A high pressure shock tube study of pyrolysis of real jet fuel Jet A

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Abstract

A typical Jet A fuel was pyrolyzed in a high-pressure shock tube at 25 and 90 atm under highly diluted conditions from 900 to 2200 K. The key species produced from the pyrolysis process were measured by gas chromatography as a function of the shock temperature. It was found that despite the compositional complexity of the fuel, the major pyrolysis products include a handful of species. They are ethylene, methane, hydrogen, propene, 1-butene, iso-butene, benzene, toluene, acetylene, 1,3-butadiene, allene and propyne, etc. Among them, ethylene is the most dominant species. The HyChem model recently proposed for the same fuel was used for prediction and comparison with the experimental data. Considering that the HyChem model was developed using shock tube and flow reactor data collected over a range of conditions significantly different from those of the current study, the agreement between the current experiment and model prediction is satisfactory. A Monte Carlo analysis was carried out that examined the sensitivities of the model predictions to the rate parameters. The results indicate that the effects of the uncertainties of *A* factors and those of activation energy are of significance in different temperature regions. Moreover, the low temperature region is dominated by the fuel pyrolysis reactions, while the high temperature region is dominated by the foundational chemistry which describes the pyrolysis and oxidation of fuel pyrolysis products.
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1. Introduction

A basic understanding of fuel combustion chemistry is critical to a better design of aircraft engines. A fundamental challenge in building reliable reaction models for jet fuels is the large number of reactions and species involved in the reaction process. For example, Jet A fuel is composed of thousands of hydrocarbon species that cannot be tracked at the level of each of these species. The approach of building a surrogate fuel mechanism [1,2] has been commonly used in the past in order to overcome this difficulty. However, surrogate fuel models are still not compact enough to enable CFD simulations of real combustor processes even after mechanism reduction. Previous studies

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[1,3–6] showed that during the oxidation of large hydrocarbons fuels, fuel pyrolysis is separated from the oxidation of the resulting pyrolysis products in high-temperature combustion. The decoupling of pyrolysis and oxidation opens up an opportunity for building simpler hybrid chemistry model for multicomponent real fuels in which the fuel decomposition is described by a small set of reactions, leading to the production of a handful of intermediates, followed by the use of a detailed chemistry model to describe the oxidation of these intermediates [7]. The products of large hydrocarbon pyrolysis are mostly small species including CH_4, H_2, C_2H_4, C_3H_6, 1-butene, benzene, and toluene. These species typically have reasonably accurate kinetic models for their further decomposition and oxidation. Based on these observations, a new chemical kinetics model for Jet A combustion, called the HyChem model, has been proposed recently [7,8]. This approach makes the assumption that the major pyrolysis processes of a multicomponent fuel are dominated by H-abstraction followed by C–C β-scission. Since the H-abstraction reactions are rate limiting, the reaction processes can be described by a small number of lumped reactions that directly form small intermediate products. For example, a long-chain alkane such as n-dodecane produces mainly CH_4, H_2, C_2H_4, C_3H_6, and 1-C_4H_8 through H-abstraction and a series of β-scission reactions, which proceed rapidly once initiated, without being significantly interfered by other reactions. The resulting species undergo further reactions to form C_2H_2, allene, propyne, etc., or are oxidized in the presence of oxygen, all of which can be modelled by a foundational chemistry model rather reliably.

As a part of the collaborative research for the HyChem model development, experiments of Jet A pyrolysis were conducted here at high pressure and in highly dilute argon mixture. All of the major pyrolysis product species were measured and compared to the results predicted by the HyChem model. Further analysis of the model was conducted using Monte Carlo simulations with an emphasis on the uncertainties in the rate parameters arising from experimental and foundational fuel and pyrolysis chemistry model uncertainties.

