Fuel-specific compact kinetic models for conventional and alternative aviation fuels

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Abstract
To be useful for computational combustor design and analysis, combustion kinetic models must be sufficiently compact so that they can be used in multi-dimensional reacting computational fluid dynamics (CFD) simulations. A second, frequently overlooked aspect of computational engine analysis is the significant variability in combustion and emissions behaviors due to fuel composition variations. Notably, many alternative fuels under consideration for certification have a reduced (or absent) aromatics fraction, which has implications for fuel performance. The present work addresses the need for fuel-specific, CFD-appropriate compact kinetic models of aviation fuel combustion. We herein demonstrate results of a kinetic model compaction and optimization scheme that transforms detailed, general kinetic models for aviation fuels (here, tested for > 3000 species) into several separate, fuel-specific compact models (≤ 30 species) for prediction of global combustion behaviors. Particular fuels addressed include a conventional Jet-A/JP-8, an isomerized paraffinic kerosene (IPK), and a natural-gas derived synthetic kerosene (S-8).

Introduction

The need for significantly reduced combustion kinetic models for modeling of real fuel combustion chemistry is well-known [1, 2]. Detailed kinetic models for even relatively simple aviation surrogate fuels may involve hundreds of species and thousands of reactions [3], which renders them intractable for CFD applications even after significant reduction. For these cases, computational costs associated with the implicit integration of the stiff chemical source term account for the majority of the computational burden for the entire reacting flow problem. Moreover, detailed chemistry often contributes negligible additional insight to analysis of simulation results, and computational predictions may still suffer from kinetic uncertainties of similar magnitude to those attributable to the flow field submodel [4].

In contrast, the simplicity and relatively low computational cost of (semi)global models of a few steps involving only a handful of species [2, 5] is offset by the inability of such models to predict combustor temperature distributions [6]; emissions (e.g., CO and non-equilibrium NO_x); and performance-constraining combustion dynamics behaviors such as lean blow-off (LBO), high altitude relight, and flashback. These global models typically lack feedback coupling of radical and small molecule chemistry with the decomposition of the assumed parent fuel molecule [2, 6-8], which is mechanistically necessary for prediction of the composition, size, and dynamics of the radical pool. The radical pool, in turn, significantly influences both emissions (e.g., NO_x) and global reactivity characteristics associated with ignition, local/global extinction, flame-out, and flame propagation. Therefore, well formulated, compact kinetic schemes on the order of a few dozen reactive species can provide a compromise between predictive fidelity in combustion behavior and computational cost. These models are

sufficiently detailed to capture the reacting flow feedback dynamics among fuel, intermediates, pollutant species, and radicals without the computational complexity associated with larger models.

While such compact models are necessary to support computational engine analysis, they are not sufficient. A second, often overlooked aspect of computational engine analysis is the significant variability in combustion and emissions behaviors due to *variations in fuel composition* (e.g., [9-11] and **Figure 1**). Many surrogate fuel formulation [12, 13] and reduced kinetic model construction approaches [14] lack consideration of *real fuel compositional variation*, which is expected to become even greater as alternative fuels are used to blend into conventional Jet A/JP-8 aviation fuels. Further, many alternative fuels under consideration for certification have a reduced (or absent) aromatics fraction, which implies reduced particulate emissions among additional implications for engine performance.

In short, robust multi-dimensional, multi-physics modeling and analysis of aviation turbine combustors requires compact CFD kinetic models that can be used
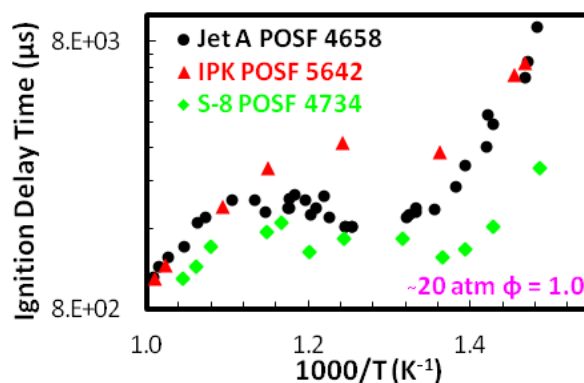

Fig. 1. Comparison of measured ignition delay times (emphasis for T ≤ 1000 K) for stoichiometric mixtures of conventional Jet A and alternative IPK and S-8 jet fuels near 20 atm [9] (Wang & Oehlschlaeger) Depending on temperature, t_{ig} varies by up to a factor of ~3.

for the compositional spectrum of conventional as well as next-generation aviation fuels. Consequently, our compact modeling approach has been developed to address *both* fuel property variation in the physical domain *and* kinetic modeling efforts in the computational domain. This permits generation of *tailor made* compact CFD models valid for a particular fuel and range of conditions.

