

AIAA 2002-0336

**Reduced Chemical Kinetic
Mechanisms for JP-8 Combustion**

C. J. Montgomery
Reaction Engineering International
Salt Lake City, UT

S. M. Cannon
CFD Research Corporation
Huntsville, AL

M. A. Mawid
Engineering Research & Analysis Co.
Wright-Patterson AFB, OH

B. Sekar
AFRL Turbine Engine Division
Wright-Patterson AFB, OH

40th AIAA Aerospace Sciences Meeting and Exhibit
14-17 January 2002
Reno, Nevada

Report Documentation Page				Form Approved OMB No. 0704-0188	
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1. REPORT DATE JAN 2002		2. REPORT TYPE		3. DATES COVERED 00-00-2002 to 00-00-2002	
4. TITLE AND SUBTITLE Reduced Chemical Kinetic Mechanisms for JP-8 Combustion				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Reaction Engineering International ,77 West 200 South Suite 210,Salt Lake City,UT,84101				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release; distribution unlimited					
13. SUPPLEMENTARY NOTES					
14. ABSTRACT					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES 11	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			

REDUCED CHEMICAL KINETIC MECHANISMS FOR JP-8 COMBUSTION

C. J. Montgomery*

Reaction Engineering International
Salt Lake City, UT

S. M. Cannon†

CFD Research Corporation
Huntsville, AL

M. A. Mawid‡

Engineering Research & Analysis Co.
Wright-Patterson AFB, OH

B. Sekar§

AFRL Turbine Engine Division
Wright-Patterson AFB, OH

ABSTRACT

Using CARM (Computer Aided Reduction Method), a computer program that automates the mechanism reduction process, six different reduced chemical kinetic mechanisms for JP-8 combustion have been generated. The reduced mechanisms have been compared to detailed chemistry calculations in simple homogeneous reactor calculations. Reduced mechanisms containing 15 and 20 species were found to give good agreement for both temperature and species concentrations (including NO) in adiabatic perfectly stirred reactor calculations for inlet temperatures from 300-1300 K, pressures from 10-40 atm, stoichiometric ratios from 0.5-2.0 and reactor residence times from 0.1 sec. to near blowout. Reduced mechanisms have also been created that compare well to available ignition delay measurements for JP-8.

INTRODUCTION

Detailed chemical kinetic descriptions of aviation fuel combustion require the tracking of hundreds of chemical species and thousands of reaction steps. For the foreseeable future, CPU time and computer memory limitations will prohibit implementation of fully detailed descriptions of combustion chemistry into 3-D CFD simulations of practical devices.

Issues such as ignition, flame stabilization, combustion efficiency, and pollutant formation are extremely important in the design of aircraft engines. Accurate simulation of these phenomena requires that significant chemical kinetic detail be retained in computer models.

Within CFD simulations, memory usage and CPU time vary linearly with the number of chemical species tracked. Methods that minimize this number while retaining essential features of the detailed chemistry are thus of great importance. The number of species required for simulation of combustion processes depends on the nature of the phenomenon, and the type of information desired from the simulation.

The recent development of comprehensive, validated, detailed mechanisms for combustion of kerosene fuels^{1,2} provides a basis for creating reduced chemical kinetic mechanisms containing few enough species to be used in a CFD simulation while accurately simulating the combustion chemistry. Reduced chemical kinetic mechanisms that can represent important aspects of the behavior of these detailed mechanism using few enough scalars that they can be implemented into CFD

*Senior Engineer, AIAA Member

†Group Leader, AIAA Member

‡Technical Director, AIAA Member

§Aerospace Engineer, AIAA Associate Fellow

simulations offer large potential improvement in the modeling of practical aviation combustors.

The approach used here is to reduce mechanisms by employing steady-state assumptions. In this work we have used CARM (Computer Assisted Reduction Method)³ a computer program that automates the reduction procedure, allowing large, detailed mechanisms to be reduced quickly. CARM produces source code for the calculation of the chemical source terms defined by the reduced mechanism that can be linked easily to a combustion simulation code.

CARM has recently been applied to combustion of hydrocarbons such as ethylene and *n*-heptane⁴, NO_x reduction in coal-fired furnaces⁵ and incineration of hazardous chemicals⁶.

In this work we apply CARM to a large detailed chemical kinetic mechanism for JP-8 combustion. The results are compared to available experiments and to detailed chemistry calculations.

