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Prediction of Non-Equilibrium Kinetics of Fuel-Rich Kerosene/LOX Combustion in Gas Generator

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Abstract

Gas generator is the device to produce high enthalpy gases needed to drive turbo-pump system in liquid rocket engine. And, the combustion temperature in gas generator should be controlled below around 1,000K to avoid any possible thermal damages to turbine blade by using either fuel rich combustion or oxidizer rich combustion. Thus, non-equilibrium chemical reaction dominates in fuel-rich combustion of gas generator. Meanwhile, kerosene is a compounded fuel with various types of hydrocarbon elements and difficult to model the chemical kinetics. This study focuses on the prediction of the non-equilibrium reaction of fuel rich kerosene/LOX combustion with detailed kinetics developed by Dagaut using PSR (Perfectly Stirred Reactor) assumption. In Dagaut's surrogate model for kerosene, chemical kinetics of kerosene consists of 1,592 reaction steps with 207 chemical species. Also, droplet evaporation time is taken into account in the PSR calculation by changing the residence time of droplet in the gas generator. Frenklach's soot model was implemented along with detailed kinetics to calculate the gas properties of fuel rich combustion efflux. The results could provide very reliable and accurate numbers in the prediction of combustion gas temperature, species fraction and material properties.

Keywords: Gas generator; Fuel-rich; Non-equilibrium; Perfectly Stirred Reactor; Fuel evaporation time

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1. Introduction

The rocket propellants are fed into the thrust chamber either by gas-pressurized feed system or turbopump feed system. Even though pressurized feeding system has advantages of simplicity in operation, the turbopump feed system is usually suitable for high thrust, long duration engines. In turbopump feed system, the major portion of the pressure required to feed propellants is supplied by pumps. Therefore, the turbopump system can be essentially applied to bigger liquid rocket engine (LRE) system with the improved performance (Huzel and Huang, 1992). Generally, the delivered temperature from gas generator should be controlled about 1,000 K or less to avoid any excessive thermal stress on turbine blade since no cooling system can be installed. Thus, combustion in gas generator is operated either with fuel-rich mixture or oxidizer rich. And the temperature uniformity of gas generator becomes one of the major issues of design and performance. The fuel rich combustion is relatively easy to implement in the liquid rocket engine even though the prediction of combustion is not easy because a non-equilibrium chemical kinetics dominates in the gas generator (NASA, 1974).

Many studies with equilibrium chemistry did not successfully predict the chamber temperature and characteristic velocity. The study of Bensky et al. (1977) was the example of the approach with equilibrium chemistry. They found the result of

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unbalanced temperature distribution was attributed to the overestimation of temperature near injector plate. Lawver (1982) suggested the new approach for the analysis of fuel rich combustion with kerosene/LOX. He could obtain the very successful prediction in combustion temperature, efflux properties and compositions by using semi global fuel decomposition with empirically fitted rates for the preliminary reaction steps. Nonetheless the good predictive capabilities of the approach as well as the details of the model are not disclosed to the public. And it is still necessary to secure a simple and effective tool for the analysis of fuel rich combustion.

Foelsche et al. (1994) proposed a simple and very efficient way of dealing with fuel rich combustion by using PSR model. They studied to predict efflux of fuel rich combustion in ram-rocket. In this propulsion system, a solid or liquid fueled rocket is employed as a gas generator to produce fuel rich efflux for subsequent combustion with air entrained from free stream. Their analysis included a finite time requirement for fuel vaporization in calculating the reactor residence time. Also, an artificial reaction temperature was implemented to maintain the reaction source in the calculation by introducing the separated temperature for chemical reaction. Then, the gas temperature was calculated from the solution of energy equation. Even though their model for fuel rich combustion was successfully applied in calculating combustion gas properties of JP-7 fuel, the combustion of more complex hydrocarbon fuel such as kerosene was not properly treated in their study. Also, their approach was intrinsically lack of the soot formation. Soot formation may be of importance in predicting performance of combustion system because soot formation and deposition may deteriorate the performance of combustion in gas generator.

Previous studies (Bensky and Wong, 1977; Lawver, 1982; Foelsche et al., 1994) on the fuel rich combustion revealed that two major factors can contribute to the poor combustion efficiency; forward reaction rate kinetics which limits the available energy in the combustion, and incomplete vaporization of the fuel rich propellant. The evaporation of oxidizer is so fast that the evaporation time can be safely neglected in the analysis. However, the vaporization time of hydrocarbon fuel is relatively longer than that of oxidizer. And the incomplete vaporization in the combustor can change the combustion mode to non equilibrium combustion. Also, the soot formation in kerosene/LOX combustion is another barrier to overcome in the computational approach.

In order to accurately model the fuel rich combustion in the computational approach, it is necessary to consider these two major factors (kinetics and vaporization) as well as the pertinent fluid dynamics and various effects in the combustion. In this regard, the perfectly stirred reactor is the proper concept used in the calculation for fuel rich combustion. And the empirical formula and thermodynamic properties can determine the vaporization time for fuel droplet. Then, the initial residence time in the reactor should be modified adequately. To implement the non-equilibrium chemical kinetics, a detailed chemical kinetics suggested by Dagaut (2002) for kerosene/LOX combustion was adopted. This kinetics has been proved a very accurate mechanism for kerosene by using the surrogated model with 1,592 reaction steps with 207 chemical species. Dagaut verified this mechanism can accurately predict the combustion in various pressure and temperature conditions. Also, since Dagaut's model did not consider the formation of precursor PAH or soot formation, the soot formation model was included by combining the well known Appel's kinetics mechanism (Appel et al., 2000). This mechanism predicts well the major, minor and aromatic species up to pyrene in laminar premixed flames of ethane, ethylene, and acetylene fuels.

