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Numerical Studies on Specific Impulse of Partially Filled Pulse Detonation Rocket Engines

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Performance analyses of pulse detonation rocket engines (PDREs) were numerically studied, focusing on partial-fill effects at ground tests. The initial detonable mixture, inert gas, fuel-fill fraction, equivalence ratio, and initial temperature of inert gas were changed as governing parameters. The simulation results were compared against those of previous studies and agreed well with them. The simulation results indicated that the initial mass fraction of the detonable mixture to total mass of the gas was the predominant factor for the specific impulse of partially filled PDREs. Based on the numerical results, a new, simple empirical formula is proposed to predict the specific impulse of partially filled PDREs.

Introduction

A PULSE detonation rocket engine (PDRE) is a device that produces thrust by using repetitive detonation waves. A number of experimental,[1–9] numerical,[10–12] and analytical[13,14] studies have been conducted regarding the performance of single-tube PDREs. Many interesting performance characteristics have been experimentally investigated in recent years. Zitoun et al.[1] and Zitoun and Desbordes[2] changed the L/D (length/diameter of a detonation tube) ratio, fill fraction α (volume fraction of the detonable gas in the tube, fuel-fill length $L_{\mathrm{fuel}}/L_{\mathrm{tube}}$), and detonation-initiation position with a $C_2H_4 + 3O_2$ mixture. They suggested that the pressure history at the thrust wall was characterized by the nondimensional time t_{CJ} [equal to L/D_{CJ}, where D_{CJ} is the Chapman–Jouguet (CJ) detonation velocity] and CJ pressure p_{CJ} and that the mixture-based specific impulse I_{sp} was not affected by initiation position. Schauer et al.[3] used a hydrogen–air mixture and examined the effect of the partial fill (α varying from 0.2 to 1.6) under multicycle operation. They showed that I_{sp} gradually increased as α decreased. Cooper and Shepherd[4] proposed an empirical formula for I_{sp} of partially filled detonation tubes by using previous experimental and numerical results with hydrocarbon fuels. Kiyanda et al.[5] examined the effect of equivalence ratio ϕ varying from 0.2 to 1.8 with an $2H_2 + O_2$ mixture. They showed that the deflagration-to-detonation transition process and I_{sp} were affected by the change of equivalence ratio. Kasahara et al.[6,7] examined effects of the inert gases in partially filled detonation tubes by using air and helium gases. They clarified that the change of inert-gas species greatly affects I_{sp}.

With regard to the numerical simulations, Li et al.[10] and Li and Kailasanath[11] studied partial-fill effects by using a $C_2H_4 + 3O_2$ mixture. They clarified the dependence of I_{sp} on α, especially at a low-fill fraction that was difficult to obtain experimentally. They proposed an empirical formula for I_{sp} of partially filled detonation tubes by using their simulation results.

A series of studies tells us that the I_{sp} of a fully filled system seems unable to exceed 200 s. The partially filled PDREs were expected to make the performance higher, and the validity of this expectation has been proved by previous studies. However, there is no model predicting the performance of the partially filled PDRE under arbitrary conditions.

In the present paper, we studied the performance of a detonation tube numerically. As governing parameters, we changed detonable and inert gases, fuel-fill fraction α, equivalence ratio ϕ, and the initial temperature of the inert gas T_{inert}. The performance analysis of the PDRE is basically assumed to take place as a ground test. Therefore, the gas pressure is always set to atmospheric pressure on the ground. Moreover, we focus on the effects of the inert gas, such as molecular weight, temperature, and quantity on I_{sp}. The simulation results were compared against the results of previous studies. Finally, we proposed a simple semi-empirical formula for I_{sp} of partially filled detonation tubes.