AUTOMATED MECHANISM REDUCTION

There are four basic steps in the formulation of a reduced chemical kinetic mechanism:

- 1) Identification of the appropriate detailed mechanism containing the essential species and elementary reaction steps.
- 2) Identification of appropriate steady-state approximations.
- 3) Elimination of reactions through use of the algebraic relations obtained in step 2.
- 4) Solution of the coupled and nonlinear set of algebraic equations obtained in the previous steps to find the reaction rates of the remaining species.

CARM automates steps 2-4, producing source code for the calculation of the chemical source terms defined by the reduced mechanism. As inputs, CARM uses a set of test problem results representing conditions of interest to rank species by the error induced by assuming they are in steady state. The subroutine produced by CARM contains code that iteratively solves the coupled, nonlinear set of algebraic equations giving the concentrations of the steady-state species. These concentrations are used along with the rates of the elementary reactions from the detailed mechanism to calculate the chemical source terms for the non-steady-state species.

DETAILED MECHANISM

JP-8 fuel is a complex mixture of thousands of hydrocarbon components that is manufactured to meet

certain property standards. The exact composition varies in time and place depending on crude feedstocks and refinery processes. Modeling JP-8 combustion requires selection of a surrogate fuel blend containing a few species with known kinetics that reproduces the essential combustion behavior of a typical batch of the actual fuel⁷.

The detailed mechanism on which the reduced mechanisms are based is an extension of the kerosene mechanism of Dagaut et al.¹ with additions for combustion of *n*-dodecane as well as other additional species². This detailed mechanism contains 201 species and 1330 reactions. This mechanism was created to simulate combustion of a 12-species surrogate mixture representing a typical batch of JP-8. Researchers at AFRL are continuing development of the detailed chemical kinetics for JP-8. Figure 1 compares JP-8 ignition delay calculated using this mechanism with measurements^{8,9}, as well as with reduced mechanisms which will be discussed below. Good agreement is found.

The purpose of this work was to develop reduced mechanisms that could be used in large eddy and RANS simulations of gas turbine combustors. Twenty species was determined to be the maximum allowable number that could be implemented into a CFD code while maintaining reasonable computer time and memory requirements. Each species in the surrogate fuel blend must be kept in the reduced mechanism or its concentration cannot be specified independently. It is also necessary to keep the major constituents of air, O₂ and N₂, as well as important product and intermediate species, CO, CO₂, H₂, and H₂O. To accurately simulate combustion of large hydrocarbons, not all radical and intermediate species can be assumed to be in steady state. Furthermore, prediction of NO_x emissions is a project goal so NO must be kept in the reduced mechanisms.

The above constraints do not allow a reduced mechanism having 20 or fewer species to be created for a 12-species fuel surrogate. Therefore, a simpler fuel surrogate was devised using only four species. This fuel blend contains by moles 34.7% *n*-C₁₂H₂₆, 32.6% *n*-C₁₀H₂₂, 16.0% C₁₀H₁₄ (butylbenzene) and 16.7% *a*-C₇H₁₄ (methylcyclohexane). This mixture represents important major classes of hydrocarbons that are present in practical fuels. Using a fuel surrogate with fewer species allows submechanisms for compounds no longer used to be removed from the detailed mechanism. This results in a detailed mechanism with 164 species and 1162 reactions.

At first we attempted to use a mixture of the above four compounds that approximated the measured concentrations of the compound classes they represent

in JP-8. However, this mixture performed poorly compared to experimental data for JP-8 ignition delay. The mixture described above has been optimized to give reasonable agreement with ignition delay measurements^{8,9} as shown in Figure 1. The 25 species ignition delay mechanism performs better at low temperatures but worse than the 20 species reduced mechanism at high temperatures. Further optimization of the species retained in the reduced mechanisms and possibly more species are needed to get better agreement with the detailed mechanism.

The four-species surrogate is expected to be sufficient to describe the overall combustion characteristics of JP-8, while more detailed surrogates, such as the 12-species mixture for which a detailed mechanism has been developed³, may be necessary for prediction of soot formation. Future work will include a more detailed surrogate, which will likely necessitate keeping more species in the reduced mechanisms.

The kerosene mechanism of Dagaut et al.¹ on which the current detailed mechanism is based uses different kinetic parameters for 34 reactions for the pressures near 1, 10, and 40 bars. These rates were the basis of reduced mechanisms created for use in the respective pressure ranges 1–10 atm., 10–25 atm., and 25–40 atm.

To predict the production of thermal NO_x, a four-step NO mechanism was added to the detailed mechanism containing the extended Zel'dovich mechanism for thermal NO formation and a step for NO dissociation. The rates for these reactions were taken from Miller and Bowman¹⁰. Future work will include a more complete NO_x model including prompt NO and N₂O pathways.

