide range of conditions. The details of initial conditions at high temperature are shown in Table 1.

Table 1. The Details of the Initial Conditions

Initial condition no.	Pressure (atm)	Temperature (K)	Chemical equivalency ratio
1	1.0	1200	0.8
2	1.0	1200	1.0
3	1.0	1200	1.2
4	1.0	1100	1.0
5	1.0	1400	1.0
6	10.0	1200	1.0
7	20.0	1200	1.0

Figures 1-3 shows the temperature variation curves under different equivalent ratios, temperatures and pressures. VFM-29 indicates that the skeletal mechanism of DME obtained by VFM method contains 29 species, and similar symbols in this paper represent the same meaning. As can be seen from the figure, the skeletal mechanisms obtained by VFM contains 28-41 species, and the skeletal mechanisms obtained by PFA contains 28-42 species. For the temperature prediction curves, the skeletal mechanisms obtained by VFM can still better reproduce the chemical kinetics of DME with the same or less species.

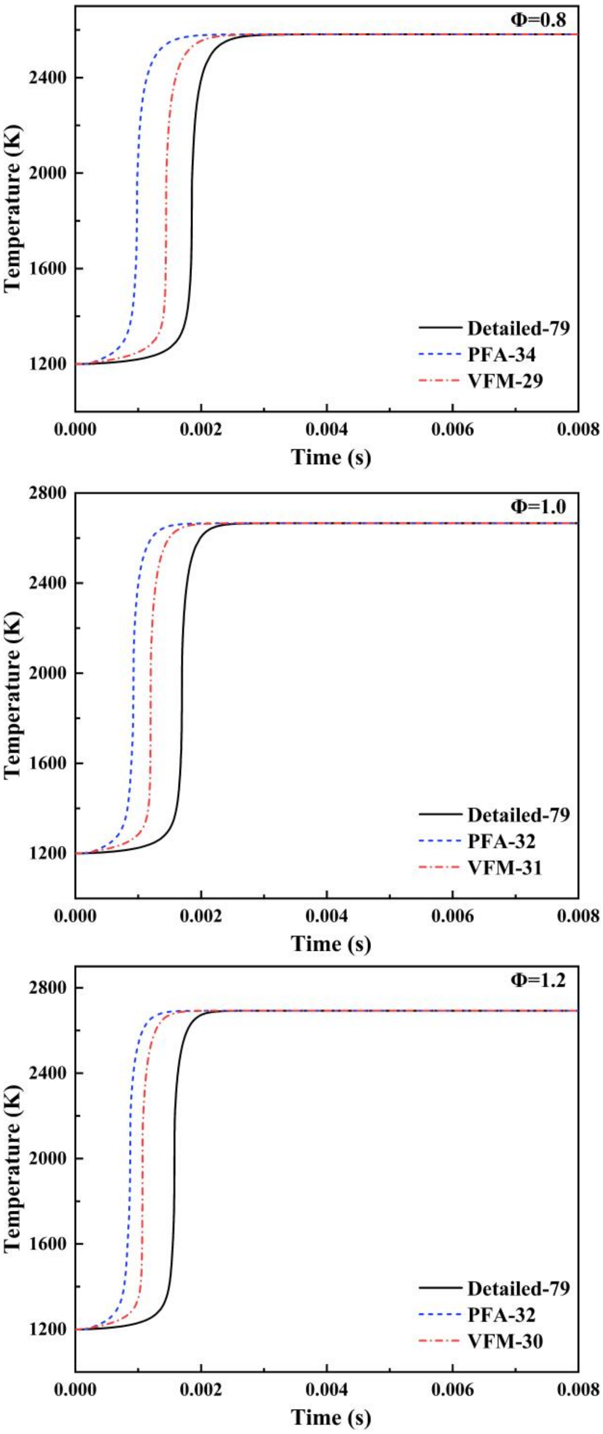

Figure 1. Comparison of Temperature Profiles in Different Stoichiometric Ratio Cases