The fuel of interest to the current study is an average Jet A (POSF#10325). This fuel is designated as A2 fuel in the recent National Jet Fuel Combustion Program [9] and has an average molecular formula of $C_{11.37}H_{21.87}$. The main components are, by mass, 20.0% n-paraffins, 29.5% iso-paraffins, 24.9% cyclo-paraffins, 6.8% dicyclo-paraffins, and 18.7% aromatics.

2. Experimental setup

Shock tube experiments were carried out in the high-pressure single pulse shock tube (HPST) at University of Illinois at Chicago. The pressure range of the HPST is between 15 and 1000 atm. Details are described elsewhere [10,11].

The HPST is connected to two gas chromatographs (GC) by an online sampling system modified from the previous setup [12]. The high-pressure post shock gas is injected into the sampling line through a pneumatic valve (lasting about 200 ms). The online injection system utilizes a narrow tube to bring the sampled gas to the GC sample loops and the pressure is stabilized before the sample is injected into the GC columns. The sampling line is treated with Silktek/Sulfinert coatings to prevent loss of hydrocarbon species throughout the sampling process, and maintained at 150 °C to prevent condensation before the sample gas enters the GC column.

Two nominal pressures (25 and 90 atm) were used for the pyrolysis experiments. The fuel concentrations were 52.3 ppm in argon for both sets of experiments. Temperatures behind the reflected shock wave ranged from approximately 900 K to 2200 K. The average nominal reaction time was 2.3 ms. The entire HPST is heated to 100 °C to prevent fuel condensation. Cleaning shocks are performed after each shock experiment, in which only argon with trace oxygen is shock heated to extremely high temperature to remove species that might remain from the last experiment.

The temperatures were obtained from calibration by two chemical thermometers [11,13], 1,1,1-trifluoroethane (TFE) [14] and cyclopropyl cyanide (CPCN) [15]. For the TFE temperature calibration, the recently updated rate parameters at the high-pressure limit from Matsugi [14] were used. Considering the uncertainties of the rate constants given by Matsugi [14] and other experimental uncertainties, $\pm$ 30 K is an estimate of the temperature uncertainty for our species profiles below 1450 K. For higher temperatures, the uncertainties can be slightly higher.

Direct measurement of the exact amount of Jet A injected cannot be easily made because of the multicomponent nature of Jet A. Consequently, we conducted total carbon experiments through CO_2 conversion to obtain the initial fuel concentration. CO_2 concentrations were obtained by making another mixture with the same concentration of fuel, but having some of the argon replaced by oxygen. A shock is generated above 2200 K to ensure complete oxidation of the fuel. The amount of oxygen used ensures that the equivalence ratio $\phi << 1$ and the fuel is fully oxidized to CO_2. The CO_2 mole fraction is converted to the mole fraction of Jet A according to the average carbon number per fuel molecule. The CO_2 conversion experiments were repeated several times, leading to the determination of 52.3 $\pm$ 1.5 ppm of initial fuel mole fraction.
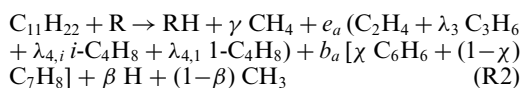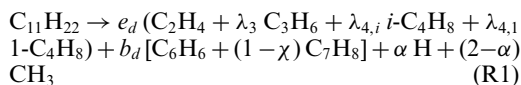
Pyrolysis products were measured and quantified using flame ionization detectors (FID). Species were identified through calibration gas compar-

isons and by GC/MS. The mole fractions of the major species were quantified by using specialty gas mixtures with argon as diluent gas.

