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Numerical Study of Contaminant Effects on Combustion of Hydrogen, Ethane and Methane in Air

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ABSTRACT

A numerical study was performed to assess the effects of vitiated air on the chemical kinetics of hydrogen, ethane, and methane combustion with air. A series of calculations in static reacting systems was performed, where the initial temperature was specified and reactions occurred at constant pressure. Three different types of test flow contaminants were considered: NO, H_2O, and a combination of H_2O and CO_2. These contaminants are present in the test flows of facilities used for hypersonic propulsion testing. The results were computed using a detailed reaction mechanism and are presented in terms of ignition and reaction times. Calculations were made for a wide range of contaminant concentrations, temperatures and pressures. The results indicate a pronounced kinetic effect over a range of temperatures, especially with NO contamination and, to a lesser degree, with H_2O contamination. In all cases studied, CO_2 remained kinetically inert, but had a thermodynamic effect on results by acting as a third body. The largest effect is observed with combustion using hydrogen fuel, less effect is seen with combustion of ethane, and little effect of contaminants is shown with methane combustion.

INTRODUCTION

When providing the proper facility stagnation conditions for testing supersonic combustors in ground-based facilities, it is necessary to heat air to an enthalpy level that matches the flight conditions. Typical heating techniques used to generate this high enthalpy include electric arcs, combustion of hydrogen or methane fuels in air with oxygen replenishment, or storage heaters. The use of an electric arc heater results in air dissociation and the generation of significant amounts of nitrogen oxides, as well as a depletion in the net level of oxygen below 21% by volume. In combustion heaters, the flow constituents are a function of the fuel used; for example, with a hydrogen burner H_2O is a primary contaminant, or with a methane heater a combination of both H_2O and CO_2 are the primary contaminants. Figures 1, 2 and 3 present the mole fractions of the constituents in the test gas as a function of total temperature (and corresponding simulated Mach number) for each of the heater types considered in this study. Due to the presence of these test flow contaminants, the combustion characteristics in a ramjet or scramjet engine can potentially be different than results obtained in clean air or actual flight. It is therefore important to understand these contamination effects to properly interpret the test data obtained in ground based experiments. The thermodynamic conditions of the air flow passing through a ramjet or scramjet combustor vary significantly across the flowpath due to the different flight Mach numbers, varying amounts of compression, the presence of flow separations, and combustion of fuel. Prior to any combustion of fuel, and with no heat loss, the local static temperature is a function of flight Mach number and local Mach number as depicted in Fig. 4. The local static pressure depends on the facility supply pressure, local Mach number, and total pressure losses through compression. For ramjet or scramjet engine systems tested in existing facilities at simulated Mach 5 to 7, the static pressure in the combustor typically ranges up to about 5 atmospheres, and there are regions of low pressure due to flow expansion through the nozzle. For the flow through a scramjet combustor the residence time is less than 1 millisecond; and for most geometries the actual times will be significantly less. Ignition and reaction of the fuel and air must take place in less than this time for performance to be attained in an engine. These ranges of relevant temperatures and pressures, and maximum allowable ignition/reaction times provide a preliminary basis to assess the potential impact of the test flow contaminants on ramjet/scramjet performance. In order to accurately assess these effects on a specific configuration a more detailed (two and three dimensional) analysis would be conducted.

Various studies[1-6] have explored the effect of NO, H_2O, and CO_2 contaminants on combustion processes, primarily with hydrogen fuel with application to hypersonic propulsion systems. These included both experi-

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mental and computational studies; a general trend from these works is that H_2O and CO_2 have a minimal influence on the kinetics of hydrogen-air combustion while NO serves to reduce both ignition and reaction times. The range of temperatures and pressure investigated and the data base with fuels other than hydrogen are limited.

The objective of the present paper is to provide an assessment of the effect of NO, H_2O and a combination of H_2O and CO_2 on combustion of various fuels including hydrogen, ethane and methane with air. The computations were performed for a static system at constant pressure, covering a broad range of initial temperatures, pressures, and chemical concentrations.

NUMERICAL METHOD

The results discussed herein are computed using the Lewis General Chemical Kinetics and Sensitivity Analysis (LSENS) program[7-9], developed at NASA Lewis. Any detailed reaction mechanism describing homogeneous, gas-phase elementary reactions can be incorporated in the LSENS code. This is an important consideration in the study of the possible effects of facility contamination, since a global model may not be available and a reduced mechanism may be insufficient. The numerical integration method is derived from a general multi-step scheme using an implicit backward difference formulation designed to solve stiff systems of differential equations encountered in the analytical analysis of combustion. The time-accurate results are computed to provide the important trends of the contamination effects to guide both future experiments and three-dimensional computations.

In this paper, two reaction models provided with the LSENS code are employed. The first is a hydrogen/air model consisting of 37 reactions involving 16 species. The second is a comprehensive hydrocarbon/air model having 133 reactions and 39 species. Description of these two models with their chemical reaction equations and the corresponding rate coefficients can be found in Ref. [9]. In computing the hydrogen combustion, the hydrogen model allows faster computational time due to a lesser number of reactions and species.

IGNITION AND REACTION TIME COMPUTATIONS

The static model represents a combustor where air or vitiated air and fuel are premixed and allowed to react spontaneously. A typical temperature history is illustrated as in Fig. 5, for three different stoichiometric mixtures. Ignition and reaction are depicted by a rapid increase to an equilibrium temperature from an initial state. The ignition delay is the time required for the mixture temperature to increase 5% of the equilibrium temperature rise. Reaction time is defined as the time increment between 5% and 95% of this temperature rise. The ignition delay time can vary considerably depending on the the mixture composition. Flow contamination can promote, impede, or even prevent ignition and reaction. For the case outlined in Fig. 5, the presence of CO_2 and H_2O results in a significant increase in ignition time. In all cases studied with clean air or with CO_2 and H_2O as contaminants the initial mole fraction of O_2 was maintained at 21%. For other cases where NO was a contaminant species, oxygen was considered depleted from dissociation. Representative mixture compositions for these cases with NO contaminant are outlined in table I.

H_2 COMBUSTION

Calculation of ignition and reaction times has been computed for hydrogen combustion with different levels of NO at four different pressures, 0.1, 1, 10 and 100 atmospheres, and initial temperatures of 800, 900, 1000, 1100 and 1200 °K. The results are shown in Figs. 6-9. Both ignition and reaction times decrease for low NO concentration then increase with increased NO concentration at lower temperature but are relatively insensitive to NO variation at high temperature. The effect of NO is generally pronounced within a temperature range for a prescribed pressure. At 0.1 atmosphere the difference from clean-air results is minimal at all initial temperatures. At 1 and 10 atmospheres, presence of NO can results in a two order of magnitude reduction in ignition and reaction times. At 100 atmospheres, the effect of NO decreases, but is present over the complete temperature range. There is a consistent increase in both ignition and reaction times for large concentrations of NO.

The influence of NO on hydrogen-air combustion is present because NO directly affects the reaction rates. It promotes chain-branching reactions when the level of NO is low, and becomes active in three-body termination reactions when NO is abundant[1,2], leading to a reduction or an increase in ignition and reaction times, respectively.

Ignition and reaction times for hydrogen combustion with H_2O contamination are presented in Figs. 10-13 for a similar range of pressures and temperatures. It is generally observed that H_2O has a small influence on the combustion process. Effects are observed at 0.1 atmosphere for the lowest temperature indicating a considerable delay or absence in ignition for increasing H_2O concentration. The reaction times remain unaffected in mixtures when ignition was accomplished. In all, the temperature range in which kinetic rates vary with pressure are confined to a more narrow range as compared to the case of NO contamination.

The H_2O contaminant is a relatively inactive species and is involved predominantly in third-body reactions.

At particular temperatures and pressures, where these third-body reactions become important, the presence of H_2O can affect the overall kinetic characteristics. For other conditions, H_2O contributes primarily to changes in the thermodynamic properties of the mixture. One specific thermodynamic effect is the reduction of equilibrium temperature due to the high heat capacity of H_2O. The equilibrium temperature is always lower than the final temperature achieved with clean air.

The influence of the H_2O and CO_2 contaminant mixture is depicted in Figs. 14-17. A very similar variation in ignition and reaction times is observed with CO_2 addition as compared with H_2O alone, suggesting no significant contribution by CO_2 to the kinetic rates. Except for the results at 800 °K and 0.1 atmosphere where combustion cannot be obtained at high H_2O and CO_2 contamination, the ignition and reaction times show small sensitivity with respect to H_2O and CO_2 concentration even up to 30% of the mixture's total composition. The results show that CO_2 does not have a significant kinetic effect on hydrogen-air combustion over the present range of temperatures, pressures and concentrations. The reason for this is that CO_2 is a stable species, which participates only in third-body reactions, with a low third-body collisional efficiency in most of the reactions. The presence of CO_2 still contributes thermodynamically by causing an additional reduction in the equilibrium temperature, below that of the combustion with H_2O, in all cases studied.