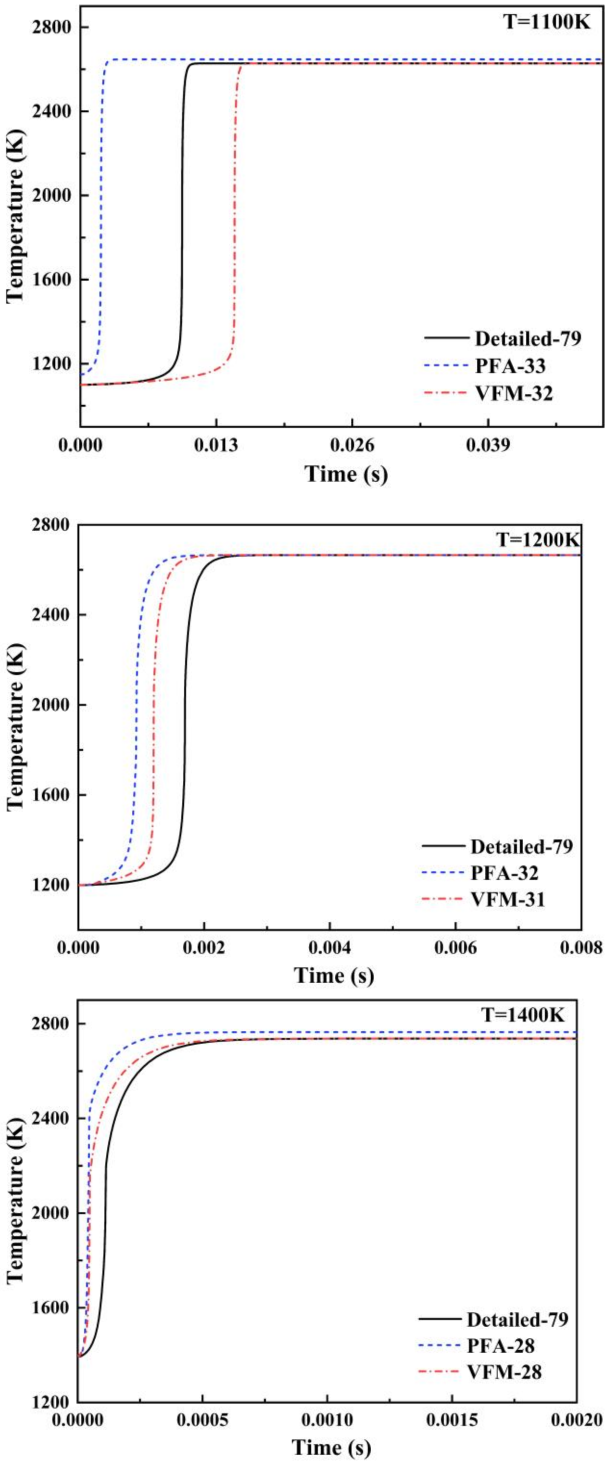

Figure 2. Comparison of Temperature Profiles in Different Temperature Cases

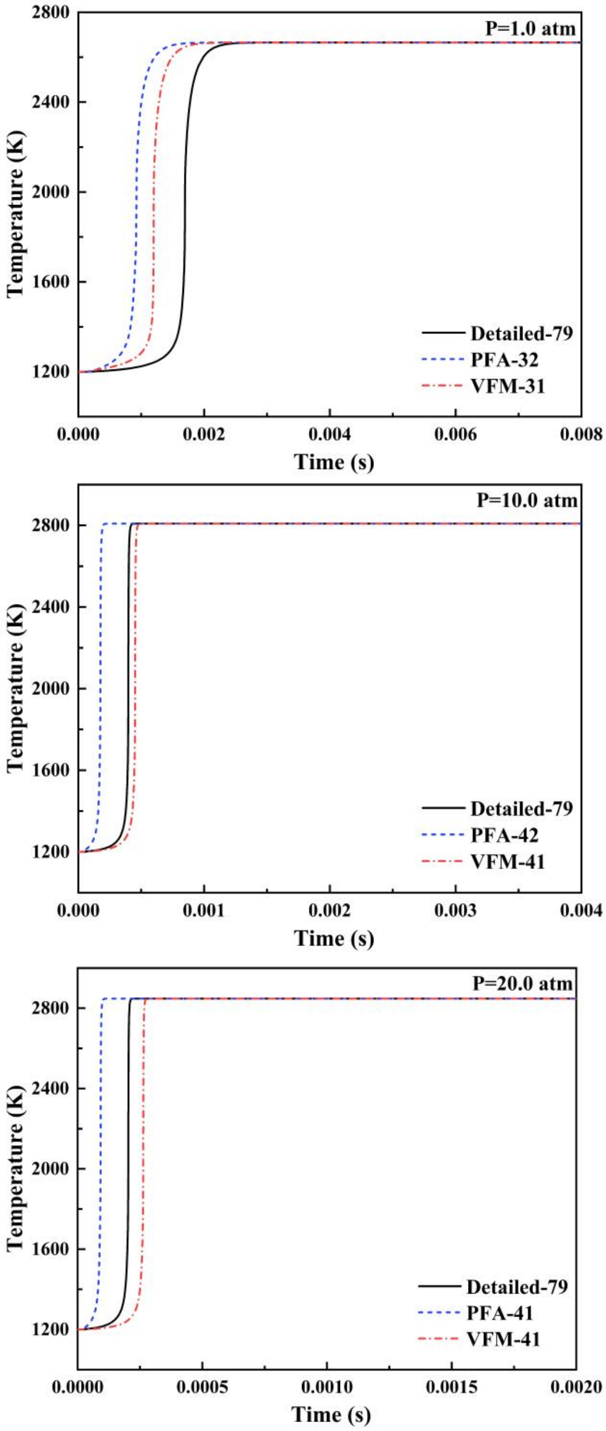

Figure 3. Comparison of Temperature Profiles in Different Pressure Cases

Figure 4 shows the concentration prediction curve of important species (CO2, O2, H2O, CH3OCH3, H and CH3) under typical conditions. As can be seen from Figure 4, the skeletal mechanism obtained by VFM contains 29 species, while the skeletal mechanism obtained by PFA contains 34 species. Although the skeletal mechanism obtained by VFM contains less species, the prediction curve of important components is still closer to the prediction curve of the detailed mechanism. For CH3, the simulation result of skeletal mechanism obtained by VFM shows the same trend as that of the detailed mechanism, while the simulation result of skeletal mechanism obtained by PFA produces two spikes, which is significantly different from the detailed mechanism simulation results. It can be seen that for the prediction of important species, the accuracy of the skeletal mechanism obtained by VFM is higher than that obtained by PFA.