RESULTS

The goal of this project has been to create reduced chemical kinetic mechanisms for JP-8 combustion that can be used in CFD simulations of gas turbine combustors. The conditions of interest are pressures from 10–40 atm., inlet temperatures from 650–1300 K and a range of fuel/air equivalence ratios so that nonpremixed combustion can be simulated.

Because experimental data on JP-8 combustion are limited, the detailed mechanism and fuel surrogate were validated against ignition delay measurements for a fuel/air equivalence ratio, ϕ , of 0.5 (fuel-lean) and an initial pressure of 1 atm. Reduced mechanisms were created using the 1 bar detailed mechanism to model these measurements using in a constant-volume plug flow reactor code. The results are shown in Figure 1. The reduced mechanisms created in this study are

summarized in Table 1. The reduced mechanism results are in reasonable agreement with the detailed mechanism results, which are in turn in reasonable agreement with the measurements. Previous experience⁵ has shown that more species are required in the reduced mechanism to model ignition delay than to model perfectly stirred reactors (PSRs).

Reduced mechanisms containing 15 and 20 species were created using the mid-pressure (10 bar) and high-pressure (40 bar) detailed mechanisms. These were compared to detailed chemistry in adiabatic PSR calculations for inlet temperatures ranging from 300–1300 K, equivalence ratios, ϕ , from 0.5 to 2.0, and PSR residence times from 0.1 seconds to a value near the blowout limit depending on stoichiometry. The mid-pressure reduced mechanisms were compared to detailed chemistry for pressures from 10 to 25 atm, while those based on the high-pressure rates were compared for pressures from 25 to 40 atm. As shown in Table 1, the 15 species reduced mechanisms for mid- and high-pressure contain identical species, while the 20-species reduced mechanisms differ by only one species; the high pressure reduced mechanism contains C₆H₆ instead of C₃H₂. Because of the similarity in makeup and behavior of the mid- and high-pressure reduced mechanisms, results will not be shown for the mid-pressure reduced mechanisms.

Adiabatic PSR calculations are good tests of a reduced mechanism's ability to reproduce the heat release and overall combustion characteristics of the detailed mechanism. Figure 2 shows plots of calculated temperature and mole fractions of O₂, CO and OH, for a range of PSR residence times. The agreement between reduced and detailed chemistry is excellent. Comparisons for other species (not shown) are of similar quality.

Figure 3 shows calculated NO mole fraction as a function of residence time for stoichiometric, fuel-lean, and fuel-rich conditions. For the three equivalence ratios, the residence times vary from 0.1 seconds down to a value close to the calculated blowout condition. Both reduced mechanisms give good agreement. For rich conditions ($\phi = 2.0$) the NO mole fraction calculated with the 15-species reduced mechanism is off by nearly an order of magnitude for some conditions. However, since both detailed and reduced chemistry predict sub-ppm NO concentrations under these conditions, this is not expected to be a significant drawback. Results for other inlet temperatures, residence times, and pressures (not shown) were similar.

Figures 4 and 5 show similar results varying respectively the inlet temperature and pressure for $\phi = 1.0$. Similar agreement is found for fuel-lean and fuel rich conditions over the same range of pressures and

inlet temperatures (not shown). Again agreement is good under nearly all conditions, with the expected result of improved agreement with detailed chemistry with fewer steady-state species under most conditions.

CONCLUSIONS

A four-species surrogate mixture representing JP-8 was found to give reasonable agreement to a more detailed 12-species surrogate and to measurements of JP-8/air ignition delay. Reduced mechanisms were created using CARM to model JP-8 combustion over a range of initial temperatures, pressures, and stoichiometric ratios.

The CARM mechanism reduction code produces reduced chemistry approximations that work well compared to detailed chemistry for mixtures of large hydrocarbons under a wide range of conditions. Reduced mechanisms produced using CARM and tested and validated against detailed chemistry are a promising way of including more detailed chemistry into CFD simulations. The reduced mechanisms described here have been implemented into the commercial CFD code CFD-ACE+ for use in large eddy simulation (LES) of gas turbine combustor instability. In this implementation improved source term evaluation times are obtained using *in-situ* adaptive tabulation (ISAT) techniques¹¹.

ACKNOWLEDGMENTS

This work has been supported with Phase II SBIR funds from the Air Force Research Laboratory, contract #F33615-00-C-2016.