The objective of present study is to develop a simple and convenient tool for the prediction of gas properties of fuel rich combustion efflux, such as combustion temperature, specific heats and specific heat ratio etc. by the use of non-equilibrium model of combustion in gas generator. PSR concept was the basis of the computational approach as a calculation code and fuel vaporization was also taken into account in the calculation procedure. A limited soot formation model was implemented in the analysis as well.

2. Numerical calculation with PSR model

In the perfectly stirred reactor (PSR), the combustion is assumed an ideal reaction. And a mixing time is assumed negligibly fast and the gas properties and temperature are also assumed spatially uniform. And this assumption can simplify the governing equation (Glarborg et al., 1990). The mass and energy equations are satisfied with appropriate consideration for the species source terms generated through the combustion process. Even with this simplification, the well stirred reactor model can provide some physically relevant results. In the stirred reactor model, the governing equations have the following form: species conservation;

$$\dot{m}(Y_k - Y_k^*) - \dot{\omega}_k W_k V = 0 \tag{1}$$

And conservation of energy;

$$\dot{m}\sum_{k=1}^{K}(Y_k h_k - Y_k^* h_k^*) + Q = 0 \tag{2}$$

where superscript(*) indicates initial conditions.

Although the governing equations are intrinsically steady, the numerical process may require the solution of the time-dependent problem to obtain the well guessed value for rapid convergence. The transient equations are then

$$\rho V \frac{dY_k}{dt} = -\dot{m}\left(Y_k - Y_k^*\right) + \dot{\omega}_k W_k V \tag{3}$$

and

$$\rho V \frac{dh}{dt} = -\dot{m}\sum_{k=1}^{K}\left(Y_k h_k - Y_k^* h_k^*\right) - Q \tag{4}$$

The steady state equations form a set of K+1 non-linear algebraic equation whereas the transient equations are non-linear ODE initial value problem with K+1 unknown.

The chemical source terms, $\dot{\omega}_k$ is the net rate of production of each species. The net rate is the summation of the individual progress of each species for each reaction. Considering a set of reactions of the form

$$\sum_{k=1}^{K}\nu'_{ki}\chi_k \rightleftarrows \sum_{k=1}^{K}\nu''_{ki}\chi_k \tag{5}$$

the term $\dot{\omega}_k$ can be written

$$\dot{\omega}_k = \sum_{i=1}^{I}\nu_{ki} q_i \tag{6}$$

where

$$\nu_{ki} = (\nu''_{ki} - \nu'_{ki}) \tag{7}$$

and the rate of progress variable is given by

$$q_i = k_{fi}\prod_{k=1}^{K}[X_k]^{\nu'_{ki}} - k_{ri}\prod_{k=1}^{K}[X_k]^{\nu''_{ki}} \tag{8}$$

In the formulation the forward reaction rate constants, k_{fi} are given by Arrhenius expression.

$$k_{fi} = A_i T^{\beta_i} exp\left(-\frac{E_i}{R_c T}\right) \tag{9}$$

And the reverse rates are calculated by the equilibrium constant determined from the thermodynamic properties for a given temperature and pressure in PSR calculation.

The present study basically utilizes a modified baseline code developed with PSR code in Chemkin II. PSR code solves the system of equations by using a damped modified Newton algorithm. This is an iterative approach which constructs a series of approximate solution vectors to the set of governing equations. In general, the n^th^ iteration will not precisely generate the solutions of governing equations, but will calculate a residual vector, $\vec{F}$ containing the updated solutions. Thus, the iteration is necessary to determine a solution vector, $\vec{\phi}$ such that

$$\vec{F}\left(\vec{\phi}\right) = 0 \tag{10}$$

In the PSR code, $\vec{\phi}$ is the solution vector of temperature and species mass fraction of each species.

$$\vec{\phi} = (T,\ Y_1, \ldots, Y_k, \ldots, Y_K) \tag{11}$$

And the residual vector $\vec{F}$ represents residual of the energy and species conservation equation.

The original stirred reactor model assumed pre-vaporized, premixed gaseous combustion by neglecting the propellant injection and vaporization issues nor ignition processes. In order to apply stirred model, however, some critical modifications should be made to incorporate these important issues in modeling the gas generator combustion within the limitations imposed by the perfectly stirred reactor idealization. One of the modifications is the droplet model implemented by classic Spalding model in the calculation code. The classic Spalding model considers the combustion of a single fuel droplet of specified diameter in a quiescent oxidizing atmosphere. Since the details of the Spalding model can be found in many sources, only the pertinent results will be included in this problem.

According to the Spalding model, a droplet lifetime can be expressed in terms of various parameters;

$$\tau_l = \frac{c_p \rho_l d_o^2}{8\lambda ln(1+B)} \tag{12}$$

where the Spalding transfer number, B is defined as:

$$B = \frac{1}{L}\left[c_p(T_\infty - T_L) + \frac{q^0 Y_{0,\infty}}{j}\right] \tag{13}$$

The fuel properties in B and τ_l are calculated from empirical correlations and thermodynamic properties. The details of fuel properties for kerosene surrogate are shown in Table 1 (Smith and Srivastava, 1986). The consideration of droplet vaporization can affect the PSR calculation in two ways. First, there is a reactor heat loss due to the enthalpy subtraction required to evaporate the fuel droplet. Secondly, the reactor residence time should be modified due to the finite time required for vaporizing the injected fuel droplets.