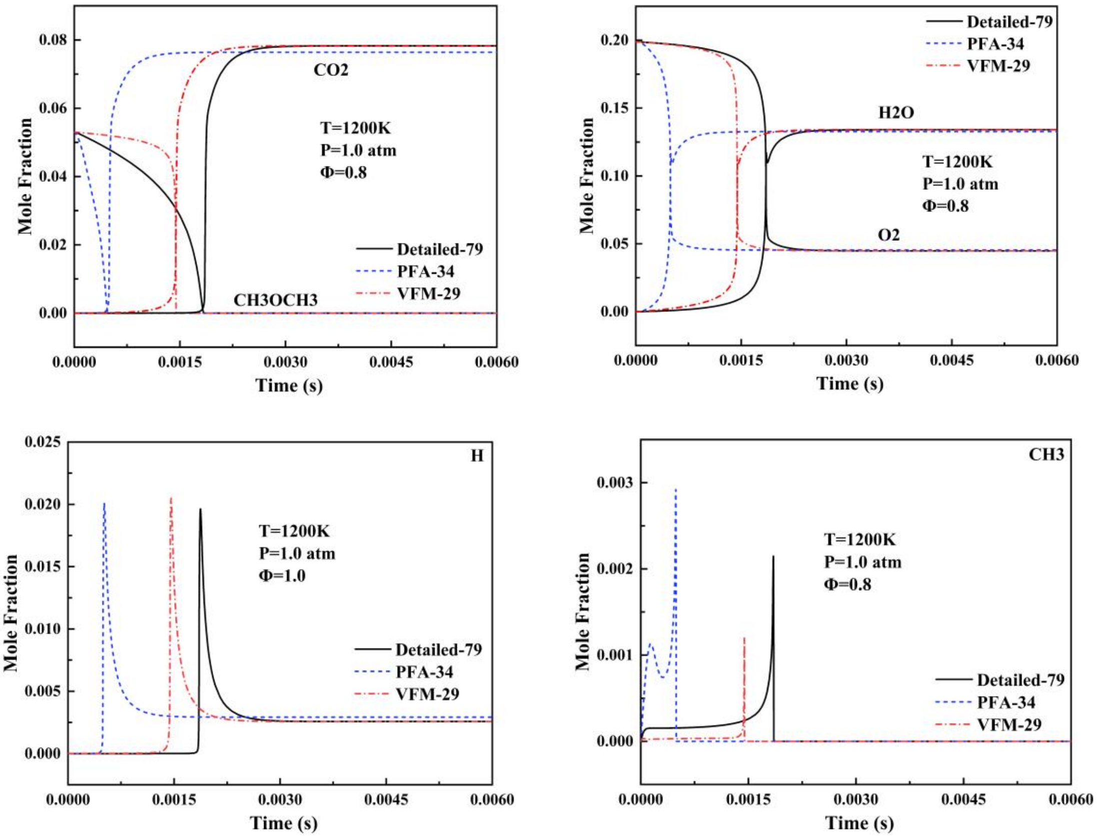

Figure 4. Comparison of Important Species Concentration Profiles in Initial Condition no.1

Table 2. CPU Time Consumption of Skeletal Mechanisms Generated by the PFA and VFM

Initial condition no.	PFA	VFM
	Time (s)	Time (s)
1	7.7	0.3
2	9.1	0.5
3	7.1	0.3
4	7.6	0.3
5	7.8	0.4
6	7.7	0.5
7	7.5	0.4

From the data in the Table 2, it can be seen that the PFA consumes one order of magnitude more CPU time than the VFM in order to obtain a high-precision skeletal mechanism.

3.2 Reduced Chemical Kinetic Model of DME at Low Temperature

The detailed mechanism of DME adopted in this paper has the characteristics of low temperature reaction and negative temperature coefficient (NTC) region. Therefore, it is very important to reduce the mechanism of DME under low temperature conditions, and the details of its verification conditions are shown in Table 2.

Figures 5-7 shows the temperature prediction curves under different equivalent ratios, temperatures and pressures. It can be seen from the Figures 5-7, in order to ensure the accuracy of the simulation results, the skeletal mechanism obtained by VFM contains at least 45 species, while the skeletal mechanism obtained by PFA has a minimum size of 47 species. Under the same working condition, the skeletal mechanism obtained by VFM contains fewer species, but the accuracy of simulation results are higher than those obtained by PFA.

Table 3. The Details of the Initial Conditions

Initial condition no.	Pressure (atm)	Temperature (K)	Chemical equivalency ratio
8	5.0	580	1.0
9	5.0	580	1.2
10	5.0	650	1.0
11	5.0	700	1.0
12	3.0	580	1.0
13	2.0	580	1.0