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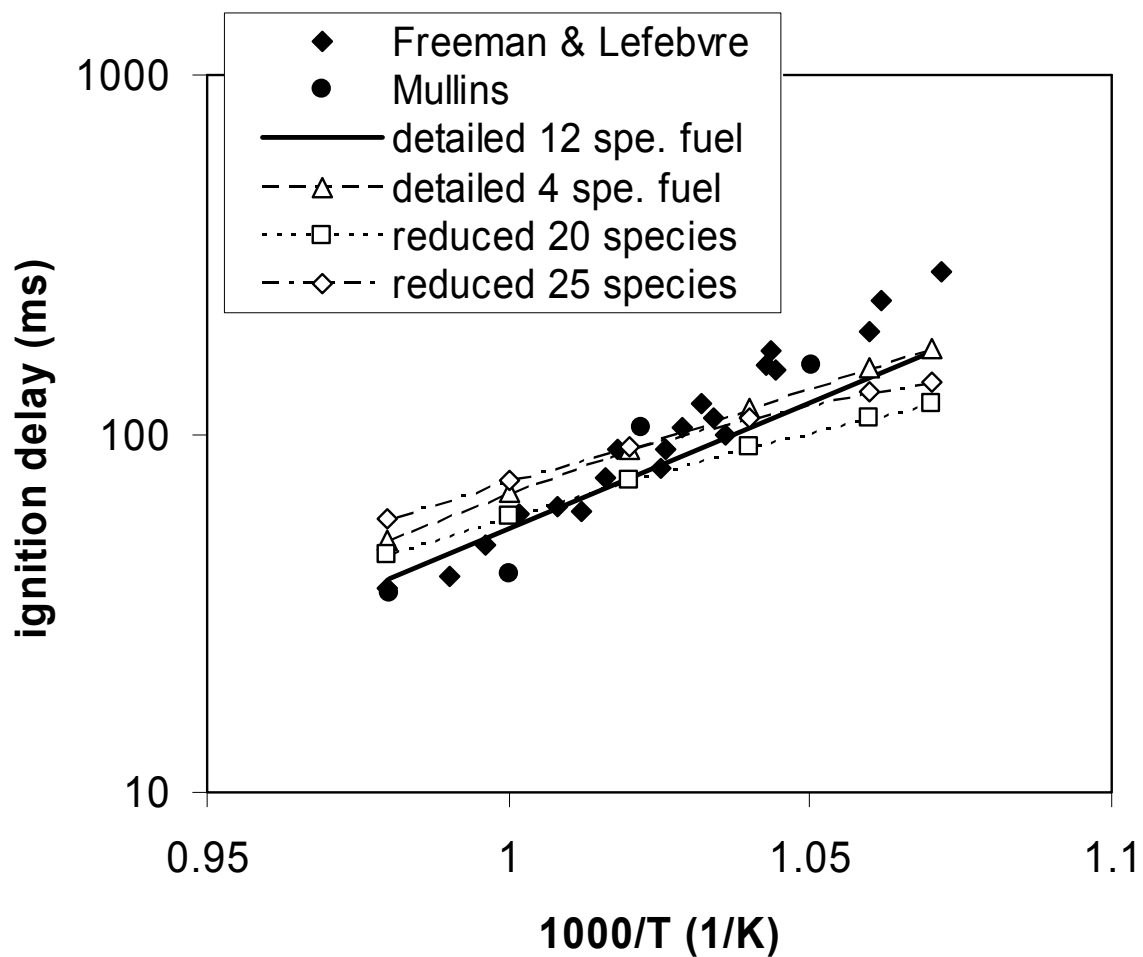


Figure 1. Measured^{8,9} and calculated ignition delay for JP-8/air, Initial pressure = 1 atm, equivalence ratio = 0.5..