C_2H_6 COMBUSTION

Ignition and reaction times are shown in Figs. 18-21. Ignition could not be achieved for mixtures at 800 °K for all pressures. Thus the results are presented for temperature of 900 °K and above. Contamination with NO generally results in the same trend observed with hydrogen combustion, which is characterized by a reduction in the ignition and reaction times over some range of temperatures and concentrations.

The main contribution of NO is to enhance ignition. Figure 18 demonstrates this characteristic since the clean air mixture did not ignite at 900 °K but a small amount of NO (1 to 1.5 %) resulted in ignition. Increasing NO concentration beyond 1.5%, the mixture again failed to ignite. The presence of NO tends to decrease ignition time, particularly at lower levels of NO. The reaction time tends to increase slightly or remains insensitive to the presence of NO.

Ignition and reaction times varying with pressure at various temperatures for mixtures with 20% H_2O contamination are shown in Fig. 22 for ethane combustion. The effect is minimal and largest at low temperature and pressure. For other level of H_2O concentration, the variations similarly show very little difference.

The effect of CO_2 and H_2O contamination on ethane combustion is illustrated in Fig. 23, and shows a variation nearly identical to the results with H_2O contamination alone. There is a small increase in reaction times. As previously observed with hydrogen combustion, ethane-air-H_2O mixtures are kinetically unaffected by the presence of CO_2. The effect of CO_2 is thermodynamic due to its large molecular weight and high heat capacity. In general, ethane combustion is insensitive to H_2O and CO_2 contamination, even at substantial levels of concentration, as was for the case for hydrogen combustion.

CH_4 COMBUSTION

Calculated ignition and reaction times for methane/air combustion with NO contamination are presented in Figs. 24-27. Methane does not easily ignite in air especially at low temperature and pressure and, in cases where combustion can be obtained, it takes a considerable time for the methane-air mixture to reach ignition and equilibrium. The overall chemical kinetics of methane combustion with NO contamination exhibits a characteristic opposite to what has been observed for hydrogen and ethane fuels. In a methane-air mixture, the effect of NO is to increase ignition and reaction times, causing combustion delay or no reaction. In Fig. 24, the clean-air mixture reacts at 1100 °K, but vitiated mixtures with any amount of NO do not at this temperature. Similarly at 100 atmospheres, Fig. 27, combustion can be achieved at 900 °K with 0 and 0.1% of NO, but mixtures with higher NO concentration do not ignite. Changes in ignition and reaction times are generally observed with small NO concentration then remain constant as the level of NO is increased. The changes appear somewhat insensitive to variations in pressure and temperature. The variations however are smaller in magnitude than in cases of combustion with hydrogen or ethane fuel where a stronger influence of NO contamination is observed.

Ignition and reaction times for methane combustion are depicted in Fig. 28 with 20% H_2O, and in Fig. 29 with 20% H_2O and 10% CO_2. These results show virtually no effect of flow contamination (H_2O or a combination of H_2O and CO_2) on the ignition time, and small influence on the reaction time.

RESULT SUMMARY

The ignition and reaction time results for the series of cases calculated in this study provide some general insight to the potential effects of test flow contaminants on ramjet/scramjet engine performance.

The results with hydrogen fuel show that the presence of NO, particularly at less than 1%, tends to promote ignition and reaction within the range of flow conditions predicted in scramjet combustors. The results for ethane

fuel with NO as a test flow contaminant show some enhancement of ignition and reaction, particularly at NO levels up to 1% and static temperature up to 1000 °K. The results for methane fuel with NO as a contaminant show a slight increase in ignition and reaction times. For many of the conditions calculated with ethane fuel and most conditions with methane fuel, the ignition and reaction times are above 1 to 10 milliseconds. For these conditions an ignition/reaction aid such as a pilot torch or injection of another (faster reacting) ignitor gas would be required.

The results with hydrogen fuel and either H_2O or the combination of H_2O and CO_2 as contaminants show a slight increase in ignition times, but the overall effects are minimal. The results with both ethane and methane fuels and either H_2O or the combination H_2O and CO_2 as contaminants show minimal effects of these contaminants on the ignition and reaction times. As explained before, for many of the conditions calculated the ignition and reaction times exceed 1 to 10 milliseconds and a pilot torch or a highly reactive ignitor gas would be required to obtain combustion in an engine.

CONCLUDING REMARKS

This study has been conducted to explore the kinetic effect of test flow contamination in air on the combustion of hydrogen, ethane, and methane fuels. The results show that the presence of NO as a contaminant could yield an enhancement of scramjet engine performance during Mach 5 to 7 testing. The presence of H_2O and CO_2 did not substantially effect the ignition and reaction kinetics for most of the cases studied. For many of these cases, however, the ignition and reaction times were too high to allow combustion in a ramjet or scramjet engine, and an ignition aid such as pilot torch or a highly reactive ignitor gas would be required to achieve combustion. For these cases (which particularly involve hydrocarbon fuels) unpiloted engine performance would not be achievable and, to assess the effects of flow contamination, additional calculations which include a candidate pilot gas should be accomplished. The overall results of this study show a potential for flow contaminant effects, but experimental data is needed to isolate these effects. Future computational efforts will include two and three dimensional analysis to explore test flow contaminant effects on specific configurations.

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NO	H_2	O_2	N_2
0.000	0.2958	0.1479	0.5563
0.005	0.2958	0.1454	0.5538
0.010	0.2958	0.1429	0.5513
0.020	0.2958	0.1379	0.5463
0.030	0.2958	0.1329	0.5413
0.045	0.2958	0.1254	0.5338

Table I: Mole fractions for hydrogen-air mixtures with NO contamination.

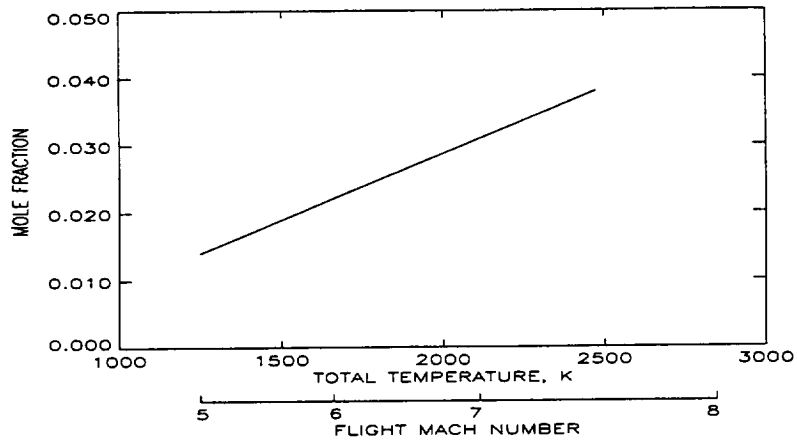


Fig. 1 Nitric oxide in electric arc-heated test facilities.

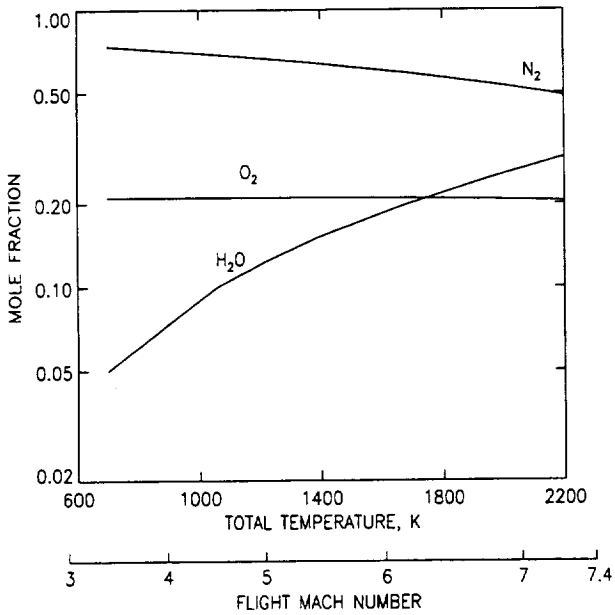


Fig. 2 Flow vitiates in H_2 combustion-heated test facilities.