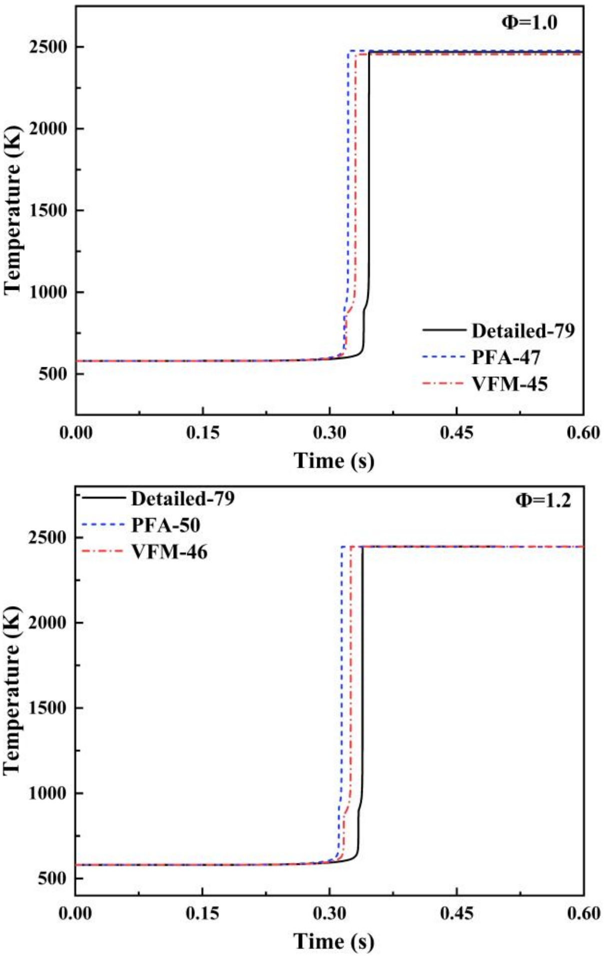

Figure 5. Comparison of Temperature Profiles in Different Stoichiometric Ratio Cases