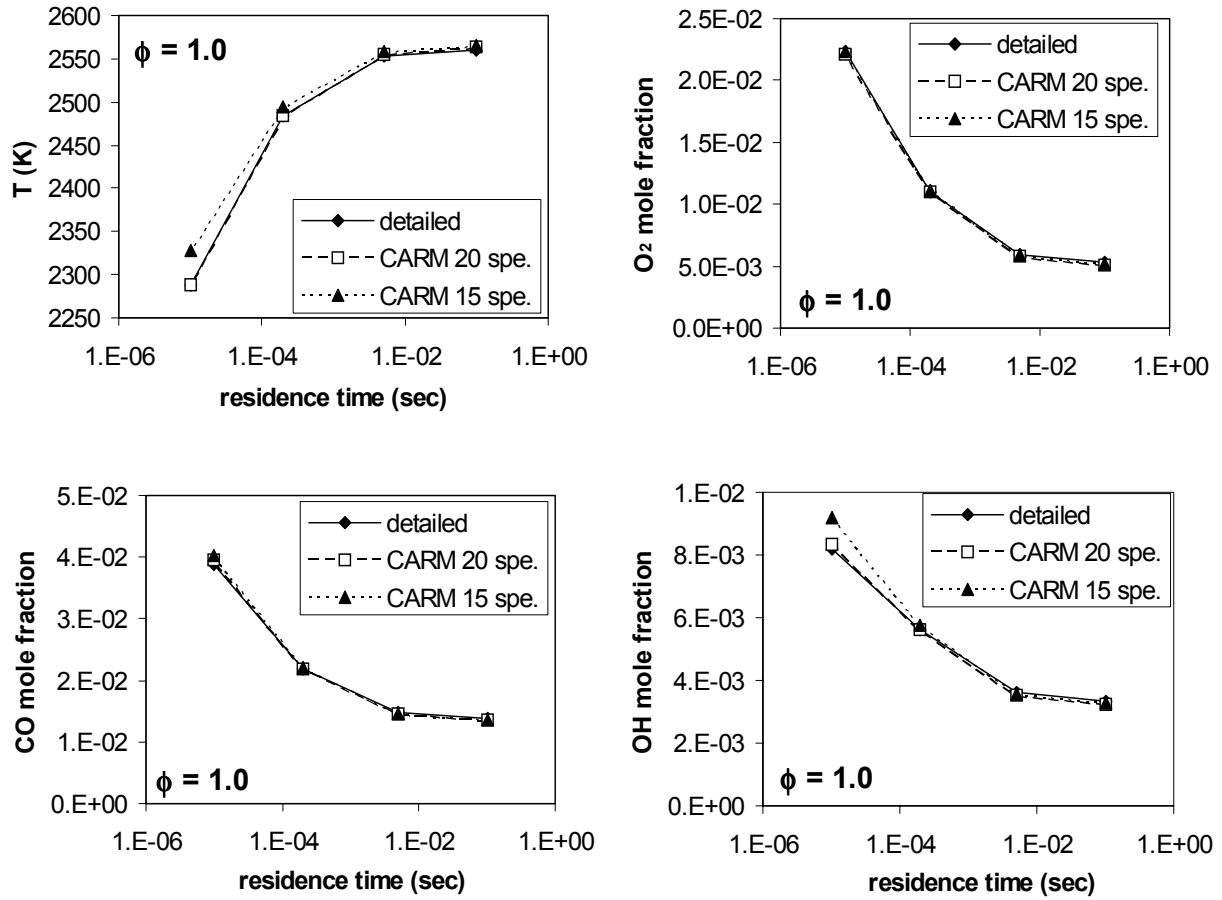


Figure 2. Calculated temperature and mole fractions of O₂, CO and OH as functions of residence time for detailed and reduced chemistry in an adiabatic PSR. Equivalence ratio = 1.0, pressure = 32.5 atm., inlet temperature = 650 K.