3. Modelling

3.1. HyChem model

The HyChem model used here was developed for the same Jet A fuel (POSF#10325). The model consists of 119 species and 841 reactions, and is comprised of a single-species, seven-reaction fuel pyrolysis submodel and USC Mech II [16] as the foundational fuel chemistry model. The fuel pyrolysis reactions are given as follows:

$$C_{11}H_{22} \rightarrow e_d \, (C_2H_4 + \lambda_3 \, C_3H_6 + \lambda_{4,i} \, i\text{-}C_4H_8 + \lambda_{4,1}$$
$$1\text{-}C_4H_8) + b_d \, [C_6H_6 + (1-\chi) \, C_7H_8] + \alpha \, H + (2-\alpha)$$
$$CH_3 \qquad \qquad \text{(R1)}$$

$$C_{11}H_{22} + R \rightarrow RH + \gamma \, CH_4 + e_a \, (C_2H_4 + \lambda_3 \, C_3H_6$$
$$+ \lambda_{4,i} \, i\text{-}C_4H_8 + \lambda_{4,1} \, 1\text{-}C_4H_8) + b_a \, [\chi \, C_6H_6 + (1-\chi)$$
$$C_7H_8] + \beta \, H + (1-\beta) \, CH_3 \qquad \text{(R2)}$$

where λ_3, $\lambda_{4,i}$, $\lambda_{4,1}$, χ, α, β and γ are stoichiometric parameters whose values were determined experimentally in Stanford shock tubes and flow reactor [7,8], and e_d, e_a, b_d and b_a are variables that can be determined from λ_3, $\lambda_{4,i}$, $\lambda_{4,1}$, χ, α, β and γ by elemental conservation. In the determination of the stoichiometric coefficients and rate parameters, two earlier speciation experiments at Stanford were conducted with higher concentrations of fuel in dilute mixtures and at lower pressures (1–15 atm): time-resolved shock tube experiments with laser diagnostics and flow reactor experiments with gas chromatography. The model was tested against global combustion properties: ignition delay, flame speed and flame extinction strain rate [7,8]. The Jet A model used here is provided in the Supplementary information.

3.2. Simulations and Monte Carlo analysis

The CHEMKINPRO 0-D homogeneous reactor model is used for simulations. All simulations were made under constant pressure of 25 atm, with a nominal reaction time of 2.3 ms. A uniform reaction time for all shock simulations was used because there is minimal difference between it and the simulation using the times measured for each shock. The parameters of the HyChem model including both submodels were studied using Monte Carlo sensitivity analysis, in which a rate parameter is randomly varied based on a prescribed probability distribution to be described later. In each simulation, the A factors or the activation energies of all, or a subset, of the reactions being studied were varied randomly and independently within a predefined range. The software package for the Monte Carlo analysis was originally built as described in

Fridlyand et al. [17] and used with small modification here.

4. Results and discussions

4.1. Experimental results

The experimental results show that at the pressures tested, the major stable product species are CH_4, C_2H_4, C_2H_2, C_2H_6, C_3H_6, pC_3H_4 (propyne), aC_3H_4 (allene), $1\text{-}C_4H_8$, $i\text{-}C_4H_8$, $1,3\text{-}C_4H_6$, C_4H_2 (diacetylene), C_4H_4 (vinylacetylene), cyclopentadiene, 1,3,5-hexatriyne, benzene, and toluene. Figure 1 presents the results for selected species. The experiments under the two pressure conditions show nearly the same results. In what follows, we will primarily use the data from 25 atm for discussion.

Ethylene is the dominant species below 1450 K. It starts to be formed at around 1050 K, and rises to its peak value at $\sim$1350 K. As the temperature rises further, C_2H_2 becomes the dominant species. An assumption, introduced earlier [7,8] and supported by the data shown here, is that C_2H_4, as well as CH_4, C_2H_6, C_3H_6, $1\text{-}C_4H_8$, $i\text{-}C_4H_8$, benzene, and toluene are the key species formed below $\sim$1400 K. The peak concentrations of C_2H_4, C_3H_6, $1\text{-}C_4H_8$, and $i\text{-}C_4H_8$ are in a decreased order, even after conversion to their contributions to the total carbon. CH_4, C_2H_6, benzene, and toluene all contribute significantly to the total carbon count. CH_4, benzene, and toluene are quite stable, and are still present in significant amounts at high temperatures. On the other hand, the concentration of $1\text{-}C_4H_8$ starts to decrease around 1200 K because of its decomposition. Like C_2H_4, aC_3H_4 and pC_3H_4 eventually decompose and are converted to C_2H_2, diacetylene, or polyacetylenes above 1400 K.