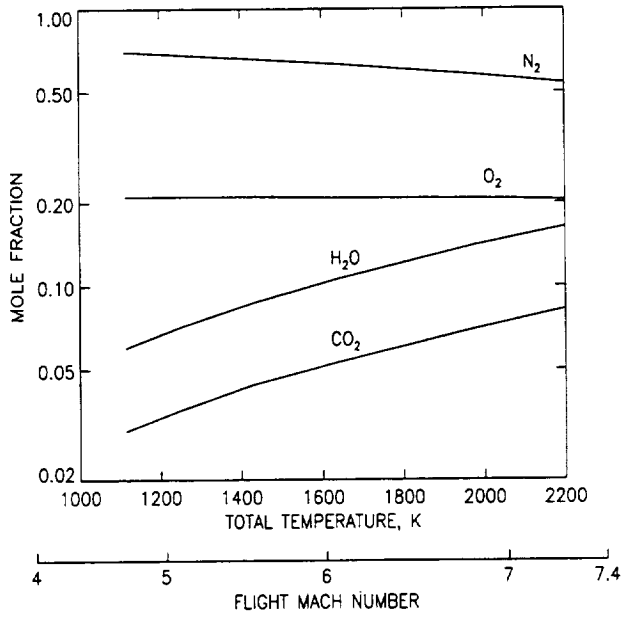


Fig. 3 Flow vitiates in CH_4 combustion-heated test facilities.

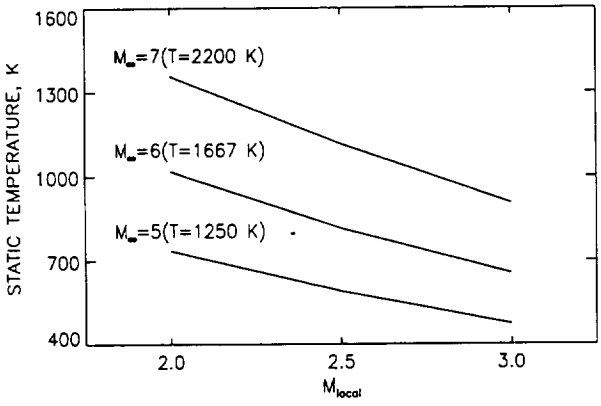


Fig. 4 Static temperature variation with local Mach number.

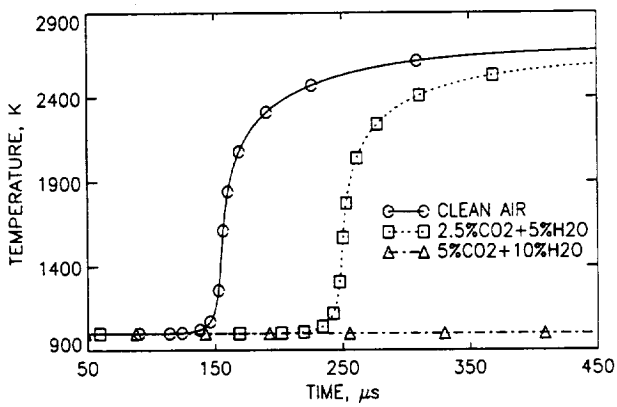


Fig. 5 Temperature profiles for hydrogen combustion at 1 atmosphere and 1000° K.

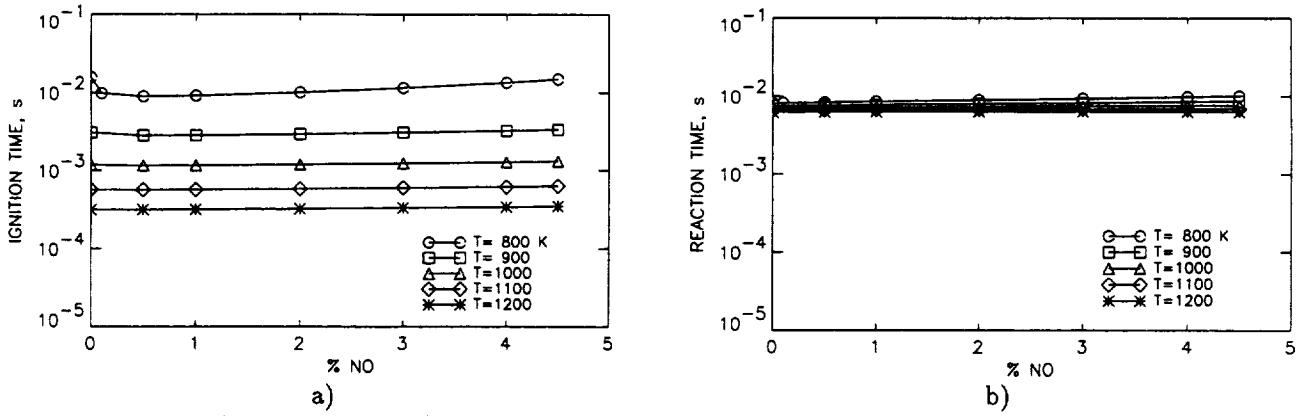


Fig. 6 Ignition, a), and reaction, b), times vs NO compositions for hydrogen fuel at 0.1 atmosphere.

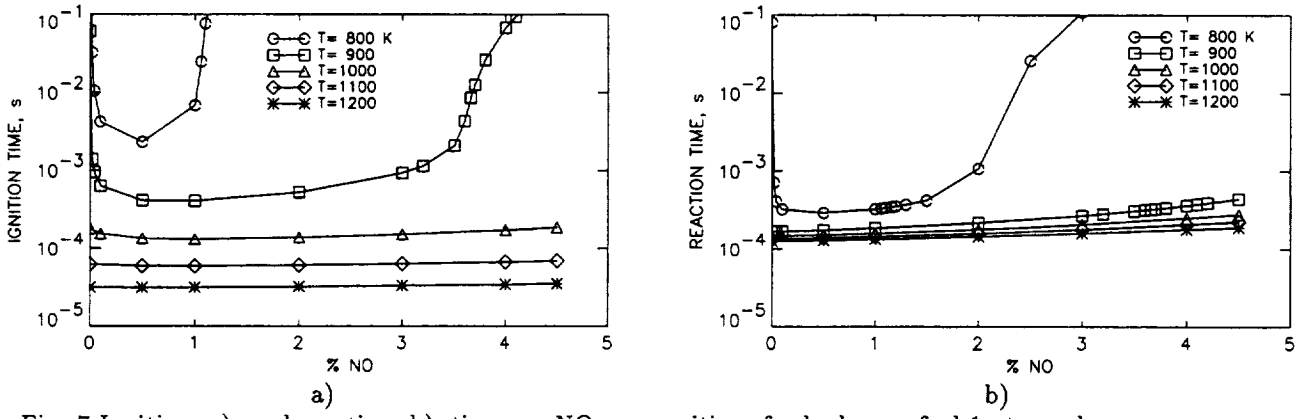


Fig. 7 Ignition, a), and reaction, b), times vs NO compositions for hydrogen fuel 1 atmosphere.

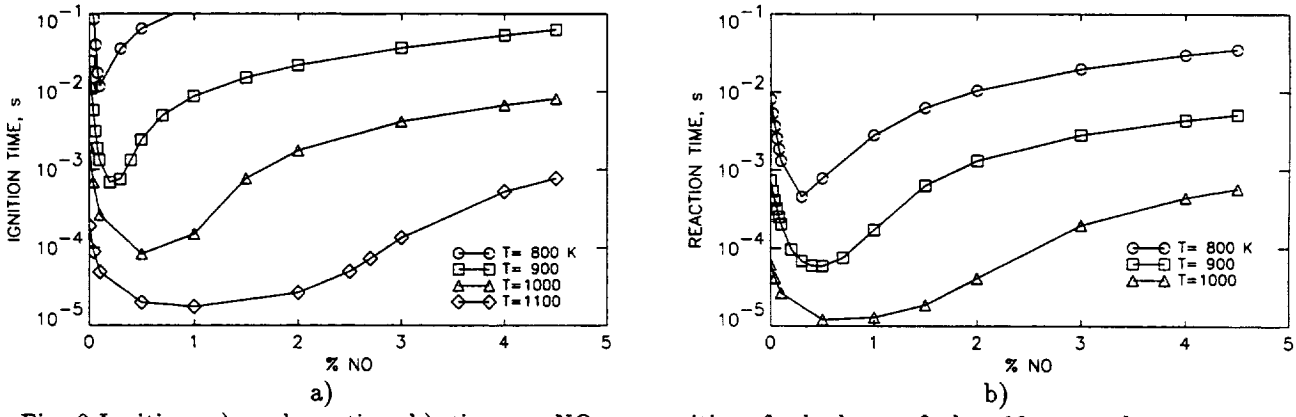


Fig. 8 Ignition, a), and reaction, b), times vs NO compositions for hydrogen fuel at 10 atmospheres.