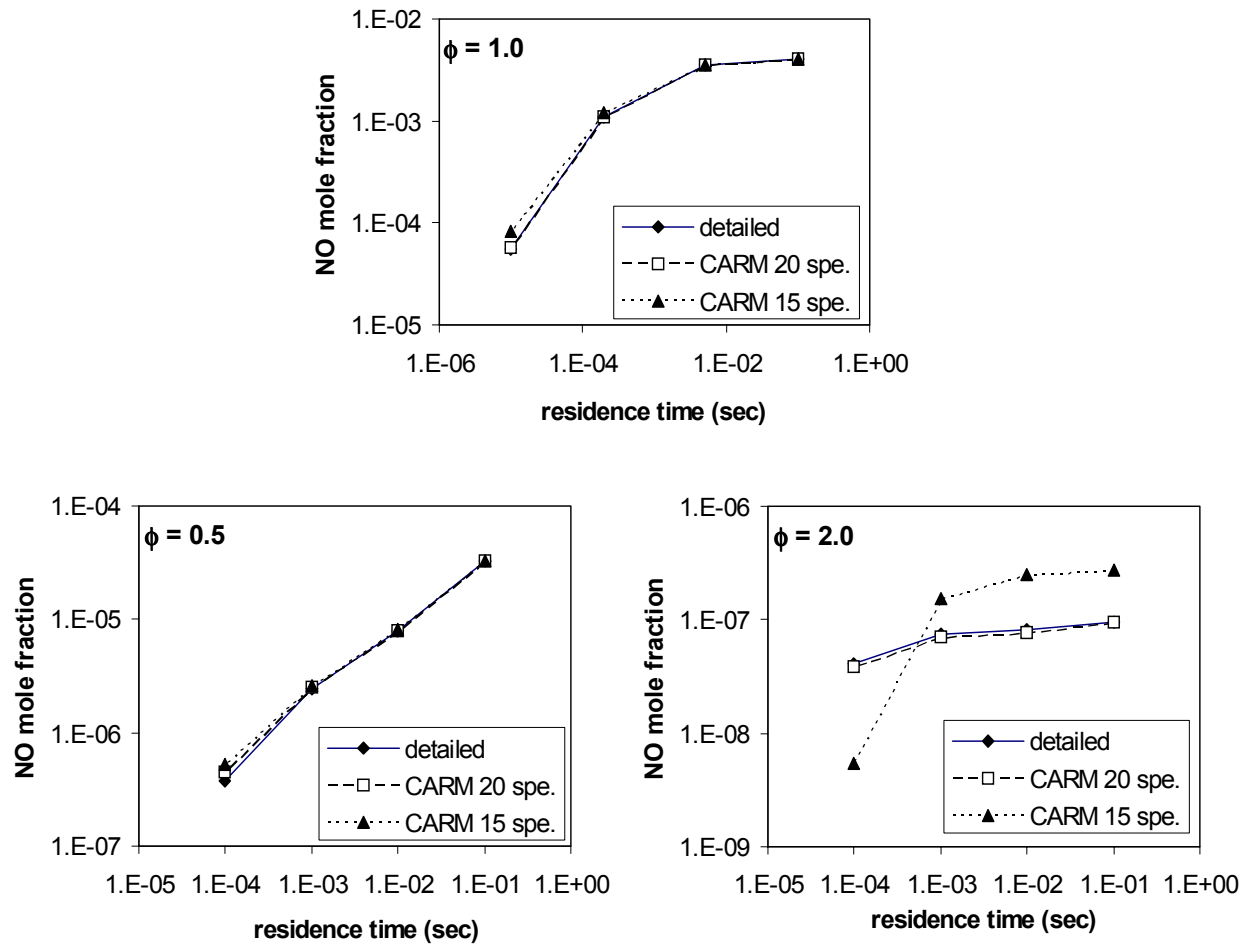


Figure 3. Calculated NO mole fraction as a function of residence time for detailed and reduced chemistry in an adiabatic PSR. Equivalence ratio = 1.0, 0.5, and 2.0, pressure = 32.5 atm., inlet temperature = 650 K.