The heat loss through the chamber wall can also affect the combustion in gas generator. A straightforward modification should be made for a given fuel type to account for the heat loss. However, no heat loss was assumed in this study. And the fuel residence time in the reactor is calculated from the total residence time by decreasing the total time by the greatest mean lifetime of a specified fuel droplet. Then, the maximum calculated lifetime for any of species needs to be subtracted from the initial reactor residence time (determined by the input mass flow rate); i.e.:

$$\tau = \tau_0 - \tau_l^* \tag{14}$$

where the superscript (*) indicates the maximum droplet lifetime. Thus the modified reactor residence time gives a lower limit for allowable combustion time. In the real conditions, the oxidizer stream vaporizes very quickly within a few percent of combustor length, whereas the combustion of vaporized fuel could proceed prior to complete evaporation. Thus, this approximation will only valid if the vaporization times are small compared to the total reactor residence time.

The followings are the equations used for the determination of evaporation time of fuel droplet in the gas generator. In order to calculate the evaporation time of fuel droplet, a few empirical constants and thermodynamic relations are required. The latent heat of vaporization, L in Spalding transfer number can be evaluated by Clapeyron equation as in Eq. (15). Here the temperature is assumed as boiling temperature and calculated by Antoine Eq. (16).

$$L = \frac{dp'}{dT}(V_g - V_l)T \tag{15}$$

$$T_b(K) = \frac{B_4}{(A_4 - log_{10}p)} - C_4 + 273.15 \tag{16}$$

As previously mentioned, kerosene can be modeled by a surrogate fuel consisted of various elements. Three major elements were used as a surrogate fuel for kerosene; n-decane, n-propylbenzene, and n-propylcyclohexane. The following equations are used to calculate vapor pressure, p' in Clapeyron equation for each three components of kerosene surrogate fuel.

n-decane: modified Wagner equation

$$ln\, p' = \frac{1}{T_r}\left[P_r^{(0)} + \Omega P_r^{(1)} + \omega^2 P_r^{(2)}\right] \tag{17}$$

$$P_r^{(i)} = N_{i,1}(1-T_r) + N_{i,2}(1-T_r)^{1.5} + N_{i,3}(1-T_r)^{2.5} + N_{i,4}(1-T_r)^5 \tag{18}$$

n-propylbenzene: Wagner equation

$$ln\, p' = \frac{1}{T_r}\left[A_1(1-T_r) + B_1(1-T_r)^{1.5} + C_1(1-T_r)^3 + D_1(1-T_r)^6\right] \tag{19}$$

n-propylcyclohexane: Riedel-Plank-Miller-2 equation

$$ln\, p' = \frac{1}{T_r}\left[A_1 + \frac{B_1}{T} + C_1 + D_1 T^2\right] \tag{20}$$

And the liquid molar volume, in Clapeyron equation is expressed as;

$$V_l = \frac{1}{\rho_l} \tag{21}$$

Also, the following Francis equation and equation of state will provide the number for V_l.

$$\rho_l(g/ml) = A_2 - B_2 T - \frac{C_2}{E_2 - T} \tag{22}$$

$$\frac{pV_g}{RT} = 1 + \frac{B_{ii}}{V_g} \tag{23}$$

The gas volume, V_g in Eq. (23) can be rewritten as

$$V_g = 1 + \frac{\sqrt{1 + 4B_{ii}\left(\frac{p}{RT}\right)}}{\left(\frac{2p}{RT}\right)} \tag{24}$$

Meanwhile, the second virial coefficient, B_{ii} in Eq. (23) should be obtained by Pitzer-curl correlations as shown below.

$$\frac{B_{ii}P_c}{RT_c} = f^{(0)}(T_r) + \Omega f^{(1)}(T_r) + f^{(2)}(T_r) \tag{25}$$

$$f^{(0)}(T_r) = f^{(0)}_{pc}(T_r) - \frac{0.000607}{T_r^8} \tag{26}$$

$$f^{(1)}(T_r) = 0.0637 + \frac{0.331}{T_r^2} - \frac{0.423}{T_r^3} - \frac{0.008}{T_r^8} \tag{27}$$

$$f^{(2)}(T_r) = \frac{A_3}{T_r^6} - \frac{B_3}{T_r^8} \tag{28}$$

$$f^{(0)}_{pc}(T_r) = 0.1445 - \frac{0.330}{T_r} - \frac{0.1385}{T_r^2} - \frac{0.0121}{T_r^3} \tag{29}$$

Figure 1 shows the schematic of the fuel rich combustion in gas generator with kerosene/LOX mixture. Since the oxidizer stream vaporizes more quickly within a short distance from the injector plate, the evaporation of fuel droplet can control the progress of chemical reaction. And the decomposition of excess fuel prevails in the gaseous oxygen environment prior to combustion reaction. Thus, a locally hot spot can be generated at the region near the injector plate, where a stoichiometric chemical reaction may take place. This hot spot can also take a role of providing the necessary heats for continuous fuel vaporization and decomposition along the gas generator.

Table 1. Physical data and empirical coefficients of kerosene surrogate.

		n-decane	n-propylbenzene	n- propylcyclohexane
Critical Temperature (K)	T_c	617.75	638.35	639.00
Critical Pressure (bar)	P_c	21.03	32.0	28.0
Heat of Reaction (cal/gm)	Q_0	10568.84	9851.32	10374.36
Vapor Pressure Correlation	A_1	Modified Wagner equation (more coefficients)	-0.81945655D+01	0.28113438D+02
	B_1		0.25824838D+01	-0.67615631D+04
	C_1		-0.49994036D+01	-0.24830113D-01
	D_1		-0.70133165D+00	0.15732895D-04
Molar Density Correlation	A_2	0.7733D+0	0.11103115D+1	0.10208874D+1
	B_2	0.76D-4	0.78414031D-3	0.70593762D-3
	C_2	-0.8D+1	0.59999990D+1	0.59999990D+1
	D_2	0.382D+3	0.62005029D+3	0.58713574D+3
B_{ii} Correlation	Ω	0.4894	0.345	0.258
	A_3	0	0	0
	B_3	0	0	0
Boiling Temperature Correlation	A_4	6.96375	6.95142	6.88646
	B_4	1508.750	1491.297	1460.800
	C_4	195.375	207.140	207.939