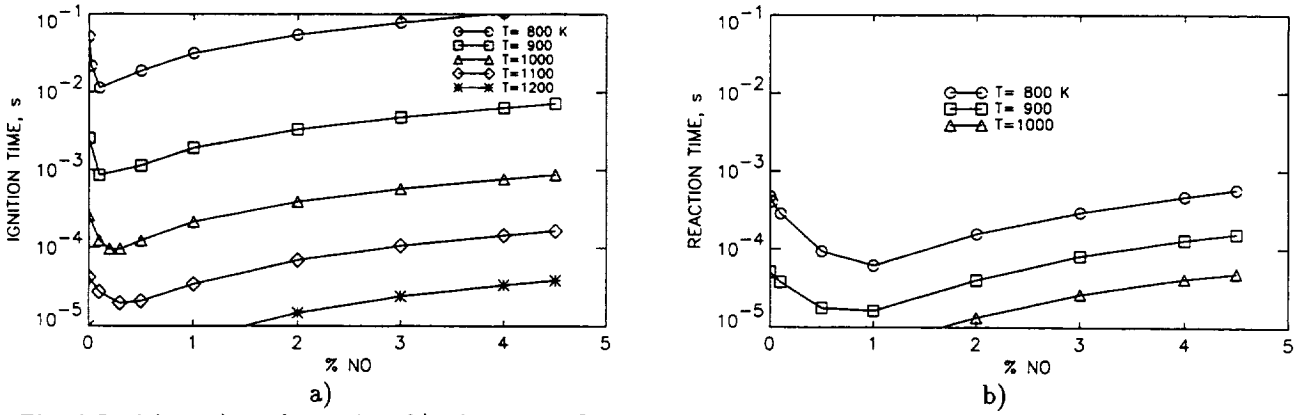
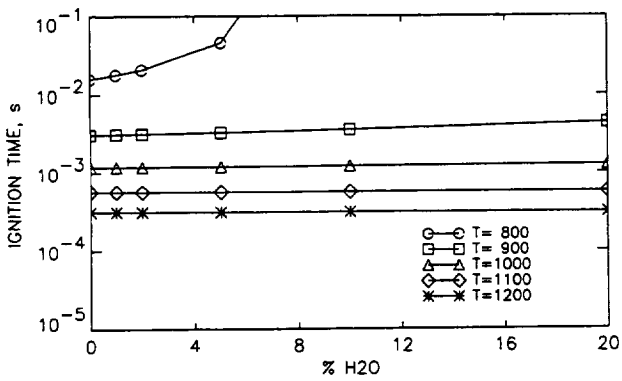


Fig. 9 Ignition, a), and reaction, b), times vs NO compositions for hydrogen fuel at 100 atmospheres.



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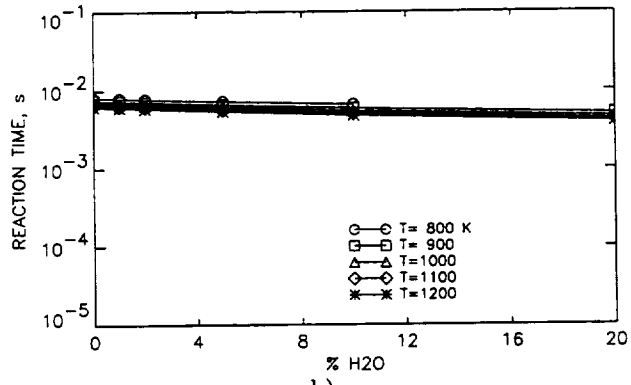
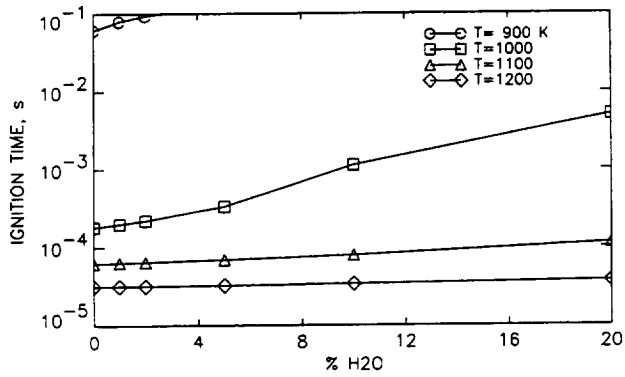
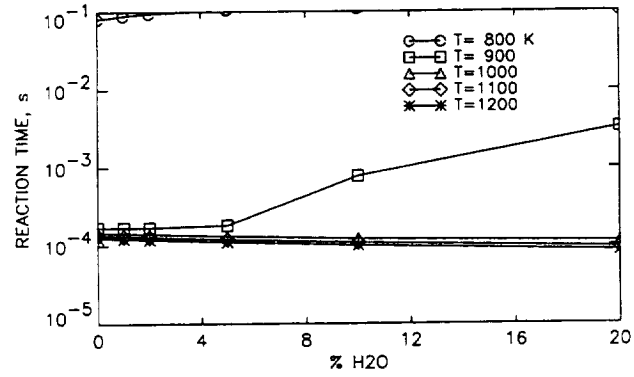


b)

Fig. 10 Ignition, a), and reaction, b), times vs H_2O compositions for hydrogen fuel at 0.1 atmosphere.

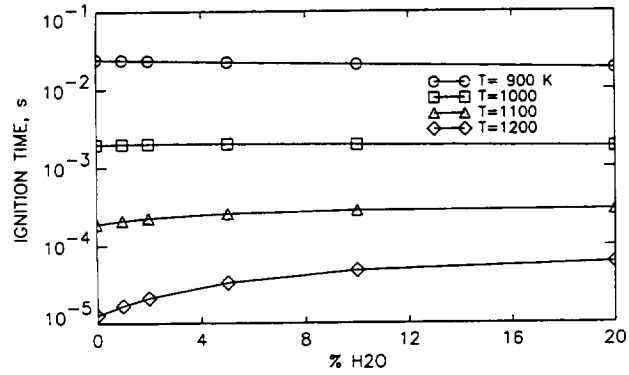


a)



b)

Fig. 11 Ignition, a), and reaction, b), times vs H_2O compositions for hydrogen fuel 1 atmosphere.



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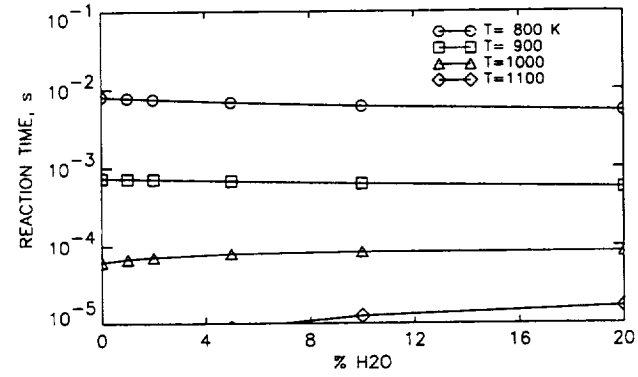
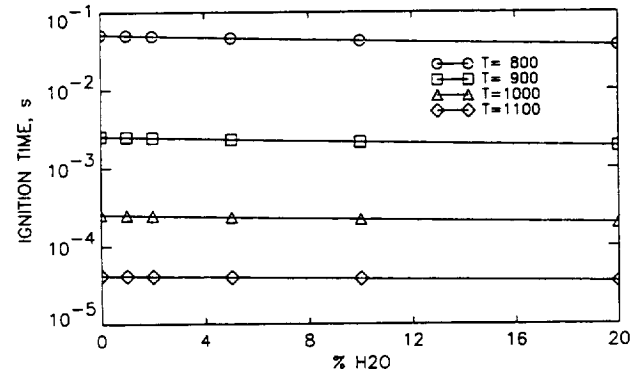


b)

Fig. 12 Ignition, a), and reaction, b), times vs H_2O compositions for hydrogen fuel at 10 atmospheres.



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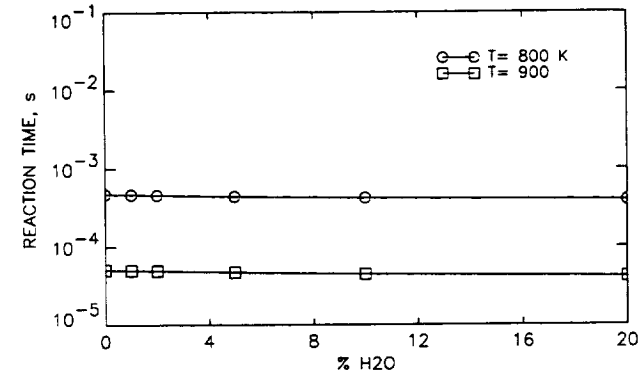

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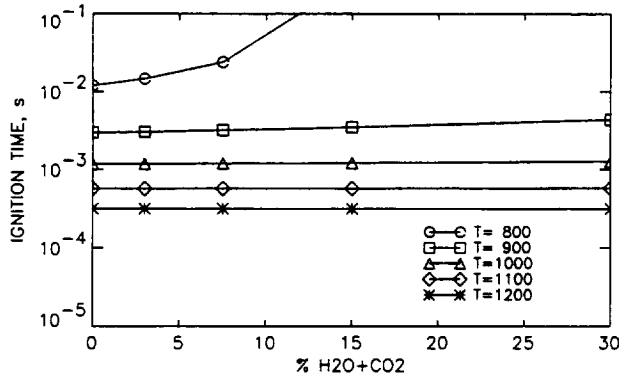
Fig. 13 Ignition, a), and reaction, b), times vs H_2O compositions for hydrogen fuel at 100 atmospheres.