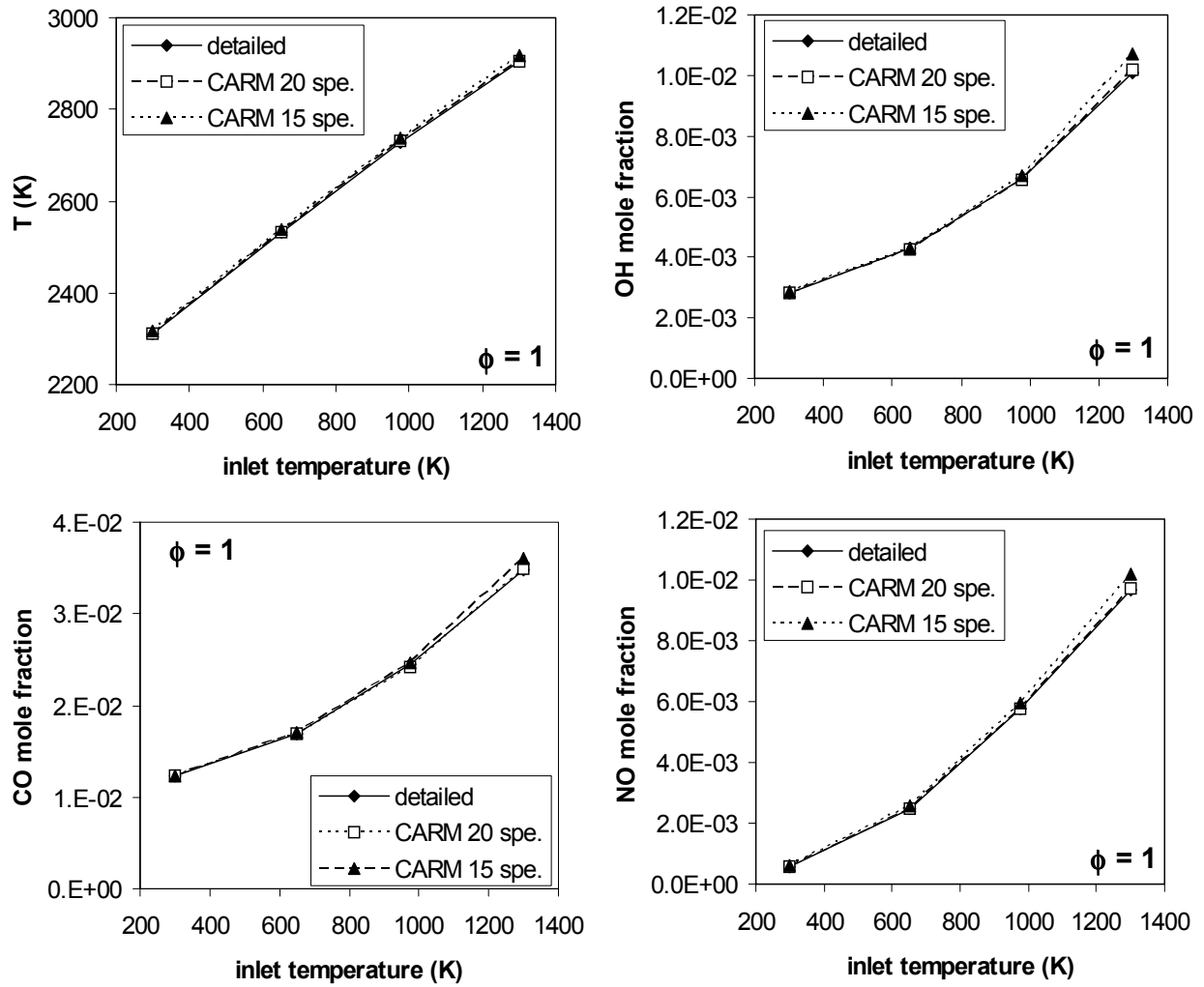


Figure 4. Calculated temperature and mole fractions of OH, CO and NO as functions of inlet temperature for detailed and reduced chemistry in an adiabatic PSR. Equivalence ratio = 1.0, pressure = 32.5 atm., residence time = 0.001 seconds.