The carbon total based on all the major products, which are the species shown in Fig. 1 and also vinylacetylene, allene, cyclopentadiene, 1,3,5-hexatriyne, is plotted against shock temperature in Fig. 2. It shows that the fuel decomposition starts at around 1050 K, the same temperature at which C_2H_4 starts to appear. At 1300 K, almost all the initial jet fuel components have broken down in about 2.3 ms reaction time to the small product species. The carbon profile flattens at around 570 ppm, which is about 96% of the initial fuel's carbon total based on the CO_2 measurement. The findings further support the assumptions of the HyChem approach: almost all the jet fuel components break down into a small number of small species rapidly at relatively low temperature compared to the combustion reaction temperature.

It should be noted that a careful comparison of the experimental data between the two pressures shows some dependency of the production of C_2H_6 and C_4H_2 on pressure. C_4H_2 production is somewhat smaller at 90 atm than at 25 atm, though the difference is small.
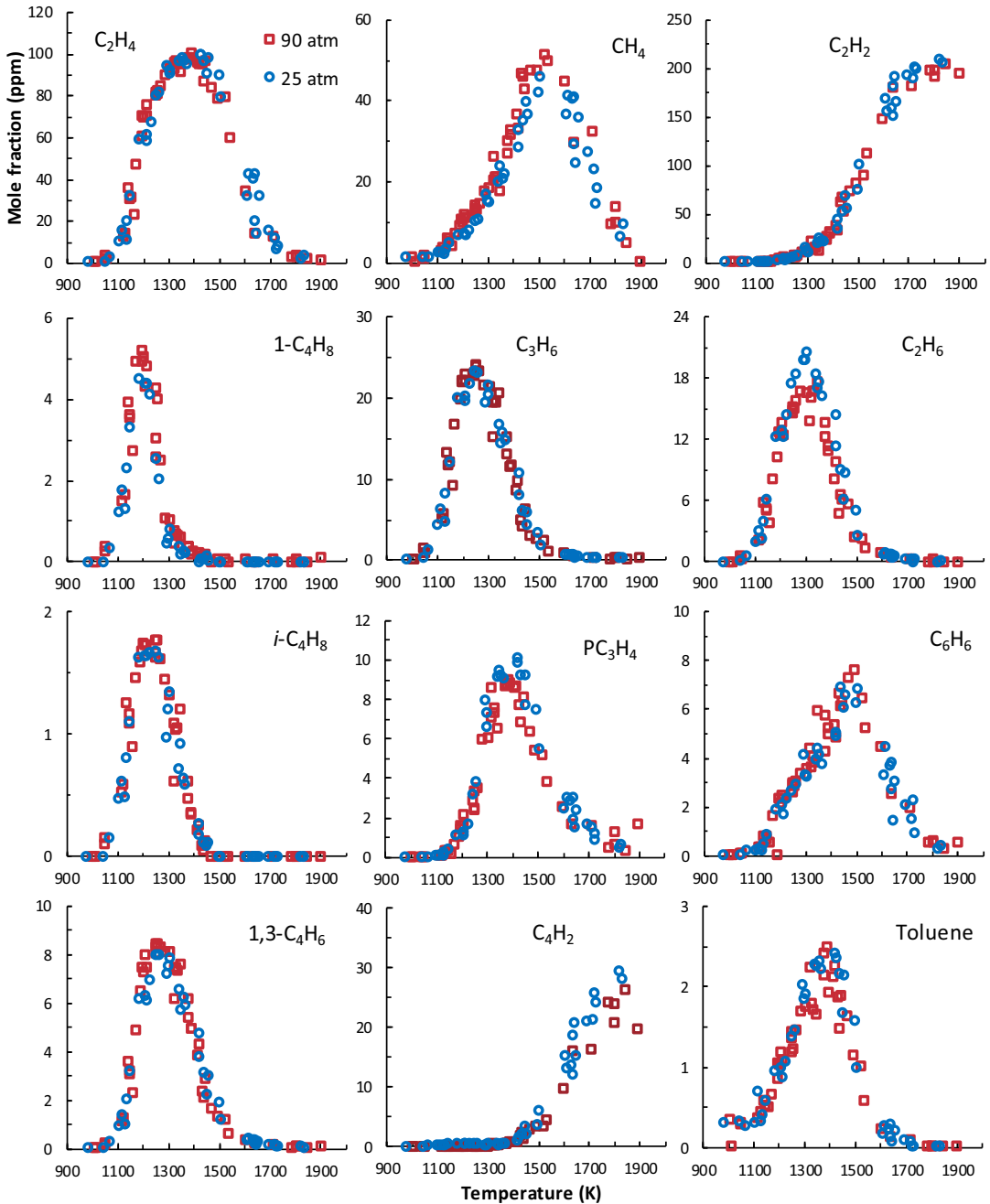
Fig. 1. Species measured at 25 and 90 atm post shock pressures (P_5) and at 900–2000 K post shock temperatures (T_5). Initial fuel mole fraction is 52.3 ppm in argon.