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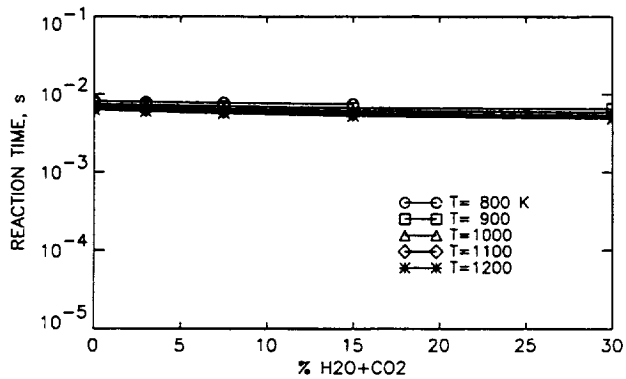
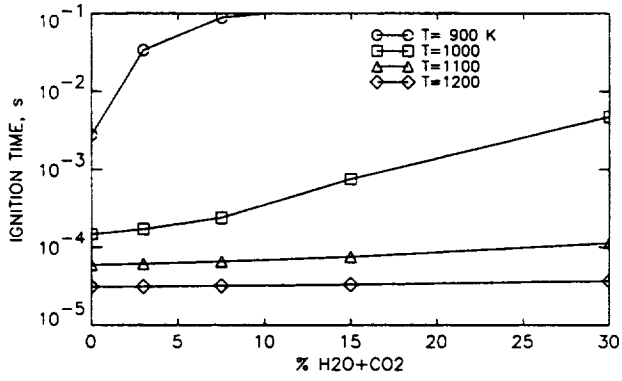


b)

Fig. 14 Ignition, a), and reaction, b), times vs H_2O and CO_2 compositions for hydrogen fuel at 0.1 atmosphere.



a)

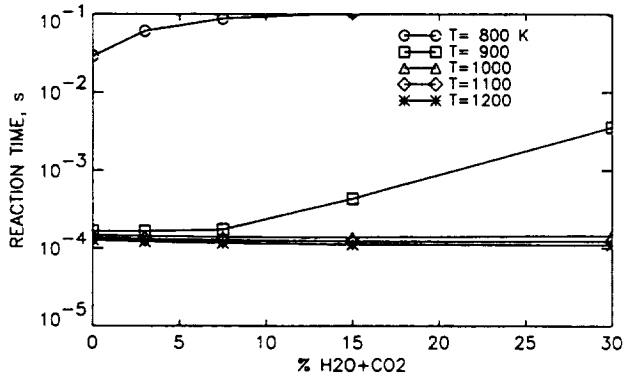


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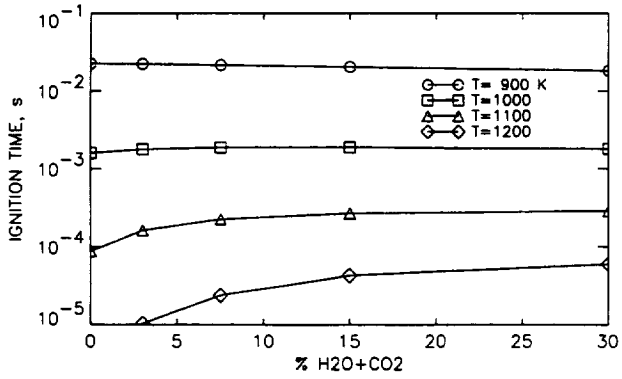
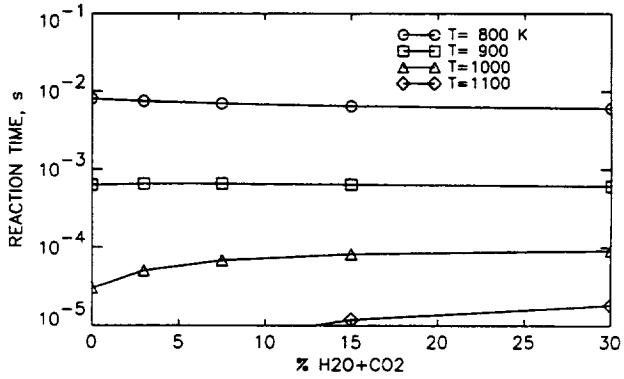
Fig. 15 Ignition, a), and reaction, b), times vs H_2O and CO_2 compositions for hydrogen fuel 1 atmosphere.

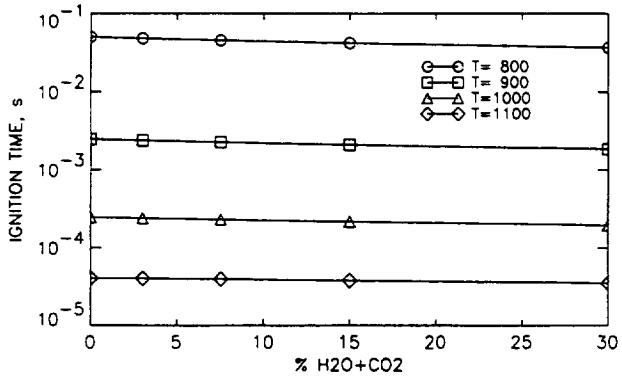


a)



b)

Fig. 16 Ignition, a), and reaction, b), times vs H_2O and CO_2 compositions for hydrogen fuel at 10 atmospheres.



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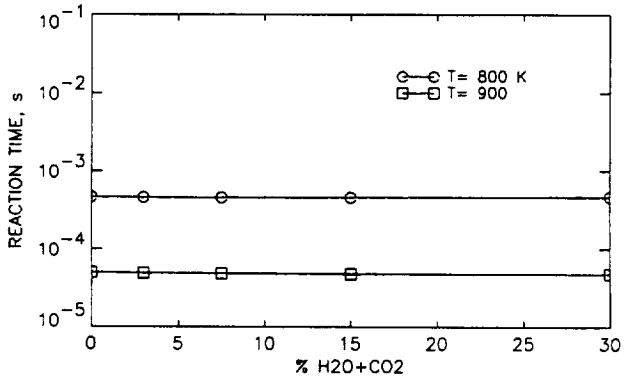

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Fig. 17 Ignition, a), and reaction, b), times vs H_2O and CO_2 compositions for hydrogen fuel at 100 atmospheres.

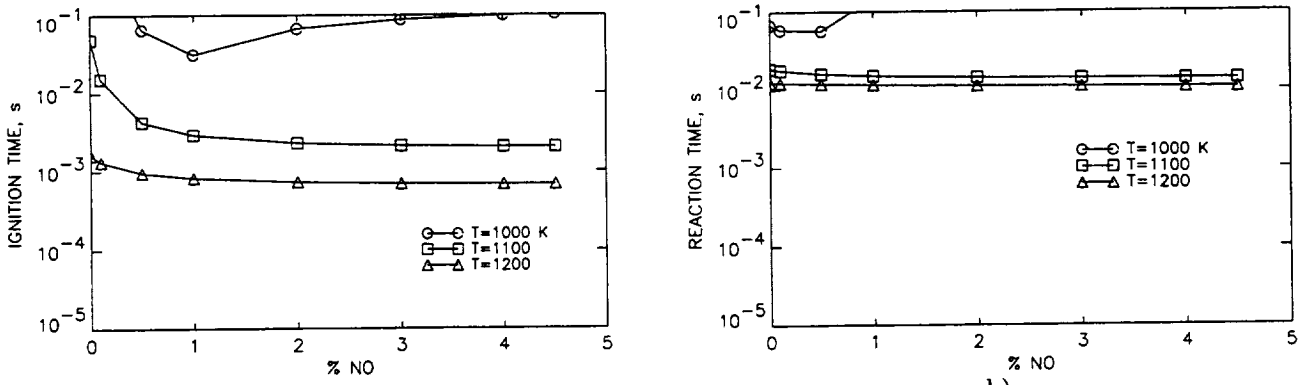


Fig. 18 Ignition, a), and reaction, b), times vs NO compositions for ethane fuel at 0.1 atmosphere.