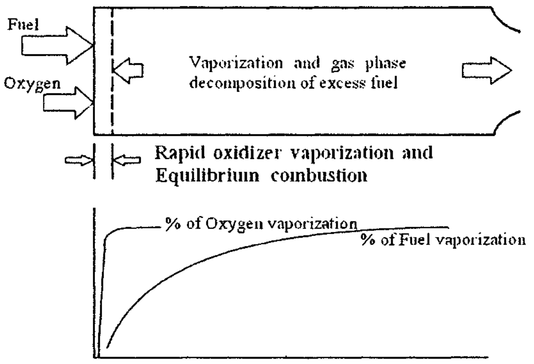

Fig. 1. Schematic of fuel rich combustion in gas generator.

The chemical reaction that occurred in the gas generator is a non-equilibrium reaction except for locally formed hot spot. And the combustion temperature gradually decreases along the axis of gas generator due to the heat subtractions by subsequent decomposition of excess fuel. It should be, therefore, noted that the numerical simulation of fuel rich combustion is not easy because the combustion temperature is too low to maintain the chemical reaction to be active in the calculation. At this point, it is useful to clarify temperatures used in the governing equations; the reaction hot temperature T_{HOT} and gas bulk temperature T_c. In real situation, the gas temperature in the reactor may be quite low compared to the reaction temperature around stoichiometric conditions. Thus, a remedy is needed to calculate the reaction temperature in fuel rich conditions. A few previous works suggested a remedy for this dilemma (Keen et al., 1993).

Since PSR assumption adopts the idea that temperature is spatially uniform, a flame kernel located near injector holding an active chemical reaction can not be accounted for in the PSR calculation. In other words, a temperature more consistent with the actual combustion of injected liquid fuel droplets should be used to drive the kinetics, effectively decoupling the fluid dynamic and chemical processes. The temperature modification is necessary to start the reactor with the proper enthalpy values consistent with a hot flame zone near the injector plate. This second temperature (T_{HOT}) better represents the stoichiometry in the flame zone than the final bulk temperature in the gas generator. And the bulk temperature can be obtained by solving the energy equation.

This model with pre-determined reaction hot temperature can also affect the gas composition in the calculation. Since the concept is applied throughout the combustion sequence, it is necessary to employ proper hot temperatures in the proper O/F range.

3. Kinetics

Practical fuels such as natural gas, diesel, gasoline and kerosene are complex mixtures of various hydrocarbons. And it is very difficult to directly simulate the chemical reaction because its detailed reaction mechanism is not still known to the society. Thus, it is necessary to have a substitution of chemical kinetic reaction for the combustion of practical fuels in terms of the mixture of typical hydrocarbons. Dagaut (2002) suggested kerosene can be modeled by a mixture of n-decane(74%), n-propylbenzene(15%) and n-propylcyclohexane(11%). In the detailed kinetics, the reaction mechanism consists of 1,592 reversible reaction kinetics and 207 species. However, it should be noted that the suggested range of a model fuel for kerosene covers only limited range of pressure and temperature; pressure ranging from 1-40 atm, equivalence ratios of 0.2-2, and temperature in the range of 500-1,300K. This applicable range of the surrogate kerosene fuel, however, does not include the equivalence ratio of fuel rich combustion occurred in gas generator. For instance, the equivalence ratio for fuel rich combustion is about 10, and this is far larger than the validated equivalence ratio of surrogate kerosene model. Even if there are differences in the equivalence ratio between the applicable ranges of surrogate fuel and kerosene, it is useful to use the surrogate fuel in predicting fuel rich natures of non-equilibrium combustion in gas generator.

4. Kinetics for soot formation

The soot formation is the result of an incomplete combustion of hydrocarbon fuel. This may be the one of the manifestation of poor combustion efficiency and the sources of environmental pollution. So the soot formation can be a critical issue in fuel rich combustion. Also, the production and deposition of soot on the turbine blade may deteriorate the system performance. Since the non-equilibrium combustion in the gas generator can cause the soot formation, the prediction of soot formation is of importance.

Dagaut's model, however, can not be extended to the prediction of soot formation because this model excludes the kinetics of the soot or PAH formation. A proper model, therefore, is required to implement the soot formation along with Dagaut's model.

Frenklach (1994) proposed that the soot formation is closely related with the production of precursor, PAH (Polycyclic Aromatic Hydrocarbon), such as pyrene($C_{16}H_{10}$) in the combustion. The initiation of soot formation is assumed to begin with the collision of precursors resulting in the production of dimer. And many researches revealed that acetylene (C_2H_2) may take the crucial role of the initiation of dimmer production. In this model, the soot formation consists of four different steps; nucleation, coagulation, surface growth and oxidation. And the specific equations for the formation can be represented by the moment concept as below;

$$\frac{dM_0^{soot}}{dt} = R_0 - G_0 \tag{30}$$

$$\frac{dM_1^{soot}}{dt} = R_1 + W \tag{31}$$

$$\frac{dM_2^{soot}}{dt} = R_2 + G_2 + W_2 \tag{32}$$

$$\cdots$$

$$\frac{dM_r^{soot}}{dt} = R_r + G_r + W_r \tag{33}$$

Here, M_r represents r^{th} moment and R, G, and W denote the nucleation, coagulation, and surface growth rate of soot formation respectively. Details of the soot formation and governing equation can be found in Frenklach and Wang, 1994.