4.2. Comparison between the model and experiments

Simulations using the HyChem model were compared with the current experimental data. Considering that the model parameters were de-

rived earlier from shock tube and flow reactor experiments [8] under thermodynamic conditions significantly different from those of the current experiments, the agreement between the current experimental data and model predictions is satisfactory. Figure 3 shows the comparisons of ma-
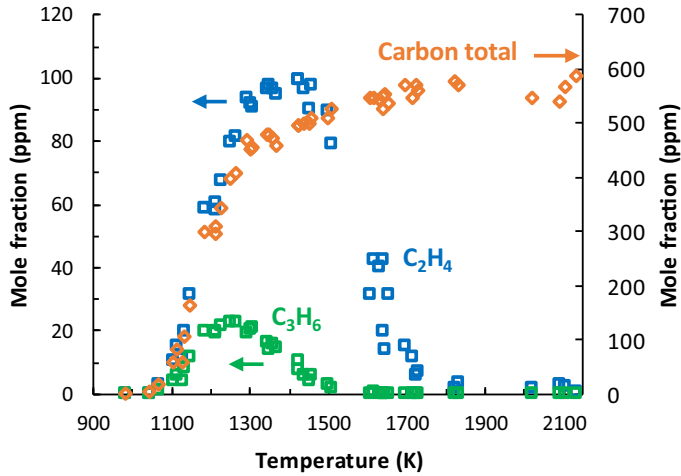
Fig. 2. Formation of C_2H_4 and C_3H_6 compared to the carbon total of all major species from pyrolysis of 52.3 ppm Jet A in argon at 25 atm with 2.3 ms of reaction time.
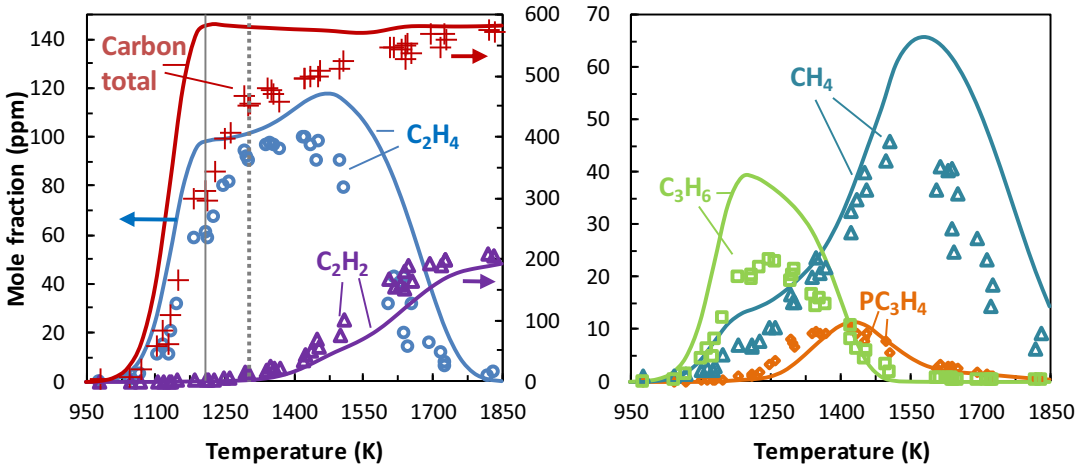