Computational Setup

All of the simulation conditions are listed in Table 1, in which the single-cycle operation is conducted. Air, helium, and argon were assumed as inert gases in partially filled cases. Although helium or argon might never be used in actual devices, our purpose was to examine how the gas species affects performance. The initial pressure and temperature were set to be 101.3 kPa and 298.15 K, respectively, in detonable gases. For inert gases, initial pressure was fixed at 101.3 kPa, but initial temperature was treated as a governing parameter. To determine the effect of multicycle PDREs, the burned gas and the purge gas must be considered as additional factors in determining performance. Because the present work is based on a single-cycle PDRE, the inert gas is set to heavy and light molecules imitating purge and burned gas and higher-temperature gas imitating burned gas. Initially, a detonation tube was filled with unburned detonable gas and inert gas, and the outside region was filled with air. The detonation propagation process in the tube was solved with a one-dimensional code. After the detonation wave reached the open

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Table 1 Simulation conditions

Detonable gas	Inert gas	Equivalence ratio ϕ	Tube-fill fraction	Temperature (inert), K
$2H_2 + O_2 + 3.76N_2$	Air	1.0	0.1–1.0[b]	298.15
$2H_2 + O_2$	Air, Ar, He	1.0	0.1–1.0	298.15
$2H_2 + O_2$	Ar, He	1.0	0.5	298.15–1192.6[c]
$2\phi H_2 + O_2$	Air	0.33–2.0[a]	0.1–1.0	298.15
$C_2H_4 + 3O_2$	Air	1.0	0.1–1.0	298.15
$C_2H_4 + 3O_2$	Air, He	1.0	0.5	298.15

[a]Refers to six cases: 0.33, 0.5, 0.67, 1.0, 1.5, and 2.0.
[b]Refers to six cases: 0.1, 0.3, 0.5, 0.7, 0.9, and 1.0.
[c]Refers to three cases: 298.15, 596.3, and 1192.6.

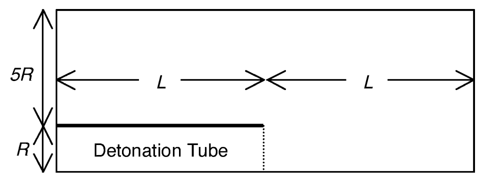
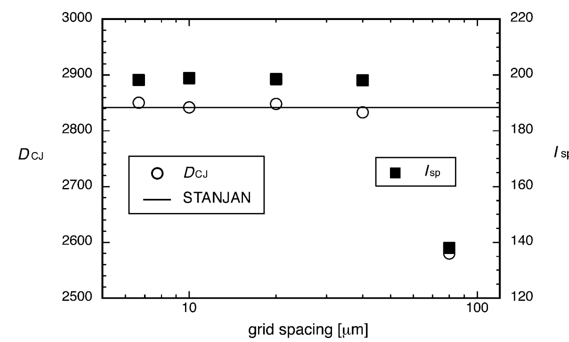


Fig. 1 Schematic of computational domain: $L = 10$ cm and $R = 0.25$ cm (hydrogen fuel) and $L = 1$ cm and $R = 0.025$ cm (ethylene fuel).

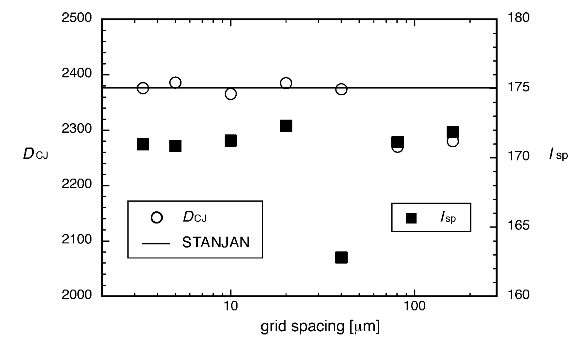
end of the tube, the flowfield in the whole computational domain was solved with a two-dimensional code. For the performance estimation of the detonation wave in the detonation tube, the one-dimensional computation gives us reasonable data. However, sometimes the interface between the inside and outside of the detonation tube causes shock or rarefaction waves. Therefore, the two-dimensional domain is prepared to estimate precisely performance in the present work. Fortunately, the higher grid resolution is not required in the two-dimensional computation because the frozen flow assumption outside of the tube works well for the performance estimation.