It should be also noted that the surrogate fuel for kerosene has more complex hydrocarbon. Since Dagaut model did not account for the formation of precursor, PAH or soot formation, the additional soot formation model was introduced to the original Dagaut's model by combining the well known Appel's kinetics mechanism (Appel et al., 2000). This mechanism well predicts the major, minor and aromatic species up to pyrene in laminar premixed flames of ethane, ethylene, and acetylene fuels. However, the capability of the Appel's mechanism in predicting the soot formation of kerosene fuel in diffusion flame nature such as in the gas generator was not verified in the open literatures. Thus, it is natural to expect some erroneous numbers in the calculation results. Even with the intrinsic limit in soot formation for kerosene combustion with modified kinetics mechanism, this approach can give at least the qualitative description for soot formation of the combustion in gas generator. Figure 2 shows the reactor temperatures calculated with original Dagaut model and modified model. As shown in the figure, the difference in the bulk temperatures is not discernable.

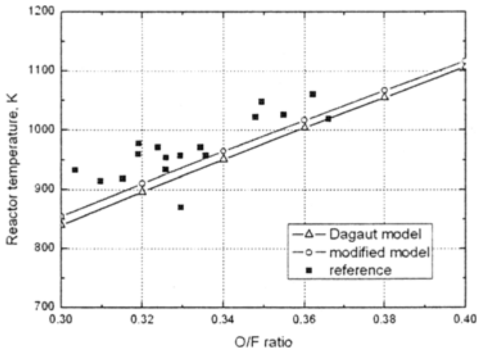

Fig. 2. Reactor temperatures calculated with original Dagaut's model and modified model.

5. Results and discussion

In order to verify the capability of the modified PSR code accounting for the droplet vaporization, the comparison of calculation results was made with the experimental data in Lawver (1982) for the chamber temperature, specific heat ratio and gas efflux composition of species. Experimental conditions are summarized in Table 2. As seen in the table, the chamber pressure was set to be the pressure of 150 atm. This pressure level is beyond the limit of valid range of pressure of 50 atm for Dagaut model for kerosene. Thus, the calculation was carried out at the pressure level of 50 atm instead of 150 atm expecting only the qualitative agreement with experimental data.

Figure 3 is the calculation results of vaporization time for three constituents of kerosene surrogate fuel

Table 2. Experimental data.

Experimental data	
P_c	150 atm / 50 atm (calculation)
Mass flow rate	16.8 kg/s
O/F ratio	0.30-0.40
Chamber volume	5092.57 cm^3

in the range of temperature of 1,000 K to 1,400 K. The droplet life time can be calculated using Eqs. (12), (13), (15)-(29). As seen in the figure, vaporization times are very insensitive to the surrounding temperature and the vaporization time of n-propylcyclohexane dominates among the surrogate components. Also, droplet life time shows a negligibly small difference for all three species if the diameter is less than 50 μm. The average droplet diameter from the injector is assumed 50 μm in the calculation. Thus, any of the evaporation time of fuel droplet of components can introduce the similar modification in reactor residence time in the calculation.

Figure 4 shows the calculation results of droplet life time at various pressure conditions of 30 to 50 atm. The empirical formula and other thermodynamic data used in the calculation are only valid at the pressure less than 50 atm. Above 50 atm, the supercritical behavior of fuel droplet is expected, and the special treatment of evaporation is required in this circumstance. The results in Fig. 4 show that the droplet life time is also insensitive to the variation of pressure level if the diameter is limited far less than 50 μm.

For the determination of reaction temperature (T_{HOT}), calculation was made with respect to various reaction temperatures at O/F ratio of 0.30 and 0.38. As seen in Fig. 5, the bulk temperature does not change very much near around 900 K and 1,000 K respectively, even though the reaction temperature varies from 1,200 to 1,600 K. Also, the residence time in the reactor shows the minimum around the temperature of 1,500 K in both cases as seen in Fig. 6. However, the difference of the residence time from the minimum value is quite much if the reaction temperature varies in the range of 1,200 K to 1,500 K. Thus, the artificial hot reaction temperature can be selected within this range if the calculation results could predict the experimental data.

The calculation result for the O_2 mole fraction can provide another guideline to choose the reaction temperature. In real combustion conditions, near stoichiometric reaction at the hot spot depletes the oxygen and the decomposition of unburned fuel prevails in the rest of the combustor. Thus, if we assume the minimum mole fraction of oxygen to be 5% after the depletion at the hot spot, this may take a role of criterion to determine the reaction temperature. Figure 7 shows the calculation result of oxygen fraction when the various reaction temperatures were adopted. As seen in the Fig. 7, the O_2 mole fraction

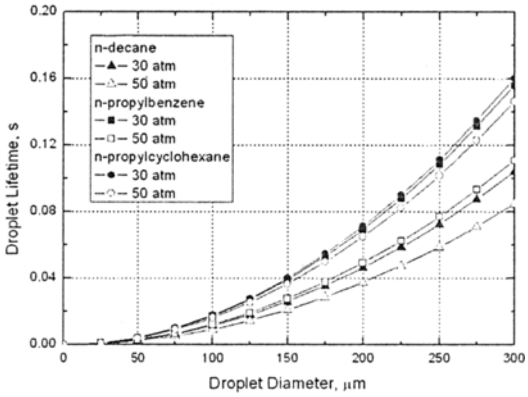

Fig. 4. Droplet lifetime of three components of kerosene surrogate fuel.