Fig. 3. Comparisons of selected experimental (symbols) and predicted (lines) species concentrations in the pyrolysis of 52.3 ppm Jet A in argon at 25 atm with 2.3 ms of reaction time. The grey vertical lines represent the approximate temperature where the ethylene concentration profile first flattens with respect to temperature for simulations (solid) and experiments (dash).

jor species. Overall, the predictions are in reasonable agreement with the experimental data for C_2H_4, CH_4, pC_3H_4, aC_3H_4 (not shown) and C_2H_2. Other key species, including C_3H_6 and $1\text{-}C_4H_8$ (not shown) are not as well predicted. For example, the model over-predicts the peak concentration of C_3H_6 by about 50%. It also overpredicts benzene and toluene concentrations quite significantly, while 1,3-butadiene is underpredicted.

The model predicts a fast fuel decomposition rate as evidenced by the comparison of carbon total profiles (Fig. 3). Likewise, the rise in the predicted C_2H_4 concentration is also more rapid than the experiment. The peak value from model pre-

diction occurs at around 1500 K, which is slightly higher than that determined by the experiment. That peak concentration predicted for ethylene is also slightly higher than the experiment. In this region (∼1500 K) and towards higher temperatures, the C_2H_4 concentration becomes sensitive to the accuracy of the foundational chemistry, as we will show later in the Monte Carlo analysis later.

Despite the difference in the model predictions and the experimental results, an examination at the carbon total and C_2H_4 profiles indicates that both the model and experiment show that the consumption of the fuel is almost entirely coupled with the production of C_2H_4. When the production of C_2H_4

levels off with respect to temperature, fuel decomposition is also complete. The turning point is shown in Fig. 3 by the two vertical lines corresponding to the temperatures at which the ethylene concentration profile first flattens with respect to temperature. The experimental results show that the carbon total due to the major species still rises as a function of temperature, while the model prediction reaches the plateau value at around 1200 K.

Overall, there are general agreements between the model and the experiment on the important species that have an impact on the subsequent oxidation chemistry in an oxidizing environment. The main difference between the experiment and model is that the model predicts a faster fuel decomposition with respect to temperature.

4.3. Monte Carlo sensitivity analysis

As discussed earlier, the HyChem model parameters were derived from the Stanford shock tube and flow reactor experiments over the pressure range of 1–15 atm. For the discrepancy observed between the model and the current experiment, there are at least two potential causes. First, the shock tube data used for HyChem parameter determination are somewhat inconsistent with the data from the current study. Second, assumptions in the fuel pyrolysis model, and especially about the pressure independency of the stoichiometric and rate coefficients, cause discrepancies at high and low pressures. In the simulation results of 25 and 90 atm shocks (presented in Fig. S1 of the Supplementary material), there is little pressure effect on major pyrolysis product mole fractions below 1400 K. The simulation results only show a small dependency on pressure at high temperatures (> 1500 K) where the chemistry is dominated by the foundational fuel chemistry model (USC Mech II), not the lumped-step pyrolysis submodel in HyChem. The fact that the current experiments also show identical fuel decomposition rates and nearly identical pyrolysis product distributions at 25 and 90 atm suggests that the HyChem parameters are indeed supposed to be independent of pressure, at least above 25 atm. While the potential causes for the discrepancies are still being investigated, we performed here a Monte Carlo analysis of the rate parameters of all the reactions in the model with respect to the experiments at 25 atm. In practice, all rate parameters in a model have uncertainties. The Monte Carlo analysis will give us a measure of the sensitivity of model predictions to the uncertainties of rate parameters with temperature. A higher sensitivity of species output to those uncertainties at a given temperature can contribute to larger discrepancies between the model and experiments at that temperature, if the model was not built upon those same experiments. The simulations comprise two sets, each of which covers a range of temperature and used 2000 model samples for each tem-