The governing equations were the one-dimensional and two-dimensional axisymmetric Euler equations. In the present study, a detailed chemical reaction model[15] was used in which eight chemical species (H_2, O_2, H, O, OH, H_2O, HO_2, and H_2O_2) and 19 elementary reactions were used to describe the reaction of hydrogen fuel. Another reduced chemical reaction model was used in which nine chemical species (C_2H_4, CO_2, CO, H_2O, H_2, O_2, H, O, and OH) and 10 reactions[16] were used to describe the case of ethylene fuel. N_2, He, and Ar were added in the original reaction models as inert gases. The algorithm used for solving these equations was Yee's non-MUSCL type total variation diminishing upwind explicit scheme.[17] These equations were integrated explicitly under the Courant–Friedrichs–Lewy number 0.1 condition, and a chemical reaction source term was treated in a linearly point implicit manner.

The computational domain is shown in Fig. 1. The tube is straight with a constant cross section and is divided into equal spacing. One end of the tube was closed, and the other was open to air. For an initiation of detonation waves in a one-dimensional code, we set an artificially high-energy core at the thrust wall of 0.4 mm for hydrogen fuel and 0.05 mm for ethylene fuel, where pressure and temperature were, respectively, 3.0 MPa and 3000 K. Two types of grid resolution, depending on the characteristics of the detonable gases, were prepared, with the grid spacing 20 μm (one-dimensional) and 100 μm (two-dimensional) in the case of hydrogen fuel and 5 μm (one-dimensional and two-dimensional) in the case of ethylene fuel. Here, the induction lengths for stoichiometric detonable gases of hydrogen–oxygen and ethylene–oxygen are 37.8 and 20.0 μm, respectively. The grid refinement study in the one-dimensional computation was carried out to confirm the validity of grid resolution on D_{CJ} and I_{sp}, and the results are shown in Figs. 2. The D_{CJ} is also compared with the data calculated via STANJAN,[18] and the I_{sp} is integrated by the pressure history on the thrust wall. Figures 2 indicate that the current grid spacing must be adequate to reproduce the characteristics for the estimation of a PDRE because we are interested in the impulse as an integrated value for the performance analysis of PDREs in the present study. Indeed, when we prepared more than 16 grid points per the induction length, the failed regime,



a) Stoichiometric hydrogen–oxygen



b) Stoichiometric ethylene–oxygen

Fig. 2 Grid refinement study for one-dimensional detonation tube computation on D_{CJ} and I_{sp}.

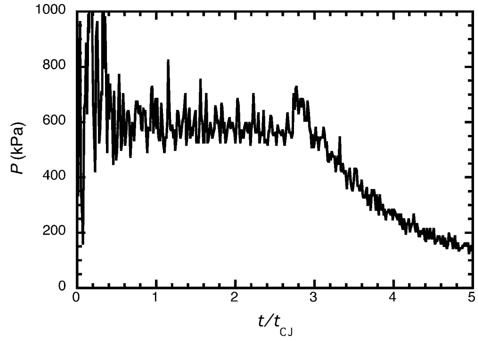
in which the burned gas separates from the leading shock wave, occurred after the initiation of detonation. We could not reproduce the stable detonation propagation under the higher grid resolution.

Multidimensional computations are required to reproduce the pressure oscillations usually observed in the experiments (Fig. 3a) because the transverse wave resulting from the multidimensions mainly affects the pressure variation in the experimental data. For the experiment in Fig. 3a, the detonation tube is 50 mm in inside diameter and 900 mm long, and $2H_2 + O_2$ mixtures are used for the detonable gas. To confirm the multidimensional effect numerically, the pressure history at the thrust wall of two-dimensional computational result is shown in Fig. 3b. The computation[19] was carried out using the simplified chemical reaction model with stoichiometric $2H_2 +$ air mixtures under the grid resolution of 10 grid points per the induction length. The history at the center of the thrust wall is indicated in Fig. 3b and oscillates during the plateau period as a result of multidimensional effects by the transverse wave in the detonation tube. The amplitude of the pressure oscillation is considered to be proper in comparison with the experimental data in Fig. 3a.