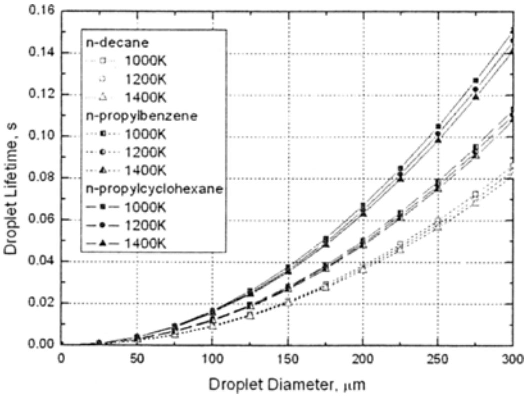

Fig. 3. Droplet lifetime of three components of kerosene surrogate fuel.

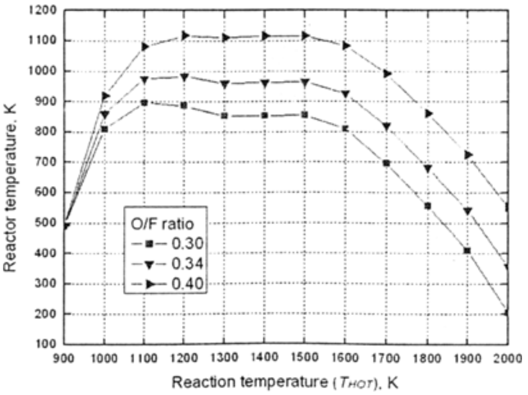

Fig. 5. Calculated reactor bulk temperature as a function of specified reaction temperature.

decreases rapidly around the reaction temperature of 1,000 K and becomes below 5% when the reaction temperature is larger than 1,100 K. Therefore, the selection of reaction temperature should be made to accommodate the real physics in the fuel rich combustion by allowing the appropriate variation of the reaction temperature at each O/F ratio. If reaction temperature would be specified as constant at all O/F ratios, say 1,500 K, this could exaggerate species mole fractions and molecular weight as well. And the reaction temperature is assumed to increase linearly from 1,200 K to 1500 K along the O/F variation in the calculation.

And Fig. 8 compares the temperature from the calculation with experimental data from Bensky and Wong, 1977. The calculation result of reactor temperature shows very good agreement with reference value in Lawver, 1982. Also Figs. 9-10 shows the

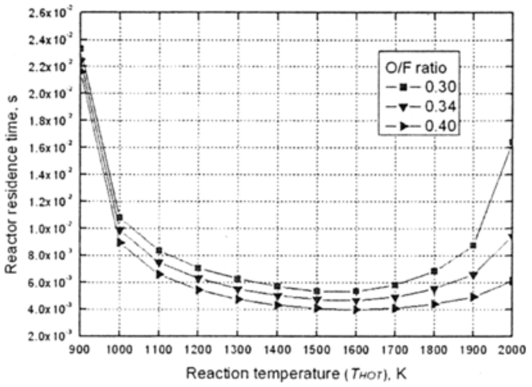

Fig. 6. Reactor residence time as a function of specified reaction temperature.

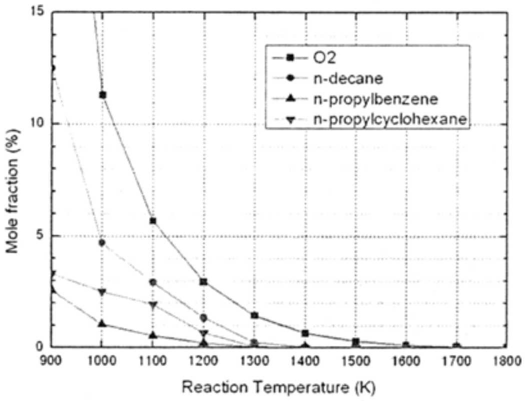

Fig. 7. Depletion of oxygen as a function of specified reaction temperature.

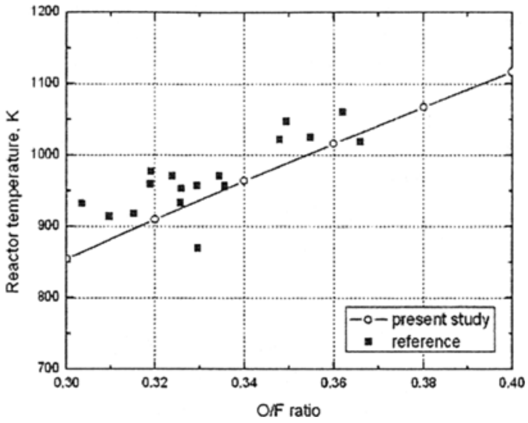

Fig. 8. The comparison of the prediction of bulk temperature with reference value.

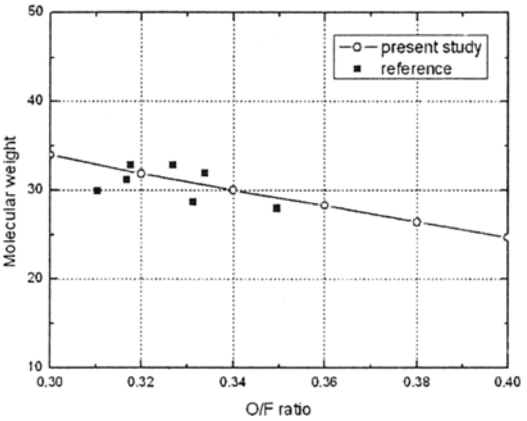

Fig. 9. The comparison of molecular weight with reference value.