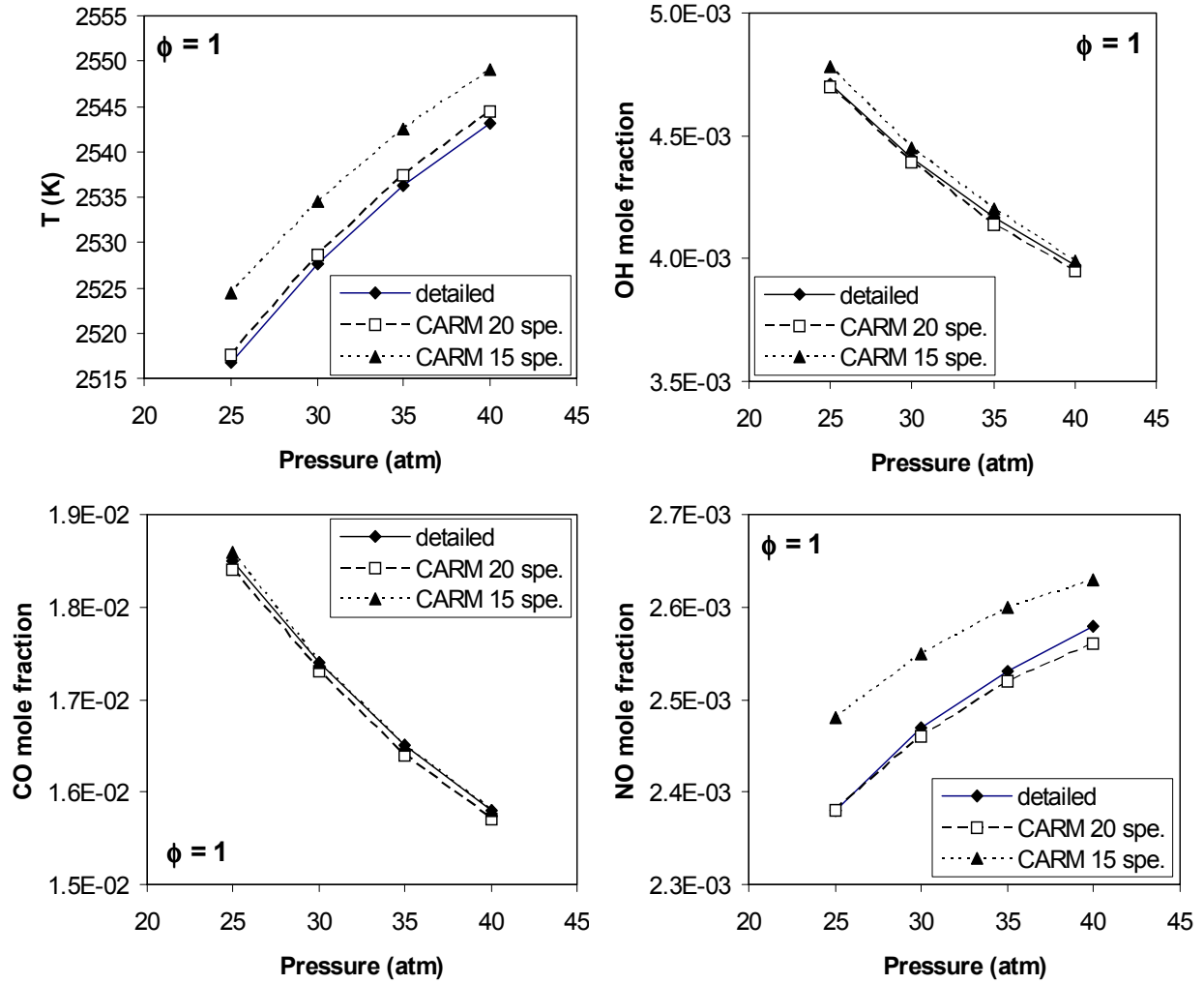


Figure 5. Calculated temperature and mole fractions of OH, CO and NO as functions of pressure for detailed and reduced chemistry in an adiabatic PSR. Equivalence ratio = 1.0, inlet temperature = 650 K, residence time = 0.001 seconds.

Table 1. Summary of reduced mechanisms described in this paper.

Mechanism	No. of species	Pressure range	Non-quasi-steady state species
Ignition 20	20	1-10 atm.	$n\text{-C}_{10}\text{H}_{22}$, $n\text{-C}_{12}\text{H}_{26}$, $\text{C}_{10}\text{H}_{14}$, $a\text{-C}_7\text{H}_{14}$, H, H_2 , O, O_2 , OH, H_2O , CO, CO_2 , CH_4 , C_2H_2 , C_2H_4 , C_3H_6 , $p\text{-C}_3\text{H}_4$, C_3H_2 , $p\text{-C}_3\text{H}_4\text{O}$, N_2
Ignition 25	25	1-10 atm.	$n\text{-C}_{10}\text{H}_{22}$, $n\text{-C}_{12}\text{H}_{26}$, $\text{C}_{10}\text{H}_{14}$, $a\text{-C}_7\text{H}_{14}$, H, H_2 , O, O_2 , OH, H_2O , CO, CO_2 , CH_4 , CH_2O , C_2H_2 , C_2H_4 , C_3H_6 , C_3H_2 , $p\text{-C}_3\text{H}_4$, $p\text{-C}_3\text{H}_4\text{O}$, C_6H_6 , C_8H_8 , $a\text{-C}_6\text{H}_{12}$, $\text{C}_5\text{H}_4\text{O}$, N_2
Mid Pressure 15	15	10-25 atm.	$n\text{-C}_{10}\text{H}_{22}$, $n\text{-C}_{12}\text{H}_{26}$, $\text{C}_{10}\text{H}_{14}$, $a\text{-C}_7\text{H}_{14}$, H_2 , O_2 , OH, H_2O , CO, CO_2 , CH_4 , C_2H_2 , C_3H_6 , N_2 , NO
Mid Pressure 20	20	10-25 atm.	$n\text{-C}_{10}\text{H}_{22}$, $n\text{-C}_{12}\text{H}_{26}$, $\text{C}_{10}\text{H}_{14}$, $a\text{-C}_7\text{H}_{14}$, H, H_2 , O, O_2 , OH, H_2O , CO, CO_2 , CH_4 , C_2H_2 , C_2H_4 , C_3H_6 , $p\text{-C}_3\text{H}_4$, C_3H_2 , N_2 , NO
High Pressure 15	10	25-40 atm.	$n\text{-C}_{10}\text{H}_{22}$, $n\text{-C}_{12}\text{H}_{26}$, $\text{C}_{10}\text{H}_{14}$, $a\text{-C}_7\text{H}_{14}$, H_2 , O_2 , OH, H_2O , CO, CO_2 , CH_4 , C_2H_2 , C_3H_6 , N_2 , NO
High Pressure 20	20	25-40 atm.	$n\text{-C}_{10}\text{H}_{22}$, $n\text{-C}_{12}\text{H}_{26}$, $\text{C}_{10}\text{H}_{14}$, $a\text{-C}_7\text{H}_{14}$, H, H_2 , O, O_2 , OH, H_2O , CO, CO_2 , CH_4 , C_2H_2 , C_2H_4 , C_3H_6 , $p\text{-C}_3\text{H}_4$, C_6H_6 , N_2 , NO