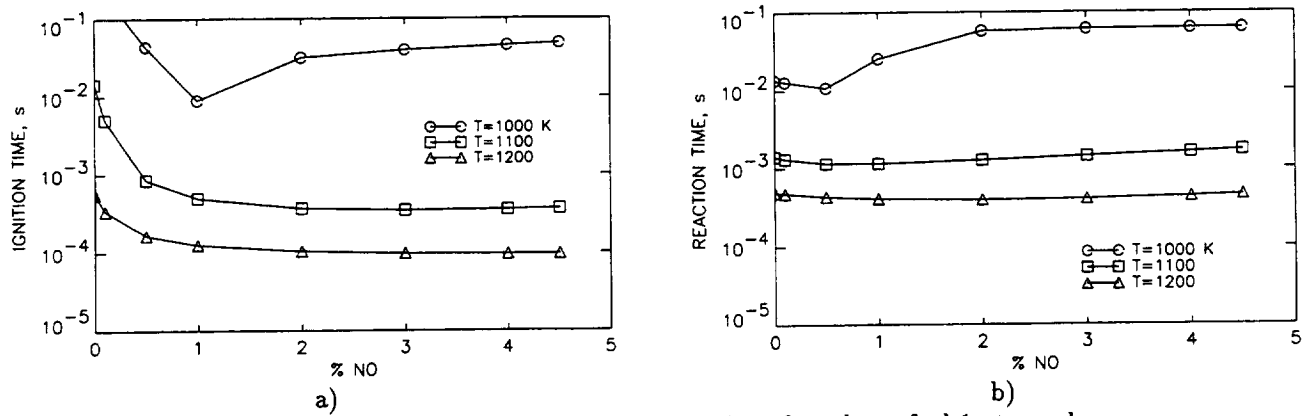


Fig. 19 Ignition, a), and reaction, b), times vs NO compositions for ethane fuel 1 atmosphere.

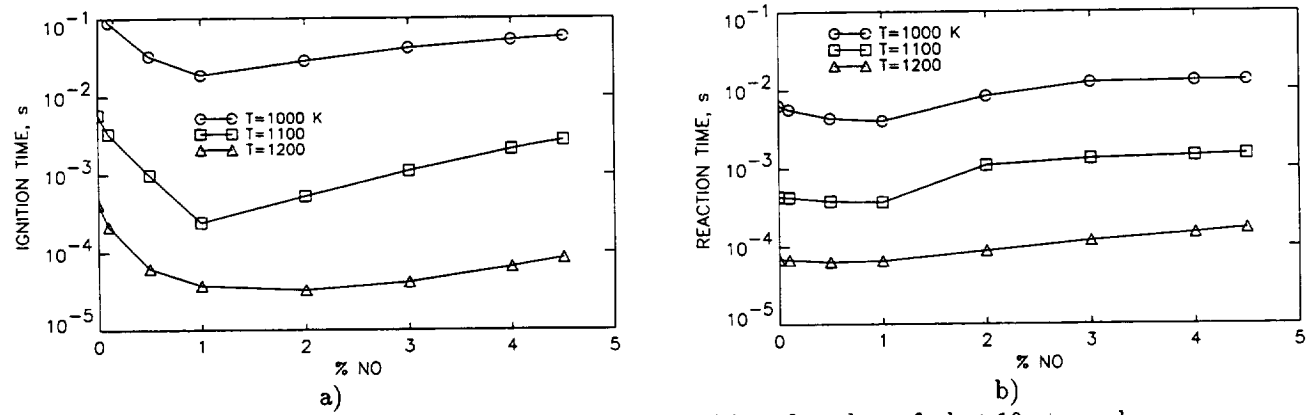


Fig. 20 Ignition, a), and reaction, b), times vs NO compositions for ethane fuel at 10 atmospheres.

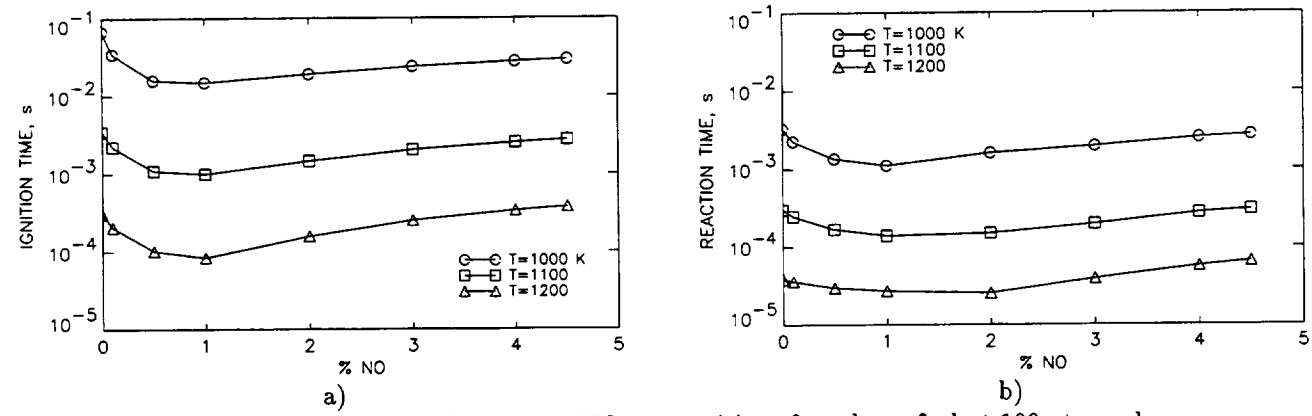


Fig. 21 Ignition, a), and reaction, b), times vs NO compositions for ethane fuel at 100 atmospheres.

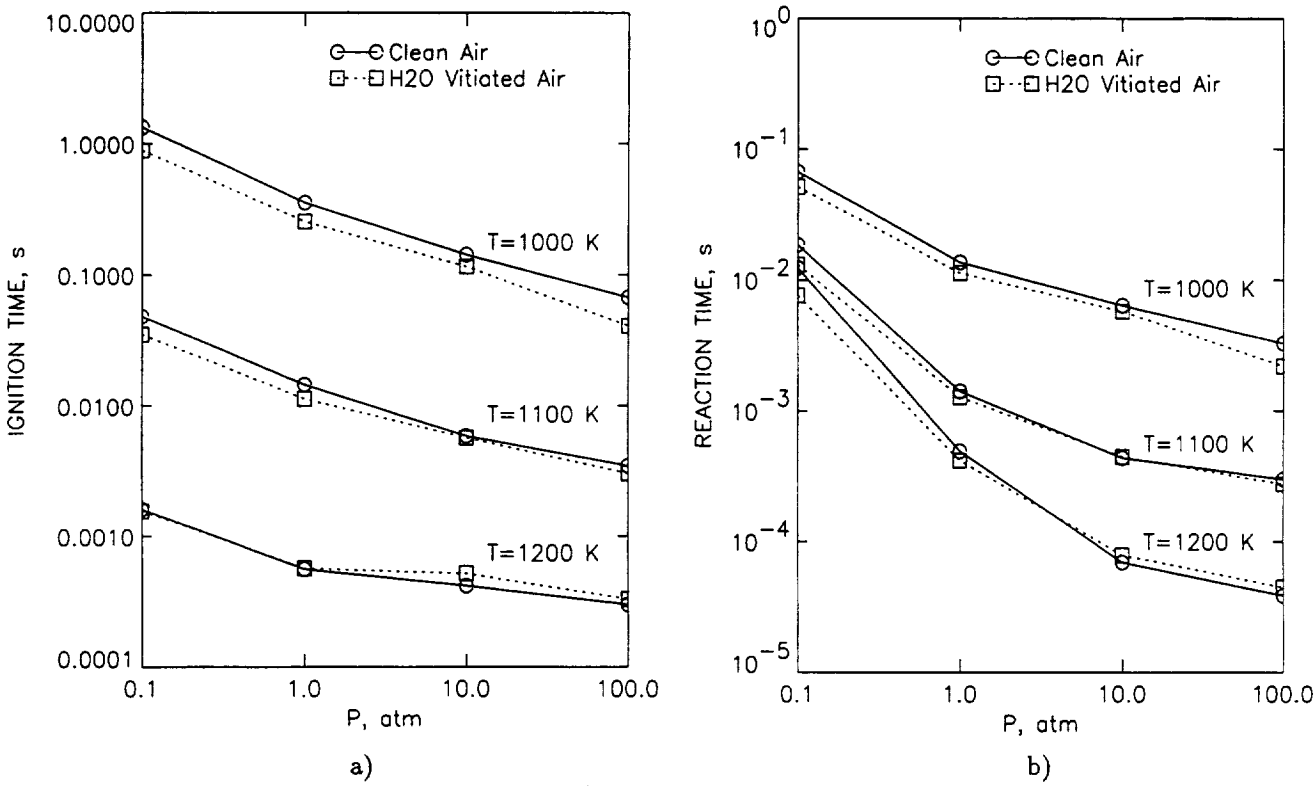


Fig. 22 H_2O contaminant effect on ignition, a), and reaction, b), times in ethane combustion.