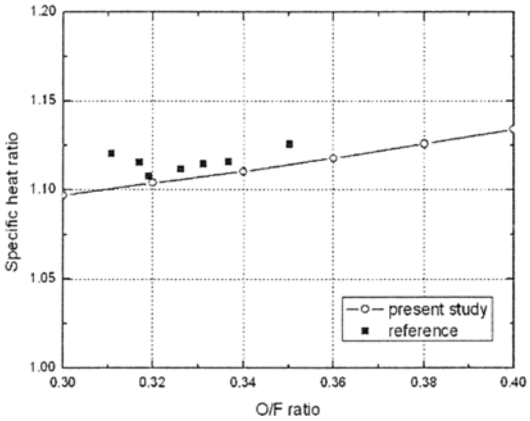

Fig. 10. The comparison of specific heat ratio with reference value.

calculated molecular weight and specific heat ratio of combustion gas and experimentally measured data from the Lawver, 1982.

The calculation provides a quite good agreement with reference value over the specified range of O/F ratio. From Figs. 11 to 16, the comparisons are made for several combustion gas compositions such as H_2, CH_4, CO_2, C_2H_4, and C_3H_6. Every mole fraction of each species but CO and H_2 shows a good agreement with experimental data. However, CO mole fraction is found to be under predicted in the calculation. This is due to the defect in the chemical kinetics for kerosene not accounting for breakdown of hydrocarbons in the high temperature environment of the reactor.

As for the soot formation, the calculation reveals soot volume fraction is the order of O (10^{-9}) in the specified O/F range in table 3. This implies the soot formation in the fuel rich combustion is negligibly small. The volume fraction found in the (Nickerson and Johnson, 1983). coincides with the calculation results in the range of O/F ratio of 0.3-0.4. The soot formation, however, increases dramatically at O/F of 0.5 and shows the maximum at 0.6 for RP-1 fuel rich combustion (Nickerson and Johnson, 1983). Figure 17 shows the calculation result of soot formation in kerosene/LOX fuel rich combustion. As mentioned previously, Dagaut's kinetic model is not suitable for the calculation of soot formation since it does not include the production and depletion kinetics of PAH, which is a precursor of soot formation. Appel's kinetics model is well known kinetic model including the formation of PAH through pyrolysis and oxidation of C_1, C_2 hydrocarbon species. However, it should be noted that kerosene is a complex mixture of C_9 or C_{10} hydrocarbons and the decomposition yields lower hydrocarbon species. And Appel's kinetics is not suitable to include the decomposition of kerosene. In spite of the intrinsic limit of Appel's kinetics, the calculation results provide a very good agreement with the results in (Nickerson and Johnson, 1983).

Table 3. Soot volume fractions at O/F ratio 0.3-0.4.

O/F ratio	0.30	0.32	0.34	0.36	0.38	0.40
Soot volume fraction (10^{-9})	3.50	3.62	3.77	3.89	4.04	4.16

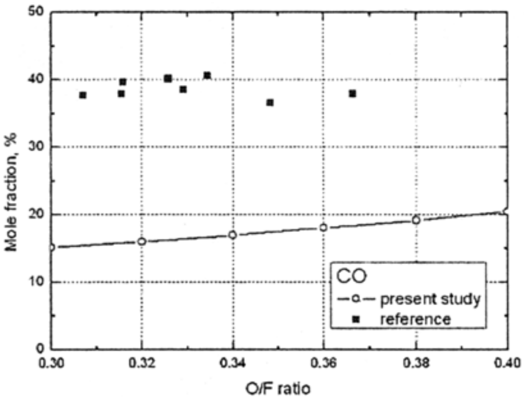

Fig. 11. Calculation of CO mole fraction (%).

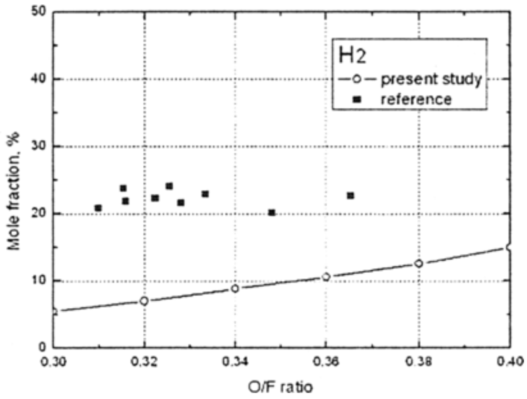

Fig. 12. Calculation of H_2 mole fraction (%).

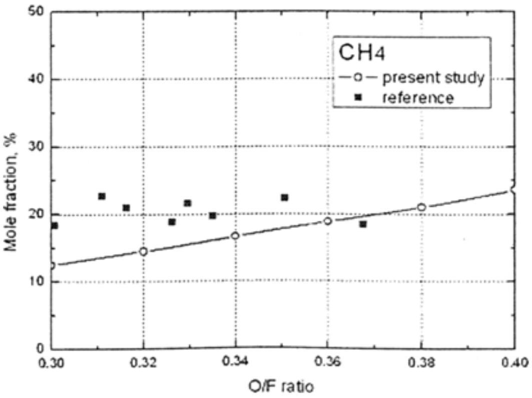

Fig. 13. Calculation of CH_4 mole fraction (%).

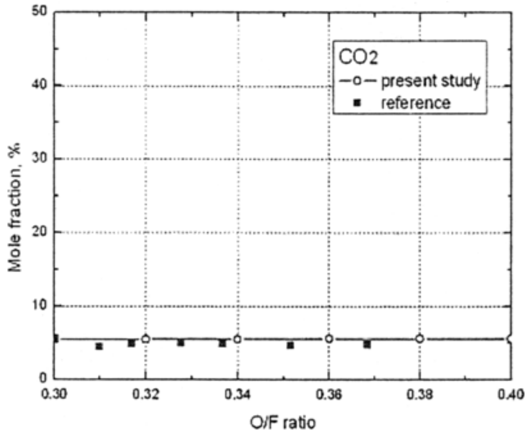

Fig. 14. Calculation of CO_2 mole fraction (%).