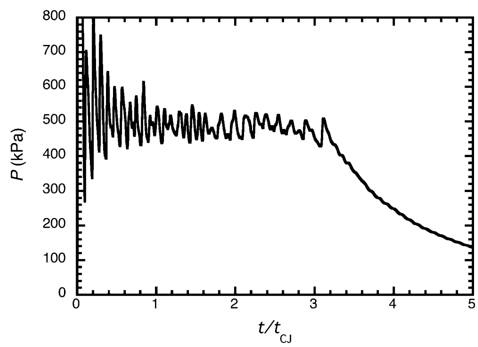
Results and Discussion

Effect of Initiation Location

The effects of the location of detonation initiation were experimentally investigated by Zhdan et al.[20] In their experiments, detonation waves were initiated at three locations, namely, at the closed end, middle, and open end of the tube, where the detonable gas



a) Experiment (detonable gas $2H_2 + O_2$)



b) Two-dimensional computation (detonable gas stoichiometric $2H_2$ + air)

Fig. 3 Pressure histories at thrust wall.

was $C_2H_2 + 2.5O_2$. Zitoun et al.[1] and Kiyanda et al.[5] carried out the similar experiments using $C_2H_4 + 3O_2$ and $2H_2 + O_2$ mixtures, respectively. It was found experimentally that I_{sp} was at almost the same level regardless of the initiation location. In the following text, the effects of the initiation location are numerically investigated with $C_2H_4 + 3O_2$ and $2H_2 + O_2$ mixtures.

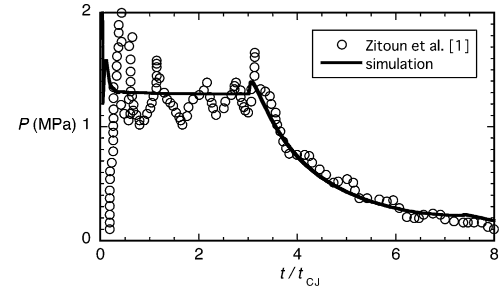
We carried out a one-dimensional analysis, described in this subsection, where the boundary condition at the open end of the tube was set to the fixed pressure when the Mach number at the open end was less than unity. Figures 4 show the pressure histories at the closed end in the cases of closed-end, (Fig. 4a) middle (Fig. 4b) and open-end (Fig. 4c) initiations. Experimental results obtained by Zitoun et al.[1] are also shown in Fig. 4. The pressure plateau was observed in Figs. 4a and 4b, but not observed in Fig. 4c. As shown in Figs. 4, the pressure histories drastically changed with changes of initiation location in the tube. As we mentioned in the "Computational Setup" section, the multidimensional computation with higher grid resolution will be required to reproduce the pressure variations in the pressure history of the experimental data. Here, we are interested in features of the thrust wall pressure history effected by initiation location, and we note that the simulation results agree well with the experimental results on the whole.

Figure 5 shows I_{sp} as a function of initiation position x_{init}/L with $2H_2 + O_2$ and $C_2H_4 + 3O_2$ mixtures. As shown in Fig. 5, I_{sp} hardly depended on the initiation location. This implies that I_{sp} is predominantly determined by energetics.

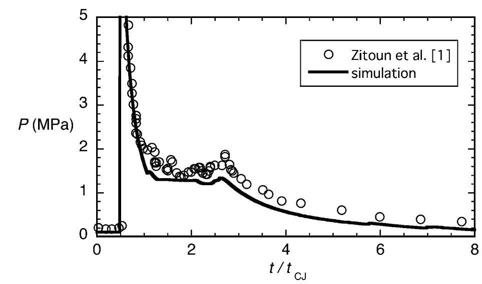
Effects of Inert-Gas Species

Figure 6 shows the pressure histories at the closed end for the detonable gas $2H_2 + O_2$ and inert gases air, helium, and argon. The fuel-fill fraction α was 0.5. After the detonation initiation at the closed end, the pressure plateau appeared. The pressure decay started after the arrival of the reflected wave from the interface between the detonable gas and the inert gas. In the cases where the inert gases were air and argon, the decay started after the pressure jump.