perature. In the first set, the A factor of every reaction was varied randomly by a uniform distribution in the ± 30% band from the nominal rate value. In the second set, the activation energies were randomly varied, with a Gaussian distribution using 5% as the 2σ uncertainty. The band, ± 30%, for the A factor is chosen as a conservative estimate for all reactions as pointed in [17]. The 5% uncertainty for E_a is a general estimate based on the uncertainty values that often occur, as can be seen in [18]. Additionally, the effect of the rate parameter uncertainties of the two submodels were also separately studied. In this additional investigation, only one submodel's parameters were randomly changed for each simulation. The results of all the Monte Carlo analysis described above are given in Fig. 4.

Uncertainties in the A factor could play a significant role in the high temperature region, while it shows a weak effect on the rise of the C_2H_4 and CH_4 concentrations in the low temperature region. In this same temperature regime, the productions of C_2H_4 and CH_4 are more sensitive to the activation energy. At low temperatures, the band from the 5% uncertainties in E_a covers the experimental results of C_2H_4 and to a large extent, also CH_4. A clear separation of the influence of the fuel pyrolysis submodel and that of the foundational chemistry submodel along different temperature regions is also observed. In Fig. 4, in the low temperature region, the red symbols overlap with the dashed lines for the cases of both A factor and E_a, while the blue symbols overlap with the solid lines. This indicates that the low temperature region is dominated by the fuel pyrolysis lumped reactions, and that the uncertainty from the foundational chemistry has negligible effect. In contrast, in the high temperature region, the blue symbols overlap with the dashed lines, while the red symbols overlap with the solid line. This indicates that in the high temperature region, the foundational chemistry becomes the dominant submodel, while the uncertainties from the fuel pyrolysis submodel show negligible effect on the species output. A further investigation in the foundational chemistry should improve the predictions in the high temperature region. The Monte Carlo analysis also shows that the experiments and model are in best agreement for a species when it has low sensitivity to both submodels in that region (around 1350 K for C_2H_4 and around 1400 K for CH_4).