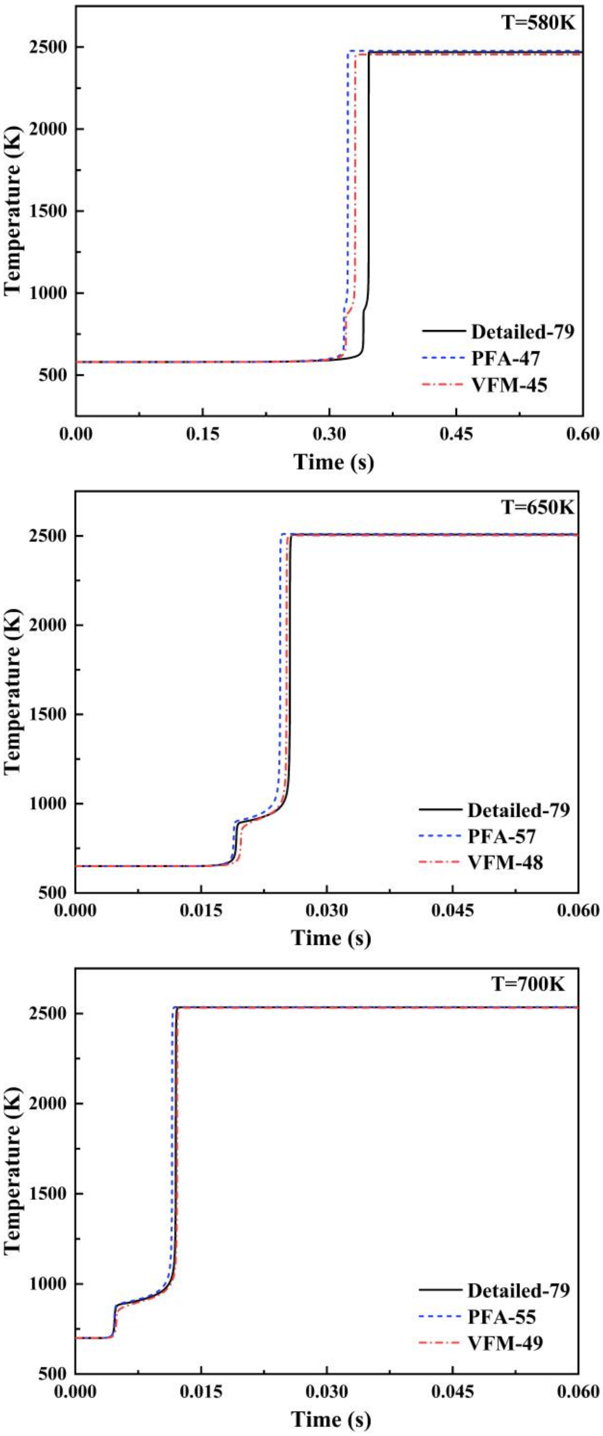

Figure 6. Comparison of Temperature Profiles in Different Temperature Cases

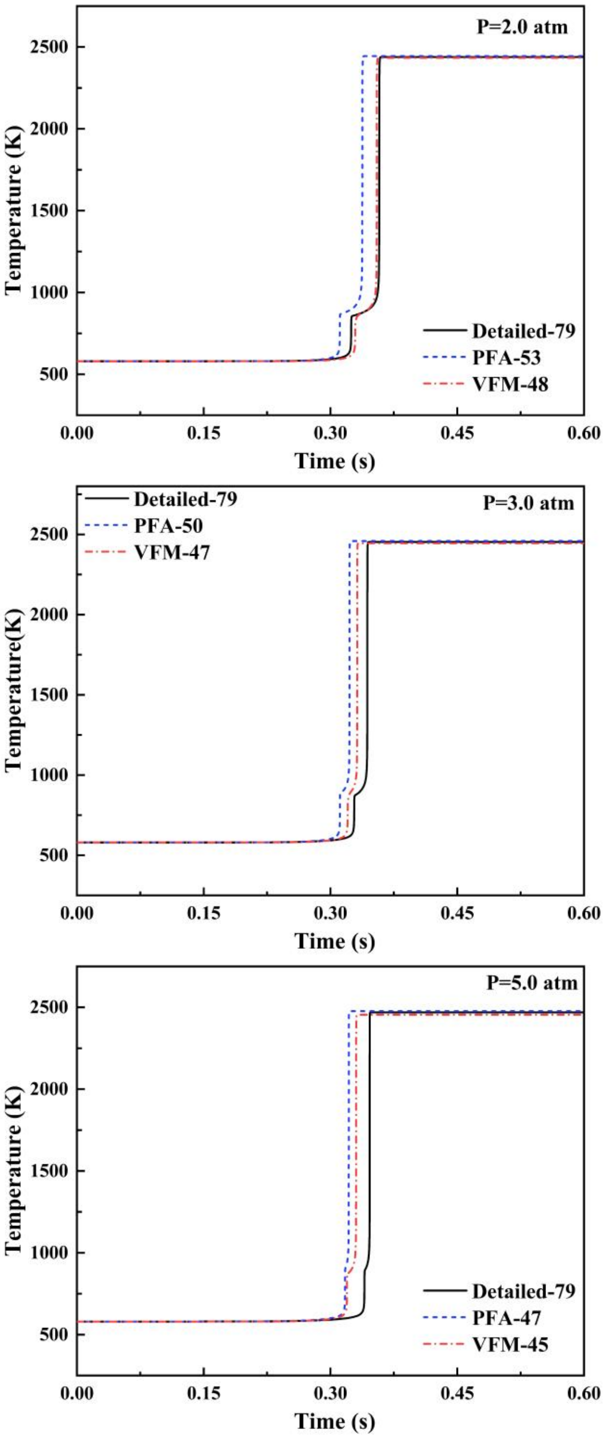

Figure 7. Comparison of Temperature Profiles in Different Pressure Cases

Figure 8 shows the concentration prediction curve of important species under typical working conditions. It can be seen from the figure 8 that the skeletal mechanism obtained by VFM contains 46 species, while the skeletal mechanism obtained by PFA contains 50 species. Compared with the simulation results of the detailed mechanism, the simulation results of the skeletal mechanism obtained by VFM are more accurate than those obtained by PFA.