Model Compaction Approach

Due to space limitations, we provide only a brief overview of our kinetic model compaction approach. For a specific conventional or alternative aviation fuel, a suitable few-component fuel surrogate can be formulated by matching particular combustion property targets (CPTs) [15-18]. In the present study, this few-component surrogate formulation is used to select detailed chemistry from the comprehensive, ~3200 species "Real Fuel 3" surrogate fuel kinetic model [19, 20] to generate a detailed kinetic model tailored to the prediction of combustion properties of the desired real fuel. However, our model compaction approach is not specific to the Real Fuel 3 detailed kinetic model, and it can accept other detailed models (e.g., [21, 22]) or experimental data (e.g., [23]) as inputs to achieve similar results as those described here.

The fuel-specific detailed kinetics model used here is reduced to a tractable size for 0-D/1-D simulations (several hundred species) using graph theory-based Path Flux Analysis (PFA) [24] over a broad range of temperatures, pressures, and equivalence ratios. The PFA procedure generates simulated combustion observables (i.e., ignition delay time, species mole fraction profiles, extinction/blow-off timescales, reaction temperature, etc.) for each [T, P, φ] condition used in the reduction. A central stipulation of the compaction approach is that the performance of the reduced kinetic model generated by PFA has high fidelity relative to the detailed surrogate kinetic model. Therefore the PFA-reduced model predictions can be used as the standard against which compact CFD kinetic model fidelity is assessed.

Using an evolutionary algorithm, reaction rate coefficient parameters in a "Seed" kinetic model are optimized to match global predictions of the PFA-reduced model across the T-P-φ space. Only fuel-related chemistry is optimized – the well-tested small species core is unchanged. This Seed model contains only a few dozen species and is of a size suitable for 3-D CFD simulations. The final product of optimization is a CFD-appropriate compact kinetic model that retains detailed model-predicted global combustion and emission behaviors inherent in the *specific aviation fuel* under consideration.

Results

Several compact models have been generated to simulate combustion of fuel-air mixtures of three real aviation fuels over the following range of conditions: initial reaction temperatures of $700 \leq T \text{ (K)} \leq 1800$;

pressures of 1 and 20 atm; and equivalence ratios of 0.6, 1.0, and 1.5. The fuels considered are

(1) POSF 4658, a typical conventional Jet A/JP-8;

(2) POSF 7629 (also known as POSF 5642 [25]), an isomerized paraffinic kerosene (IPK) produced by Sasol; and

(3) POSF 4734, a natural-gas derived synthetic kerosene (S-8) produced by Syntroleum.

Few-component surrogates for each of these fuels have been previously developed (and tested for POSF 4658 and POSF 4734) by matching combustion property targets of (1) average molecular weight (MW), (2) overall fuel H/C ratio, (3) derived cetane number (DCN), and (4) threshold sooting index (TSI) [15-17]. These few-component surrogate formulations appear in **Table 1**, and have been used to specify fuel composition inputs for simulations with the comprehensive Real Fuel 3 model and its subsequent reductions by PFA. The PFA-reduced kinetic models developed by this process serve as optimization targets/performance benchmarks for compact model development.

Table 1. Few-component surrogate compositions for real fuels (1)-(3) used to generate PFA-reduced benchmark models for subsequent compaction.