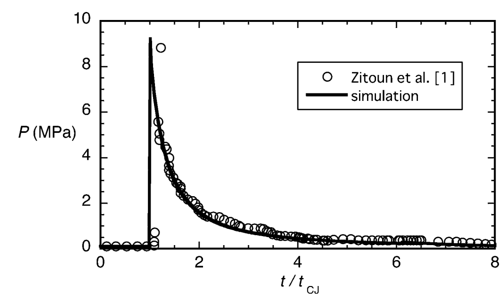
Figures 7 show the pressure in the space–time plane for the cases where the inert gases were air and helium. The reflected wave in Fig. 7a consists of the preceding compression wave and the following rarefaction wave. This preceding compression wave produced the pressure jump at the closed end shown in Fig. 6. A similar level



a) Closed-end initiation



b) Center initiation



c) Open-end initiation

Fig. 4 Pressure histories at closed end with change of initiation location with $C_2H_4 + 3O_2$ fully filled in tube.

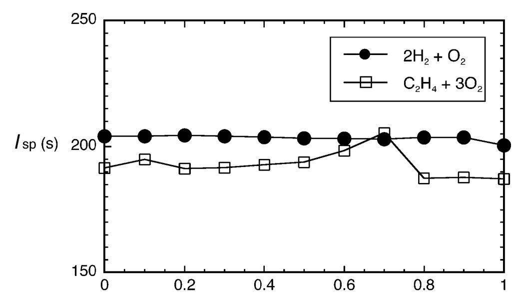


Fig. 5 Specific impulse as function of initiation location.

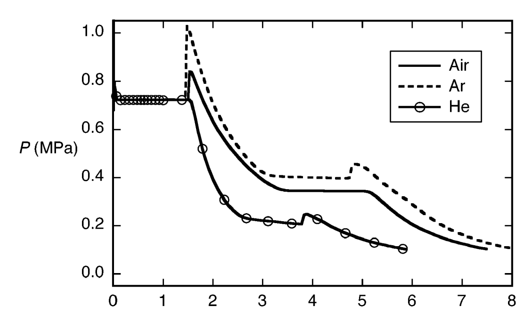
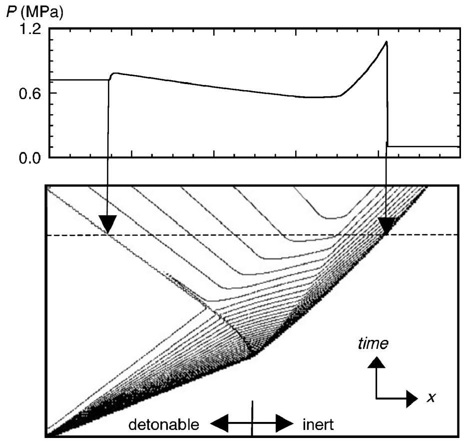
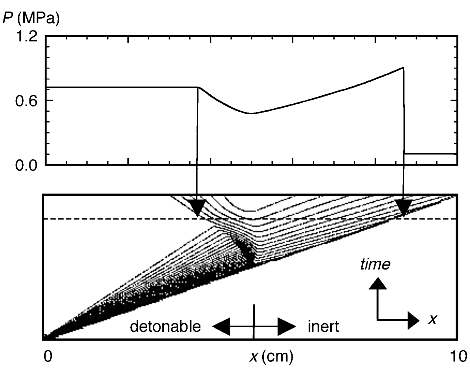


Fig. 6 Pressure histories at closed end in case of $\alpha = 0.5$, where detonation wave was initiated at closed end (detonable gas $2H_2 + O_2$ and inert gases air, Ar, and He).



a) Inert gas air



b) Inert gas He

Fig. 7 Pressure in space–time plane, $\alpha = 0.5$ (detonable gas $2H_2 + O_2$ and inert gases air and He).