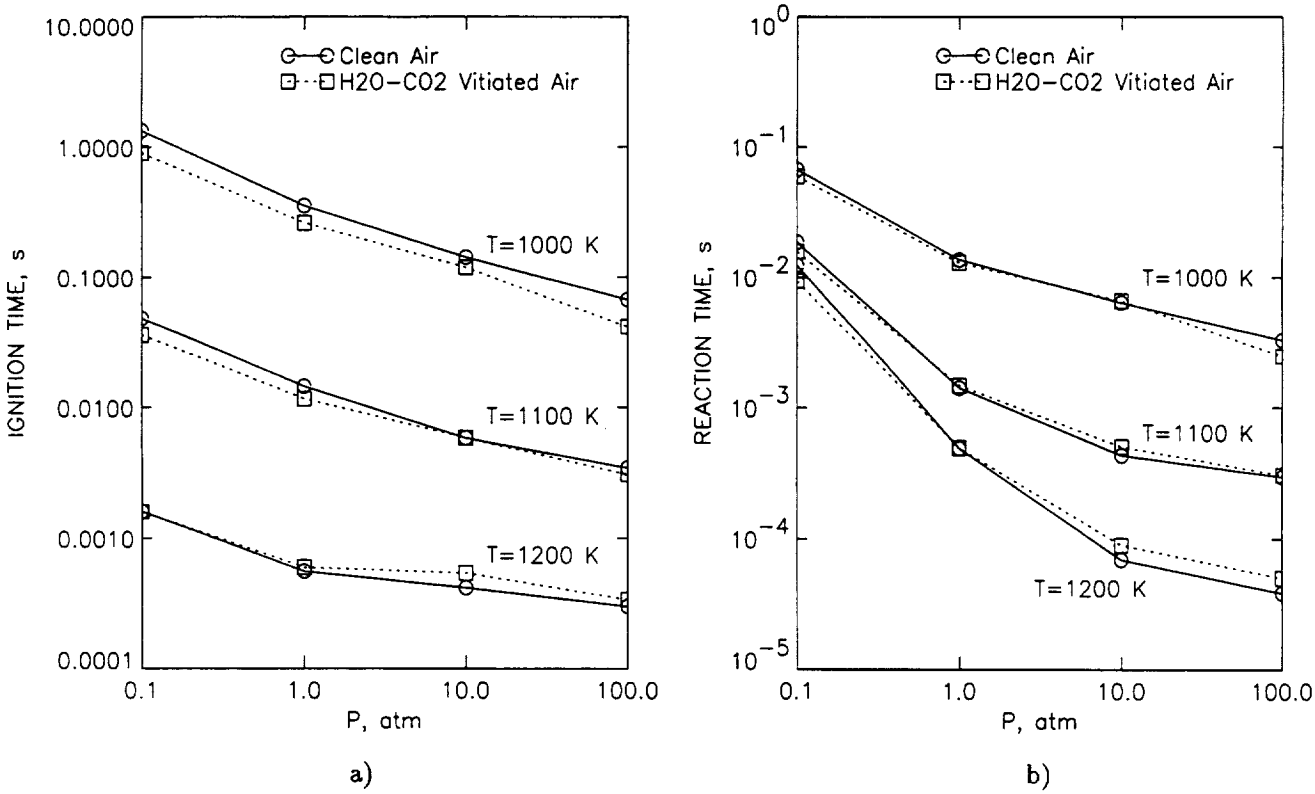
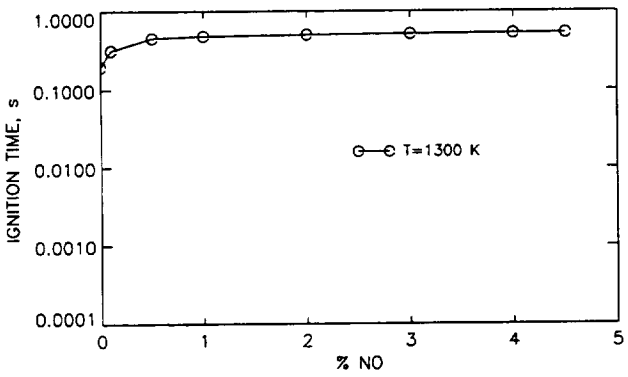


Fig. 23 H_2O and CO_2 contaminant effect on ignition, a), and reaction, b), times in ethane combustion.



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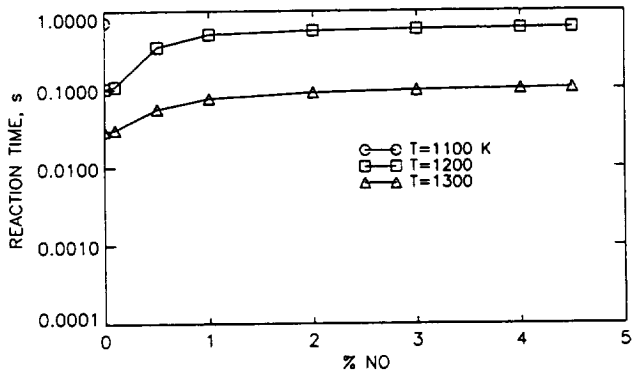
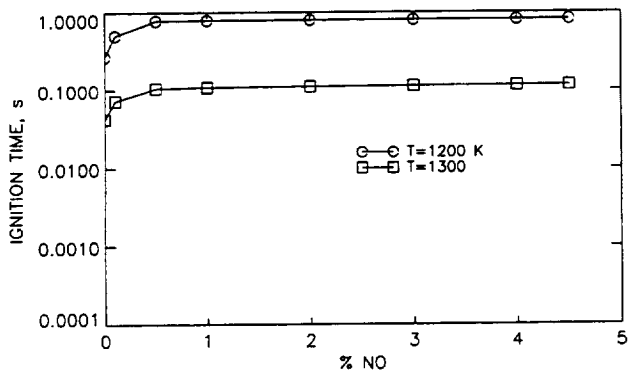


b)

Fig. 24 Ignition, a), and reaction, b), times vs NO compositions for methane fuel at 0.1 atmosphere.



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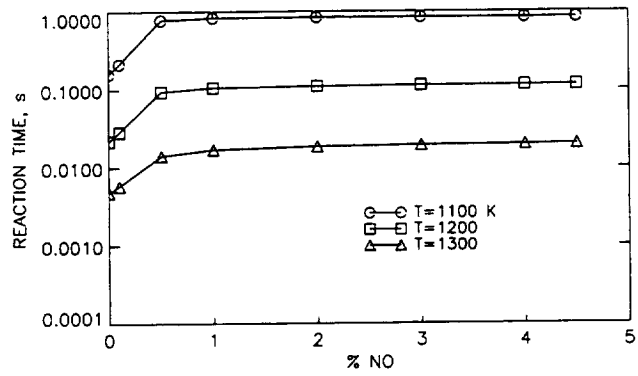
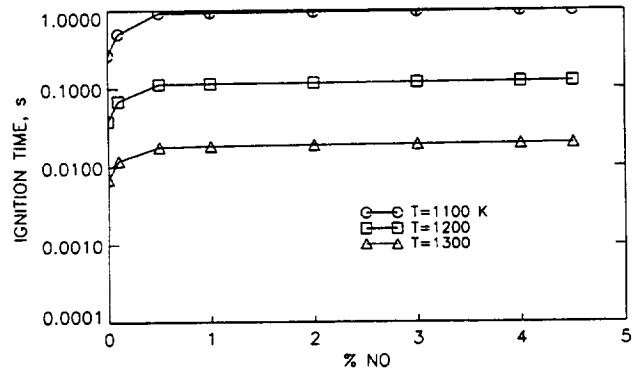
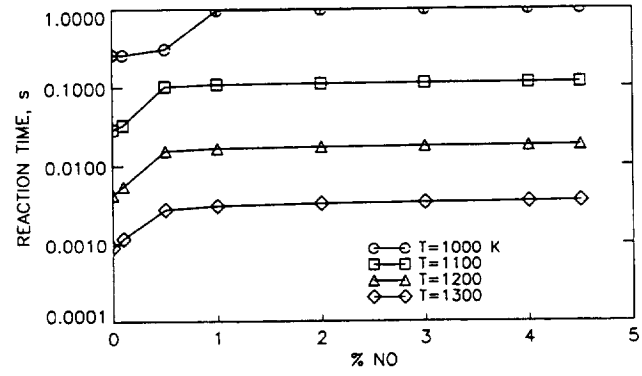


b)

Fig. 25 Ignition, a), and reaction, b), times vs NO compositions for methane fuel 1 atmosphere.

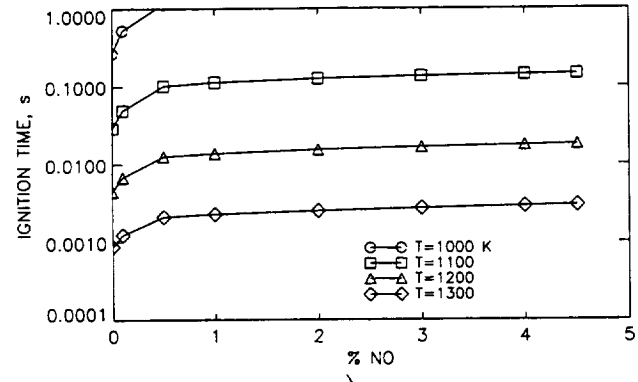


a)



b)

Fig. 26 Ignition, a), and reaction, b), times vs NO compositions for methane fuel at 10 atmospheres.