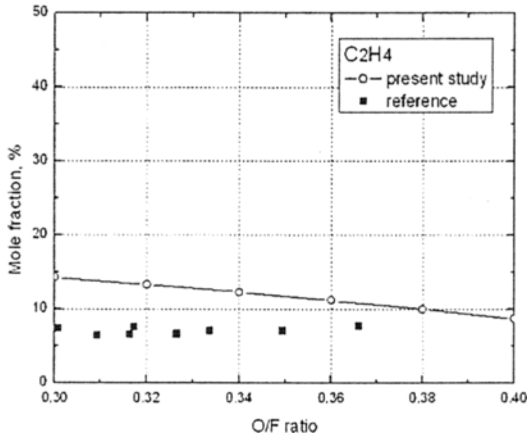

Fig. 15. Calculation of C_2H_4 mole fraction (%).

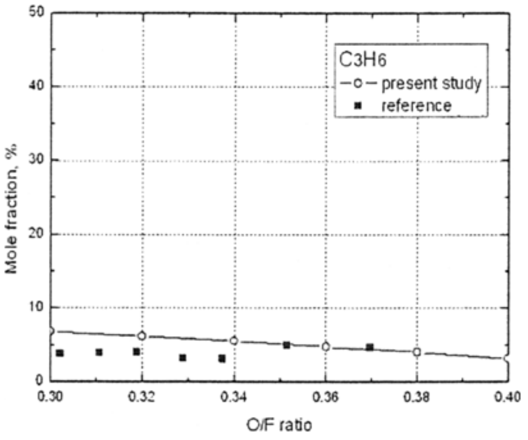

Fig. 16. Calculation of C_3H_6 mole fraction (%).

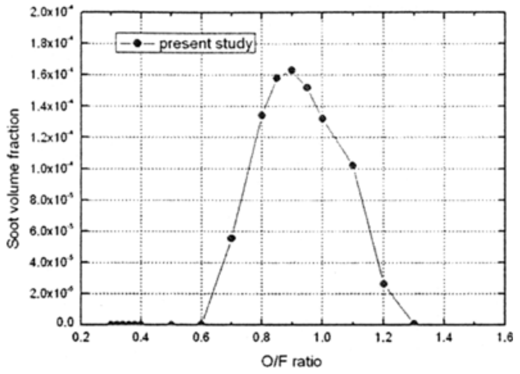

Fig. 17. Characteristics of soot volume fraction in fuel rich Kerosene/LOX combustion.

6. Conclusion

This study aims to develop the efficient analysis model for the non-equilibrium chemical reaction of kerosene/LOX in the fuel rich gas generator with detailed kerosene kinetics developed by Dagaut and soot formation mechanism. The calculation code was developed based on PSR (Perfectly stirred reactor) assumption. The calculation accommodates the effect of droplet vaporization on the reactor residence time and soot formation. In Dagaut's surrogate model for kerosene, chemical kinetics of kerosene consists of 1,592 reaction steps with 207 chemical species. Also, droplet evaporation time is taken into account in the calculation with the implementation of reaction hot temperature decoupling the reaction temperature in the governing equations. The results could provide very reliable and accurate numbers in the prediction of combustion gas temperature, species fraction and material properties except for CO and H_2 mole fractions. This approach can be used to calculate the fuel rich combustion other than Kerosene/LOX mixture such as methane, diesel, etc. at the design stage. Also, the prediction of soot formation shows a quite good qualitative agreement with reference value even with the intrinsic limit of soot formation mechanism. And a further study is required to tune up the gas properties in the combustion gases.

Nomenclature

A_i : Arrhenius expression pre-exponential factor for i^{th} reaction

B : Spalding transfer number

B_{ii} : Second virial coefficient

c_p : Specific heat at constant pressure
d_o : Nominal initial droplet diameter
E_i : Arrhenius expression activation energy for ith reaction
$\vec{F}$: Vector containing the energy and species continuity equations residuals
h_k : Specific enthalpy per unit mass of species k
h_{k^o} : Inlet specific enthalpy of species k
j : Stoichiometric fuel-oxidant mass ratio
k_{fi} : Forward rate of ith reaction
k_{ri} : Reverse rate of ith reaction
$\dot{m}$: Mass flow rate through reactor (gm/sec)
p : Reactor pressure in the reactor
p' : Non-dimensional pressure in vapor pressure correlation
q^o : Heat of reaction (cal/gm)
Q : Reactor heat loss
R_c : Universal gas constant
T : Reactor temperature (K)
T_∞ : Temperature at infinity or reactor temperature (K)
T_L : Temperature at the droplet surface (K)
T_r : Non-dimensional temperature in vapor pressure correlation
V : Reactor volume (cm^3)
V_g : Gaseous molar volume of fuel
V_l : Liquid molar volume of fuel
W_k : Molecular weight of species k
X_k : Mole fraction of species k
$[X_k]$: Molar concentration of species k
Y_k : Mass fraction of species k
$Y_{o,\infty}$: Oxidizer mass fraction at infinity
Y_k^* : Inlet mass fraction of species k

Greek Symbols

β_i : Non-Arrhenius temperature exponential for i^{th} reaction
δ : Finite difference in Jacobian update scheme
ε : User specified tolerance for convergence of numerical solution
λ : Gas phase thermal conductivity (cal/sec/cm/K)
ρ : Mixture density (gm/cc)
ρ_l : Droplet liquid density at the boiling point temperature
$\vec{\varphi}$: Solution vector of temperature and species mass fractions
τ : Reactor residence time
$\dot{\omega}_K$: Molar rate of production per unit volume of species k
Ω : Acentric factor

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