Fuel	Surrogate Composition (mole fraction)	Ref.
Conventional Jet A/JP-8 (1)	0.295 iso-octane 0.404 n-dodecane 0.228 n-propylbenzene 0.073 1,3,5-trimethylbenzene	[16]
Sasol IPK (2)	0.607 iso-octane 0.057 n-dodecane 0.301 iso-cetane 0.035 n-hexadecane	[20]
Syntroleum S-8 (3)	0.481 iso-octane 0.519 n-dodecane	[17]

For each real fuel (1)-(3), a compact model has been generated by representing the base fuel as a single-component surrogate fuel molecule C_nH_m, where integral values of n and m have been selected to most closely represent the MW and H/C ratio of the real fuel. **Figures 2-4** provide some comparison of the predictive performance of each of these compact models relative to their respective high-fidelity PFA benchmarks. The legends in these figures designate the number of species "_xxx" that comprise the corresponding PFA-reduced or compact model for the indicated Jet A, IPK, or S-8 fuel. For global combustion behaviors such as homogeneous ignition, flame propagation, and PSR extinction, the compact models generally perform well against the significantly more detailed (hundreds of species) PFA-reduced models.

While representation of the real fuel as a single-component surrogate fuel presents *a minimal limit* for compaction (and hence reduced computational burden), it is reasonable to expect that a more complex surrogate
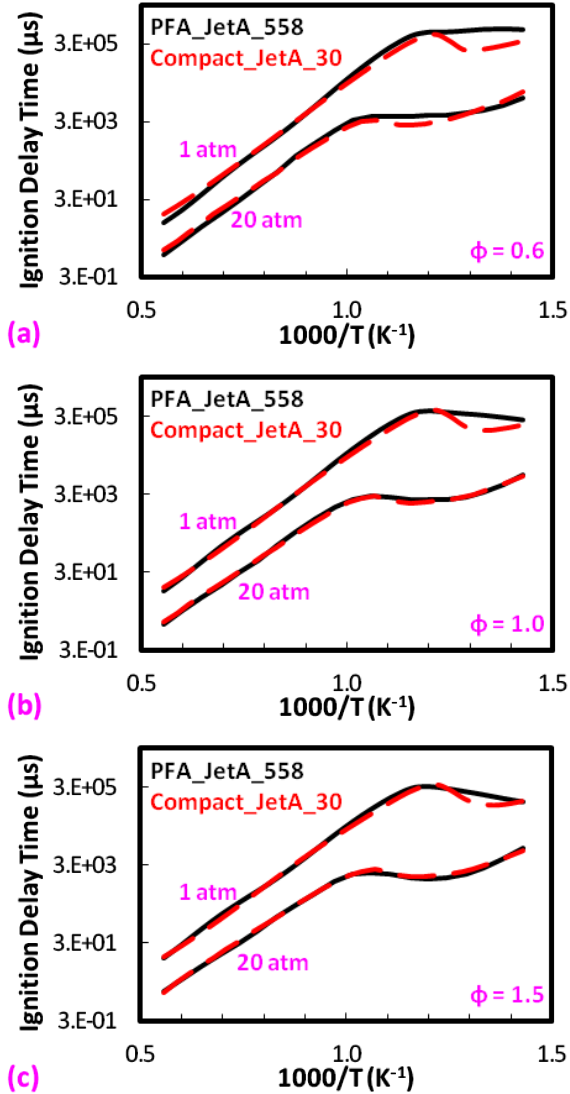
Fig. 2. Computed ignition delay times at noted pressures and equivalence ratios for fuel-air mixtures of conventional Jet A/JP-8 POSF 4658. Comparisons between 1) the 558 species PFA-reduced model used as the compaction target (black lines) and 2) a 30 species compact model (red lines). (For interpretation of color references used in this and following figures, please refer to the original digital version of this document).

fuel formulation might permit improved compact model predictions relative to the PFA benchmark. This is explored in **Figure 4** for the case of the Syntroleum S-8 fuel. The figure compares simulation results of a 30 species single-component fuel compact model (Compact_S8_30), a 36 species 2-component surrogate fuel compact model (Compact_S8_36), and the benchmark 473 species PFA-reduced model for the 2-component surrogate fuel (PFA_S8_473). The two-component models employ the S-8 surrogate composition indicated in **Table 1**. Additional comparison against a single-component compact model developed for high temperatures ($\geq$ 1000 K) is discussed below.

The Compact_S8_36 2-component surrogate fuel model performs as well or better than the 1-component Compact_S8_30 model for characteristic temperatures of $\geq$ 800 K found in homogeneous ignition, PSR extinction and major species evolution, and laminar flame propagation. For homogeneous ignition over the lowest range of temperatures considered here, the Compact_S8_36 model diverges from the PFA-reduced benchmark and Compact_S8_30. This may be due to incomplete convergence of the compact model optimization or incomplete mechanistic description of the fuel chemistry. Compact_S8_36 does not include any low temperature species/reactions for the iso-octane fuel component, and for this reason, predictions of this particular model must be regarded as preliminary.