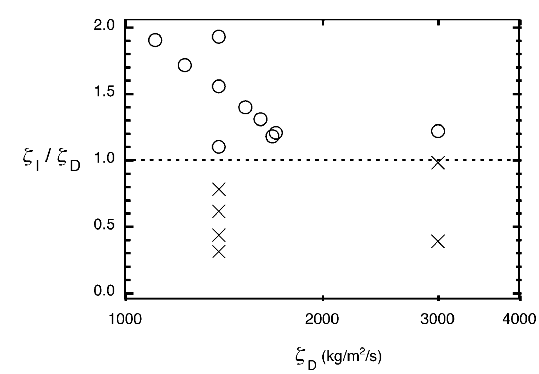


Fig. 8 Relation between ζ_D and impedance ratio: ○, compression and ×, rarefaction.

of pressure jump appeared regardless of the change of α. However, in Fig. 7b, the reflected wave was a rarefaction wave, and, therefore, the pressure jump was not observed as shown in Fig. 6. The relation between the impedance of detonable and inert gases determines the feature of the reflected wave. The generalized acoustic impedance consists specific-heat ratio γ and the pressure ratio of the incident shock wave p_2/p_1. Here, p_2 denotes the pressure of von Neumann spike of the CJ detonation wave running in the tube. This impedance is described as follows[21]:

$$\xi_{\mathrm{D}} = \sqrt{(\rho_D p_1/2)[(\gamma_D + 1)(p_2/p_1) + (\gamma_D - 1)]}$$

$$\xi_{\mathrm{I}} = \sqrt{(\rho_I p_1/2)[(\gamma_I + 1)(p_2/p_1) + (\gamma_I - 1)]}$$

Here, the subscripts D and I denote the detonable and inert gases, respectively.

Figure 8 shows the relation between the generalized acoustic impedance of detonable gas ζ_D and the impedance ratio ζ_I/ζ_D in the case of a fuel-fill fraction of $\alpha = 0.5$. This impedance ratio less than unity makes the reflected wave a rarefaction wave, and that larger than unity makes it a compression wave.

Table 2 Specific impulse in fully filled cases

ϕ	D_{CI}, m/s	$I_{\mathrm{sp,full}}$, s
	$2H_2 + O_2 + 3.76N_2$	
1.0	1979.1	122.30
	$2\phi\, H_2 + O_2$	
0.33	2083.8	138.58
0.5	2323.9	157.34
0.67	2522.5	172.66
1.0	2841.6	195.56
1.5	3177.9	217.12
2.0	3408.9	226.99
	$C_2H_4 + 3O_2$	
1.0	2376.1	179.85

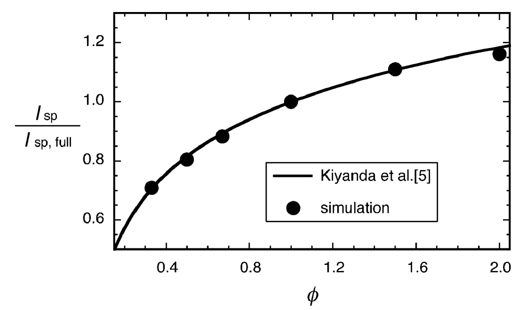


Fig. 9 Normalized I_{sp} as function of equivalence ratio with $2\phi H_2 + O_2$.

Comparison with Previous Studies

To confirm the reliability of the simulation results for single-cycle operation, we compared them against previous studies. Table 2 shows specific impulse in fully filled cases obtained by integrating the pressure history at the closed end, denoted by $I_{\mathrm{sp,full}}$.

Kiyanda et al.[5] investigated effects of the equivalence ratio ϕ between 0.2 and 1.8 in H_2–O_2 cases experimentally. Present simulation results with six values of ϕ ($2\phi H_2 + O_2$, $\phi = 0.33$, 0.5, 0.67, 1.0, 1.5, and 2.0) in the H_2–O_2 system were compared against their experimental results. Figure 9 shows the dependence of the specific impulse on the equivalence ratio, where the specific impulse I_{sp} is detonable-gas based and normalized by that in the stoichiometric case $I_{\mathrm{sp,stoic}}$. The solid curve shows a fitted curve based on the Kiyanda et al. experimental results. As the ϕ increased I_{sp} also increased. The simulation results were in good agreement with the experimental ones for a wide range of ϕ.