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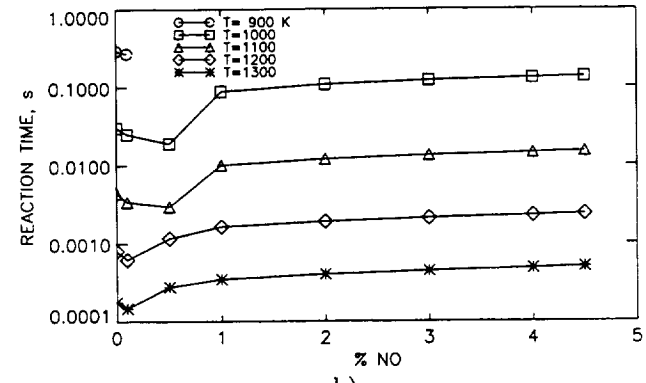
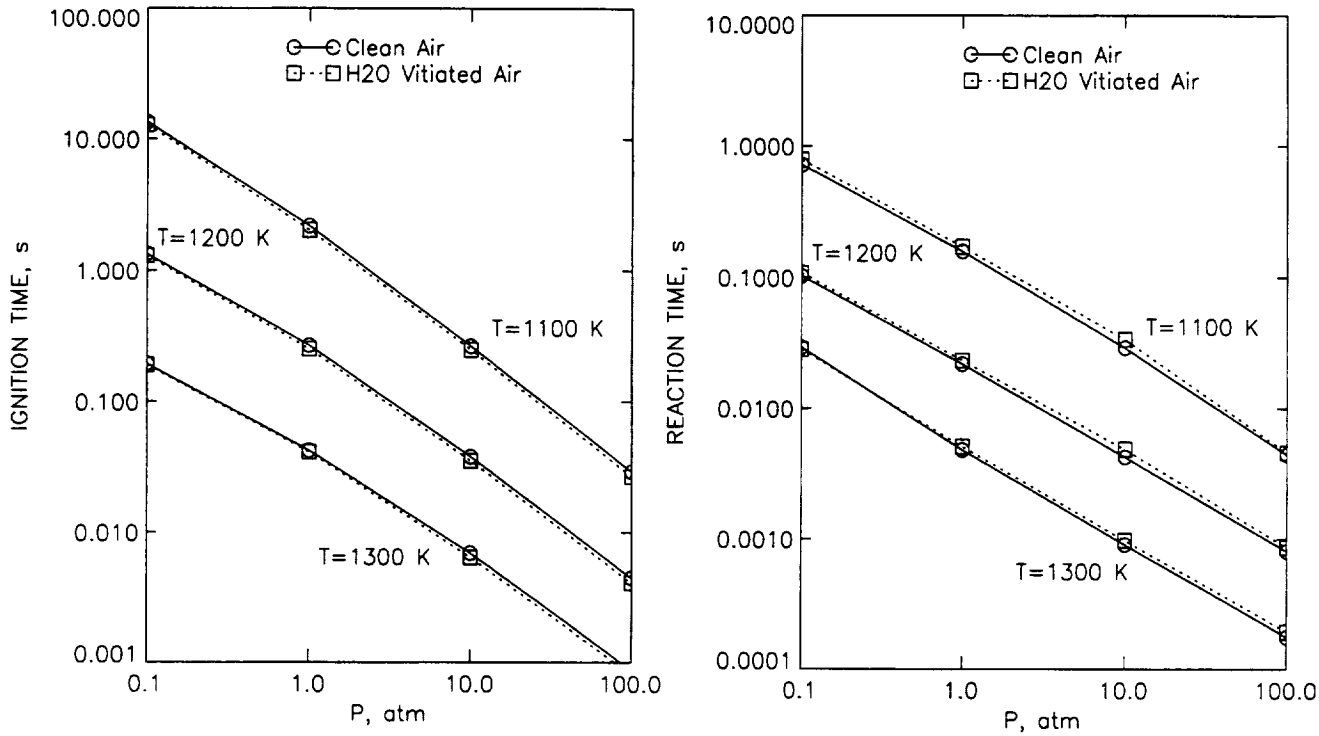


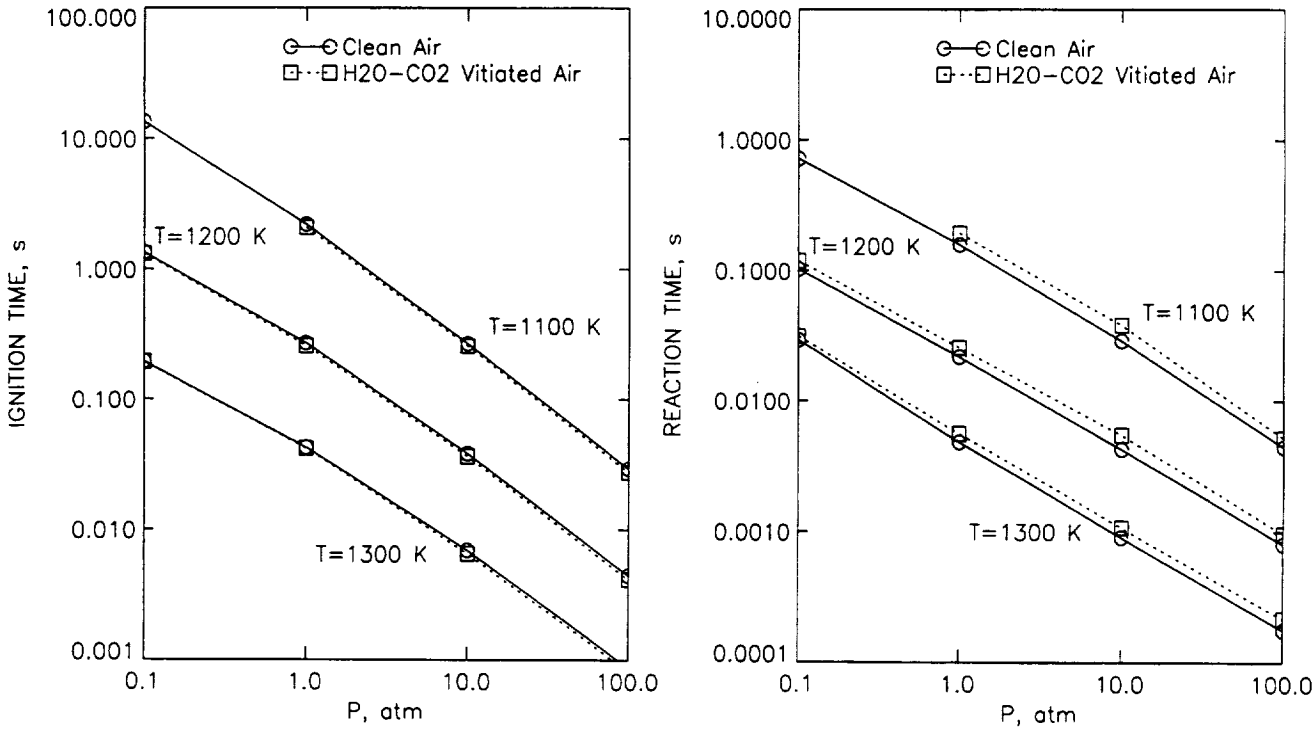
b)

Fig. 27 Ignition, a), and reaction, b), times vs NO compositions for methane fuel at 100 atmospheres.



a) b)

Fig. 28 H_2O contaminant effect on ignition, a), and reaction, b), times in methane combustion.



a) b)

Fig. 29 H_2O and CO_2 contaminant effect on ignition, a), and reaction, b), times in methane combustion.

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13. ABSTRACT (*Maximum 200 words*)

A numerical study was performed to assess the effects of vitiated air on the chemical kinetics of hydrogen, ethane, and methane combustion with air. A series of calculations in static reacting systems was performed, where the initial temperature was specified and reactions occurred at constant pressure. Three different types of test flow contaminants were considered: NO, H_2O, and a combination of H_2O and CO_2. These contaminants are present in the test flows of facilities used for hypersonic propulsion testing. The results were computed using a detailed reaction mechanism and are presented in terms of ignition and reaction times. Calculations were made for a wide range of contaminant concentrations, temperatures and pressures. The results indicate a pronounced kinetic effect over a range of temperatures, especially with NO contamination and, to a lesser degree, with H_2O contamination. In all cases studied, CO_2 remained kinetically inert, but had a thermodynamic effect on results by acting as a third body. The largest effect is observed with combustion using hydrogen fuel, less effect is seen with combustion of ethane, and little effect of contaminants is shown with methane combustion.

14. SUBJECT TERMS

Contaminants; Hydrogen; Methane; Ethane; Ignition time delay; Reaction time; Scramjet; Combustor

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