In any case, the tradeoff for the comparable, possibly slightly better, overall predictive fidelity of Compact_S8_36 relative to Compact_S8_30 is the increased size of the kinetic model. Assuming that CFD computational costs scale roughly with the cube of the number of model species, simulations with 2-component fuel surrogate Compact_S8_36 will incur approximately 75% more in computational cost than the Compact_S8_30 single-component fuel representation. Clearly, more complex surrogate fuels such as the 4-component surrogates for Jet A or IPK (**Table 1**) may incur even greater computational costs if a more complex fuel specification (than the single-component constructions used for **Figures 2 and 3**) is used as a basis for compact model development.

Figure 4 also demonstrates a reduction in the number of species (and hence reduction of CFD computational burden) that may be obtained by restricting the parameter space over which the compact model is required to perform. In addition to the comparisons described earlier, the figure also shows predictions of a single-component fuel compact model optimized from $1000 \leq$ T (K) ≤ 1800. This 27 species high-temperature model Compact_S8_27 is based on the 30 species base single-component compact model optimized from $700 \leq$ T (K) ≤ 1800, though 3 species (and 7 reactions) corresponding to global low temperature chemistry behavior have been removed and the entire model has been re-optimized. Over the restricted parameter space considered, the modified model predicts ignition, flame propagation, PSR heat release rate, and PSR extinction as well as the base compact model.

Though the modified compact model may only be predictive in its restricted parameter space, it is relevant to note that this inflexibility is only apparent. Individual CFD simulations often consider restricted ranges of T-P-φ space (e.g., [2, 6]), and the computational cost of model compaction is much less than the cost of a CFD simulation. Hence a tailor made compact model for fuel and relevant T-P-φ range may lead to more efficient CFD computations than would be possible with a compact model developed for a more comprehensive range of T-P-φ. For example, model fidelity at high pressure is unnecessary for prediction of a behavior

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such as high altitude relight. Accordingly, one strategy for effective use of compact models may be to generate several smaller, condition-appropriate compact models for a fuel of interest instead of generating one larger, more general compact model.

Conclusions

This work presents the results of a methodology to develop *fuel specific,* CFD-appropriate compact combustion kinetic models (on the order of 3-4 dozen species) from more general, detailed models (of hundreds or thousands of species). Particular real jet fuels considered here include a conventional Jet-A/JP-8, an isomerized paraffinic kerosene (IPK), and a natural-gas derived synthetic kerosene (S-8). For global combustion behaviors such as homogenous ignition delay time, PSR species profiles and extinction timescale, and laminar burning velocity, the predictions of the ~30 species compact models developed for these fuels generally well-emulate the predictions of more detailed (hundreds of species) kinetic models over a wide range of T-P-φ parameter space.