Schauer et al.[3] and Kasahara et al.[6] investigated effects of the fuel-fill fraction α, where the stoichiometric H_2–air and H_2–O_2 mixtures were used, respectively. In Figs. 10, the simulation results are compared against their experimental results, where air ($O_2 + 3.76N_2$) was used as the inert gas. Although the experimental data[3] in Fig. 10a were obtained under multicycle operation (12 and 16 Hz), the simulation reproduced the experimental results well in both cases shown in Figs. 10a and 10b.

Empirical Formula

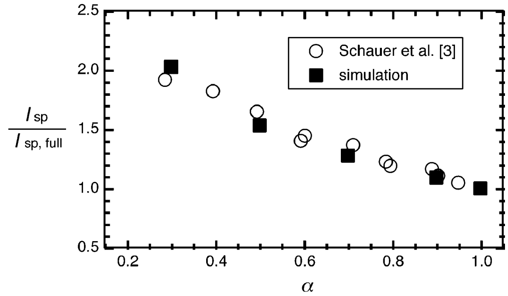
For the $C_2H_4 + 3O_2$ mixture, an empirical formula was proposed by Li and Kailasanath,[11] described as follows:

$$I_{\mathrm{sp}}/I_{\mathrm{sp,full}} = a - (a-1)/\exp[(L_t/L_f - 1)/8]$$

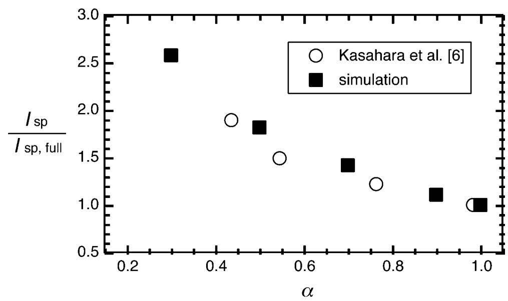
where a is a constant that was determined empirically and was recommended to be between 3.2 and 3.5, L_t is detonation-tube length, and L_f is fuel-fill length. In contrast, Cooper and Shepherd[4] also proposed an empirical formula for hydrocarbon fuels, described as follows:

$$I_{\mathrm{sp}}/I_{\mathrm{sp,full}} = 0.794 + 0.206(V^0/V), \qquad (0 < V/V^0 < 0.073)$$

$$I_{\mathrm{sp}}/I_{\mathrm{sp,full}} = 3.6, \qquad (0.073 < V/V^0 < 1)$$



a) Detonable gas $2H_2 + O_2 + 3.76N_2$ and inert gas air



b) Detonable gas $2H_2 + O_2$ and inert gas air

Fig. 10 Normalized I_{sp}, detonable-gas based, as function of fuel-fill fraction.

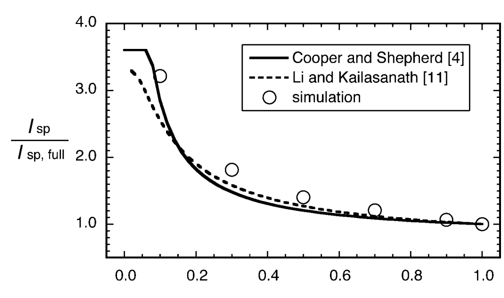


Fig. 11 Normalized I_{sp} detonable-gas based, as function of fuel-fill fraction (detonable gas $C_2H_4 + 3O_2$ and inert gas air, $a = 3.3$).

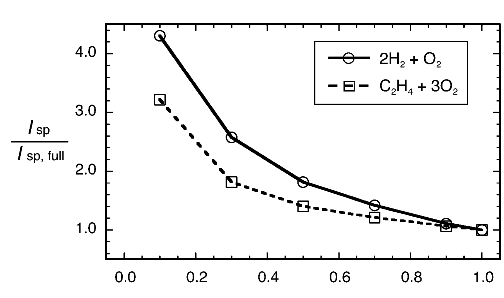


Fig. 12 Normalized I_{sp}, detonable-gas based, as function of fuel-fill fraction (detonable gases $2H_2 + O_2$ and $C_2H_4 + 3O_2$ and inert gas air).

where V is the tube volume filled with detonable gas and V^0 is the total volume of the tube. Figure 11 shows the comparison between the simulation results and their empirical formulas. As shown in Fig. 11, the simulation results agreed well with their empirical formulas.