It should be noted that under oxidative conditions, the oxidation chemistry is coupled with pyrolysis chemistry above 1400 K and as such the oxidative chemistry can impact the pyrolysis product distribution in a major way. The level of difference observed in the model pyrolysis predictions above this temperature does not necessarily translate to a significant difference in the predicted combustion responses. This shock tube study, along with model analysis, serves the purpose of presenting
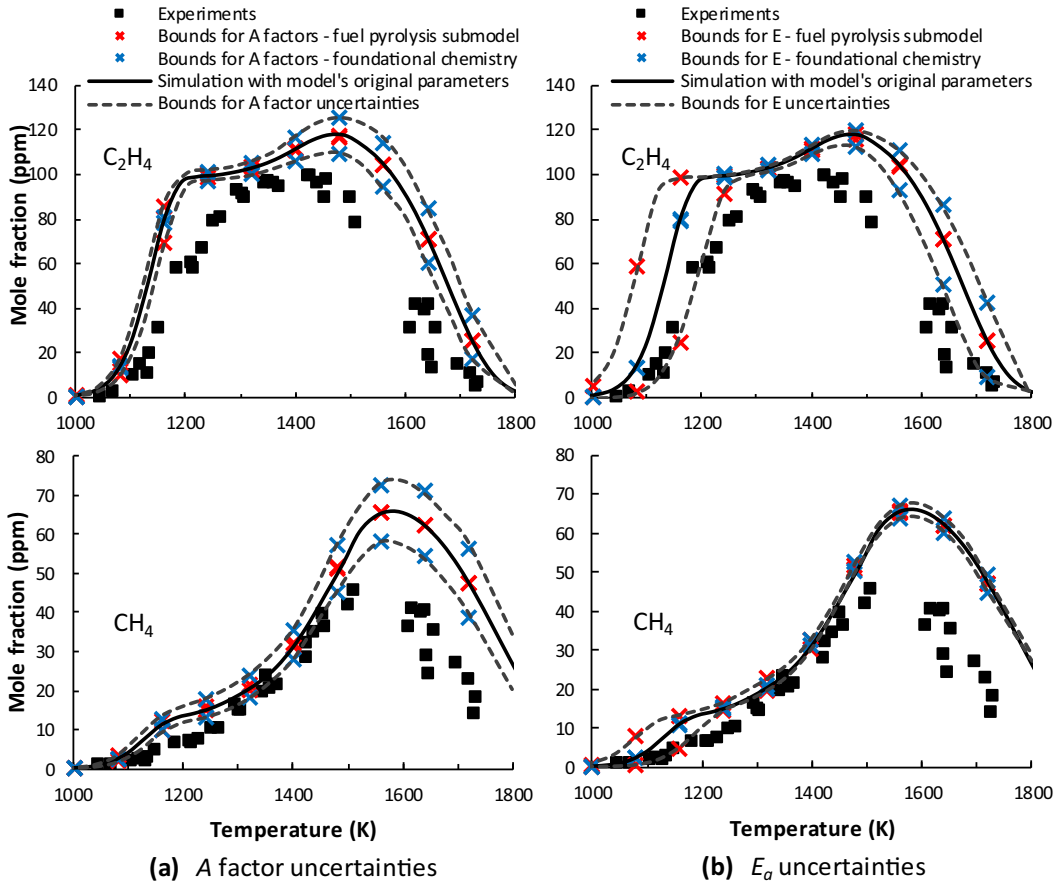
Fig. 4. Monte Carlo results of the sensitivities of C_2H_4 and CH_4 to (a) the A factor and (b) the activation energy E_a. Symbols are experimental data at 25 atm. Solid lines are nominal predictions, and dashed lines represent 95% confidence intervals from (a) the A factor sampling within a $\pm 30\%$ uniform distribution for each A factor and (b) E_a sampling with a Gaussian distribution using 5% as the 2σ. The coloured symbols represent bounds when the rate parameters of either only the fuel pyrolysis submodel (red) or only the foundational chemistry submodel (blue) are varied. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

experimental data under conditions (high pressure and highly dilute fuel/argon mixture) different than those from which the model was developed (lower pressure and high fuel concentration). To this end, the results of the sensitivity analysis motivate future studies in real fuel combustion chemistry, especially in understanding the limitations in model assumptions.

5. Conclusions

A shock tube study of the species formed from the pyrolysis of a typical Jet A was performed at 25 and 90 atm in highly diluted fuel/argon mixtures. The experimental results were compared with predictions of the HyChem model recently developed from lower-pressure shock tube and flow reactor experiments on the same fuel. The experimental data acquired in the current study support an important assumption of the HyChem modelling approach, in that the pyrolysis of the multicomponent Jet A fuel occurs rather fast, and the fuel fragments into a handful number of simple stable species that have well-defined pyrolysis and oxidation kinetics. Considering that the HyChem model was developed from thermodynamic conditions considerably different from those used in the current study, the agreement between model simulations and experiments is satisfactory. Monte Carlo sensitivity analysis of the model rate parameters gives a better understanding of the model. The results indicate that below 1250 K, the production of ethylene and methane is largely sensitive to the activation energies of the fuel pyrolysis reactions, while above 1500 K, the predictions are more sensitive to the A factors of the rate coefficients in the foundational fuel chemistry model.

Acknowledgements

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.proci.2018.05.136.

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