Acknowledgements

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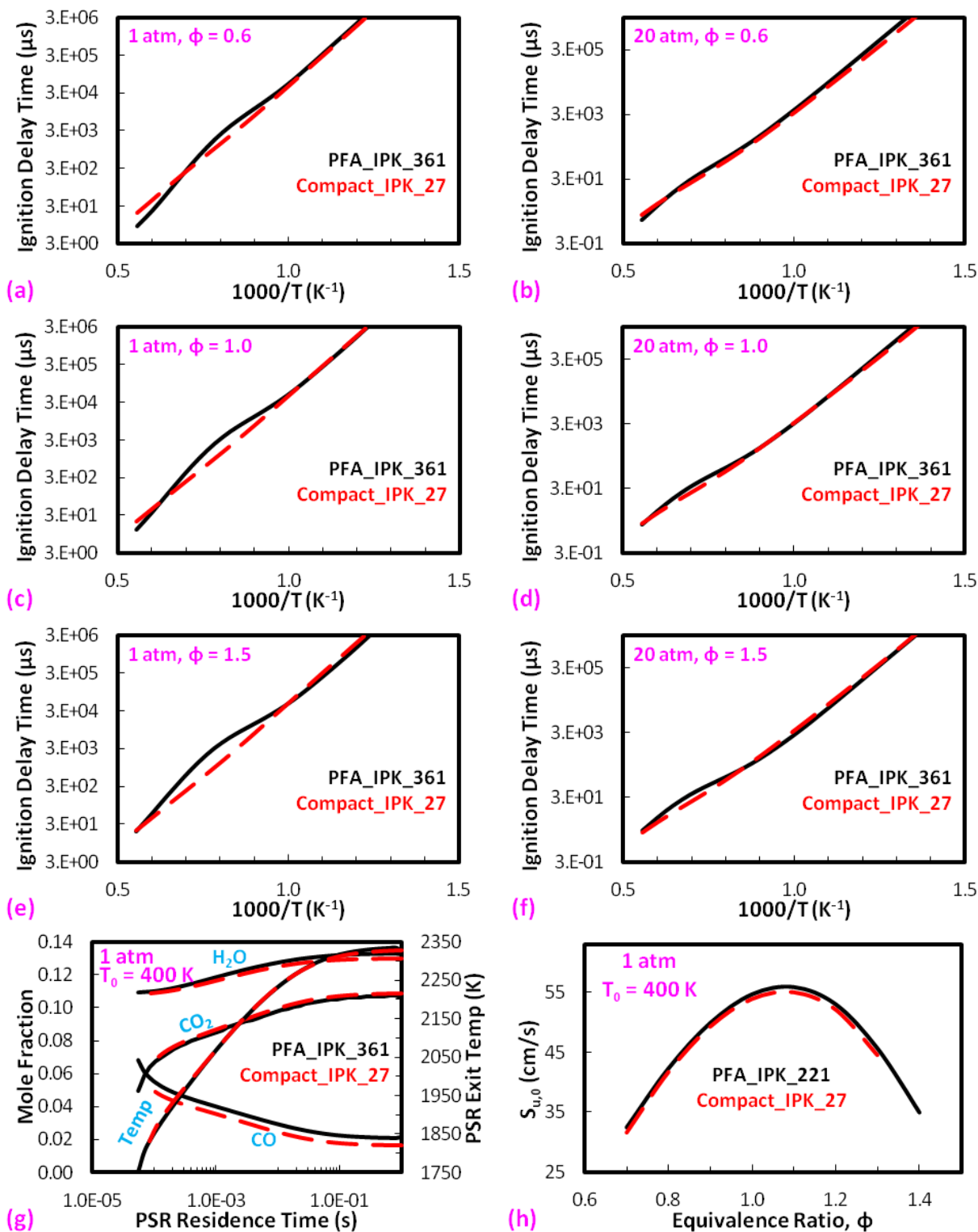
Fig. 3. Sasol IPK POSF 7629 (POSF 5642) kinetic model computations for fuel-air mixtures.