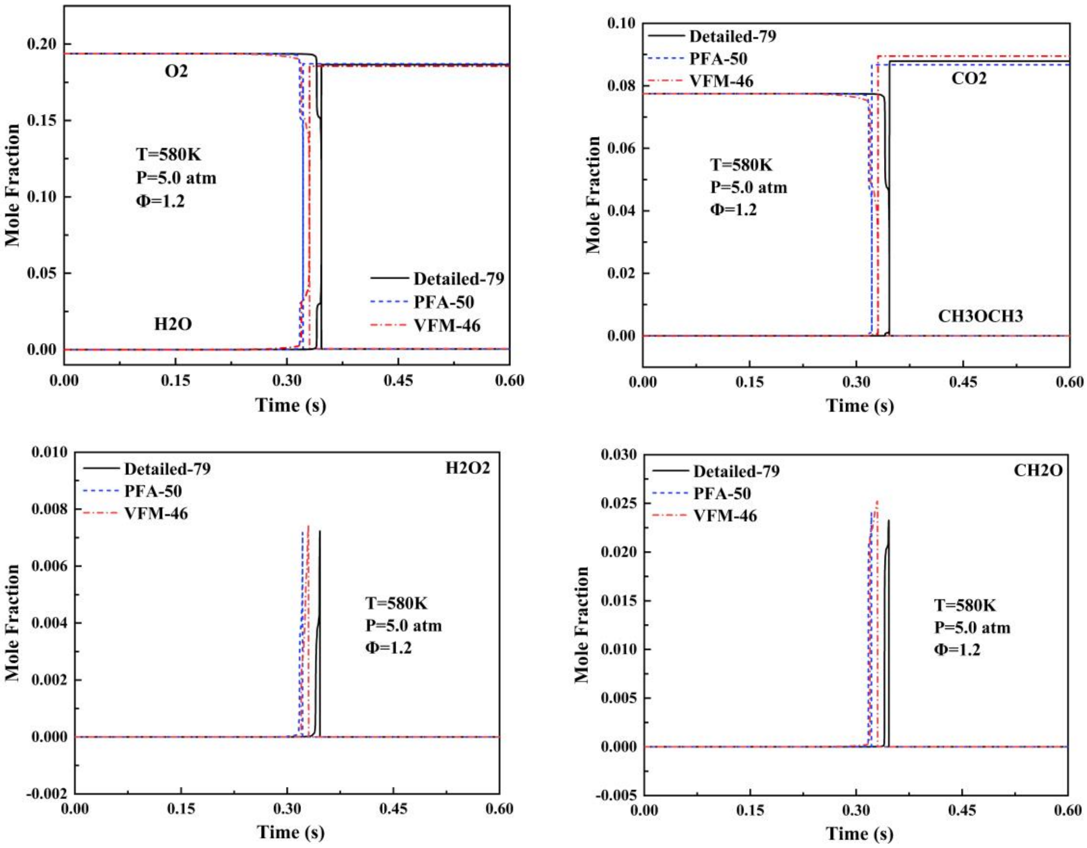

Figure 8. Comparison of Important Species Concentration Profiles in Initial Condition no.9

Table 4. CPU Time Consumption of Skeletal Mechanisms Generated by the PFA and VFM

Initial condition no.	PFA Time (s)	VFM Time (s)
8	7.5	0.2
9	8.1	0.3
10	9.5	0.5
11	9.1	0.3
12	8.9	0.4
13	8.7	0.2

Similarly, the CPU time consumed by PFA and VFM to obtain the reduced mechanisms for different operating conditions is shown in Table 4. From the data in the Table 4, it can be seen that under a wide range of working conditions, compared to the PFA, the VFM can save one orders of magnitude in CUP time.

4. Conclusion

In this work, reduced chemical kinetic models of DME are obtained based on variance filtering method. The results show the skeletal mechanisms obtained by this method ensure the computational efficiency at the same time can also effectively identify and eliminate the redundant species.

Under high temperature conditions, the skeletal mechanisms obtained by VFM contain 28-41 species, and the skeletal mechanisms obtained by PFA contain 28-42 species. Under low temperature conditions, the skeletal mechanisms obtained by VFM contain 45-49 species, and the skeletal mechanisms obtained by PFA contain 47-57 species. The results show that at the same working condition, The size of skeletal mechanism obtained by VFM is smaller than that obtained by PFA, and the reduction accuracy of VFM is higher than that of PFA, whether it is temperature curve prediction or important component concentration prediction. Moreover, the VFM can save one order of magnitude in CUP time compared to PFA.

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