Panels (a)-(f): computed ignition delay times (shown for $t_{ig} \leq 3$ sec) at noted pressures and equivalence ratios. Comparisons among 1) 361 species PFA-reduced model used as the compaction target (black lines) and 2) a 27 species compact model (optimized for $700 \leq T$ (K) ≤ 1800, red lines). Panel (g): computed CO, CO_2, H_2O and exit temperature vs. residence time profiles for an adiabatic, isobaric (1 atm) perfectly stirred reactor (PSR) with reactants initially at 400 K; lines as identified in (a)-(f). Panel (h): computed laminar burning velocities for reactant mixtures at 1 atm and 400 K; black line is for 221 species PFA-reduced model, red line as identified in (a)-(f). Neither PSR simulations nor burning velocity simulations were used as targets for compact model development.
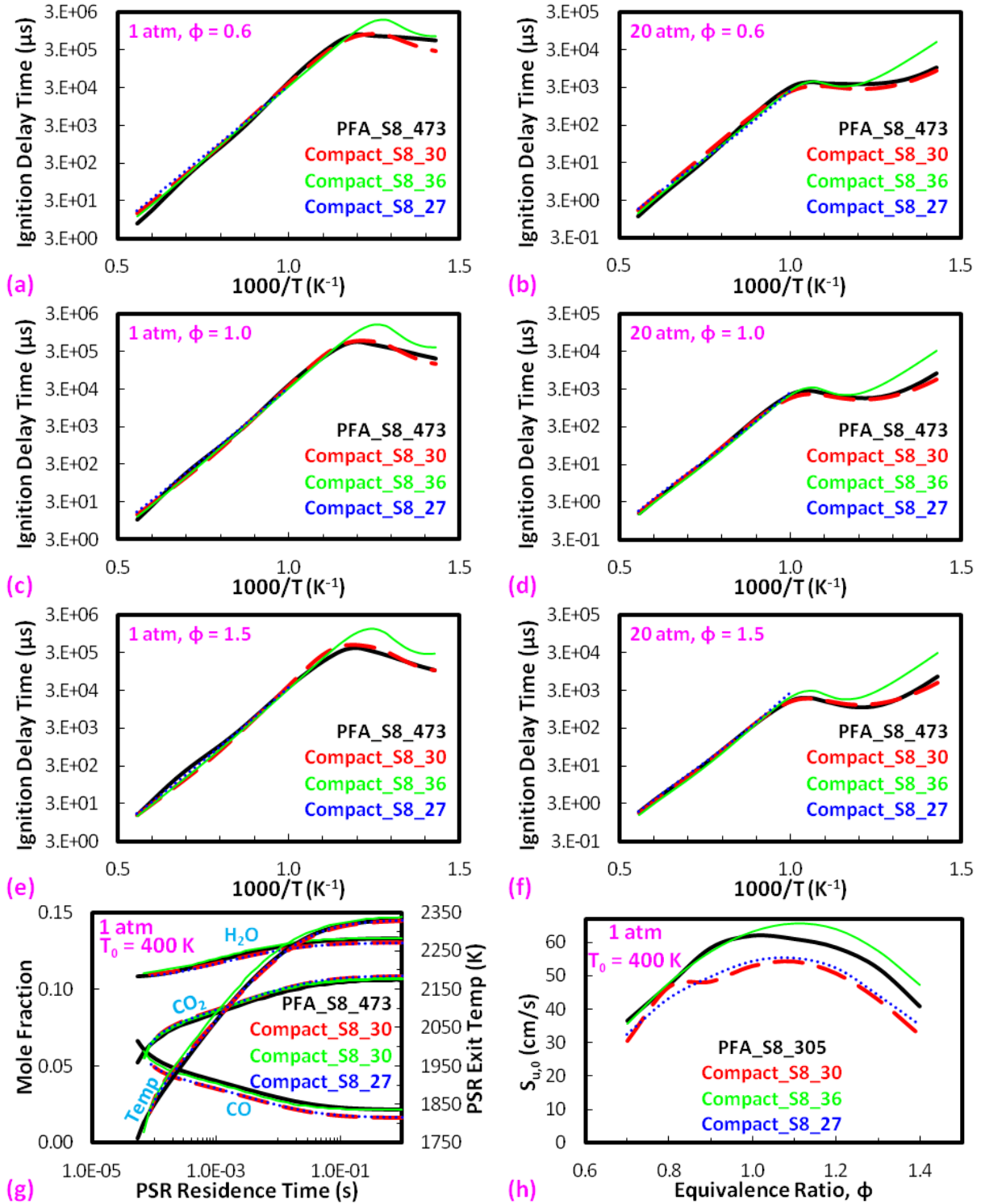
Fig. 4. Syntroleum S-8 POSF 4734 kinetic model computations for fuel-air mixtures.

Panels (a)-(f): computed ignition delay times at noted pressures and equivalence ratios. Comparisons among 1) 473 species PFA-reduced model used as the compaction target (black lines), 2) 30 species, single-component fuel compact model (for $700 \leq T$ (K) ≤ 1800, red lines), 3) 36 species, two-component fuel compact model (for $1000 \leq T$ (K) ≤ 1800, blue lines) and 4) 27 species, single-component fuel high temperature compact model (for $1000 \leq T$ (K) ≤ 1800, blue lines). Panel (g): computed CO, CO_2, H_2O and exit temperature vs. residence time profiles for an adiabatic, isobaric (1 atm) perfectly stirred reactor (PSR) with reactants initially at 400 K; lines as identified in (a)-(f). Panel (h): computed laminar burning velocities for reactant mixtures at 1 atm and 400 K; black line is for 305 species PFA-reduced model, other lines as identified in (a)-(f). Neither PSR simulations nor burning velocity simulations were used as targets for compact model development.