Figure 12 shows the simulation results in the cases where the detonable gases were $C_2H_4 + 3O_2$ and $2H_2 + O_2$ mixtures. As shown in Fig. 12, the fuel-fill fraction α does not work as a universal governing parameter. Based on the discussion of the initiation location, the universal governing parameter should be in close relation to the heat released by combustion in the tube. Here, we try to find a simple empirical formula for predicting $I_{sp}/I_{sp,full}$. As the universal governing parameter, we examine the ratio of the heat released by combustion

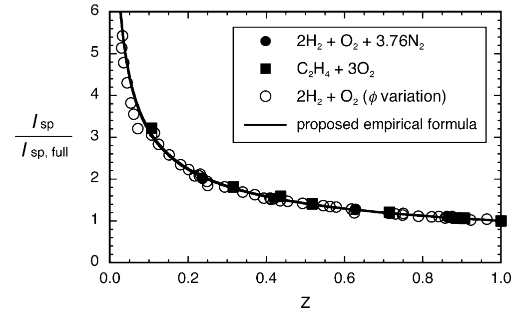


Fig. 13 Normalized I_{sp}, detonable-gas based, as function of Z.

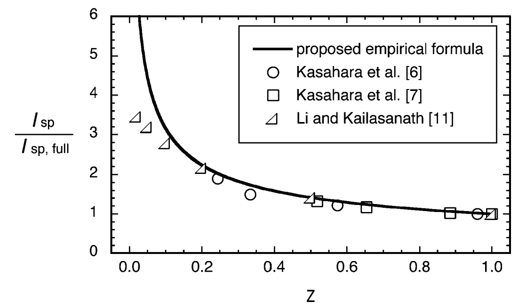


Fig. 14 Comparison between proposed empirical formula and previously reported results.

per unit mass of the gas in the tube between partially filled and fully filled cases. That is, we examine the ratio $(Q_P/m_P)/(Q_F/m_F)$, where Q is the total heat released by combustion in the tube, m is the total mass of the gas in the tube, and subscripts P and F denote the partially filled and fully filled cases, respectively. When the species and initial thermodynamic state of the detonable gas are determined, the heat released by combustion per unit mass of the detonable gas is uniquely determined. Therefore, we can write the following relation:

$$Q_F/m_F = Q_P/m_P Z$$

where Z is the mass fraction of the detonable gas in the tube. The parameter Z is in relation to the parameter α as

$$Z = \frac{m_{\text{detonable}}}{m_{\text{detonable}} + m_{\text{inert}}} = \frac{\rho_{\text{detonable}} \cdot \alpha}{\rho_{\text{detonable}} \cdot \alpha + \rho_{\text{inert}} \cdot (1 - \alpha)}$$

By the use of parameter Z, the ratio $(Q_P/m_P)/(Q_F/m_F)$ is written by Z. In conclusion, we look for a simple empirical formula for predicting $I_{sp}/I_{sp,full}$ in terms of Z. Figure 13 shows the simulation results of $I_{sp}/I_{sp,full}$, which is the ratio of the detonable-gas based specific impulses between the partially filled and fully filled cases of the same species and the initial thermodynamic state of the detonable gas, as a function of Z. Figure 13 contains all of the results of the simulations summarized in Table 1. Based on the results summarized in Fig. 13, we propose a new simple empirical formula for predicting $I_{sp}/I_{sp,full}$,

$$I_{sp}/I_{sp,full} = 1\Big/\sqrt{Z}$$

This empirical formula is also shown in Fig. 13, and it agrees with the simulation results where the average error was 2.6%. This formula approaches infinity at $Z = 0$. Actually, it is difficult to eliminate the effect of initial energy input or the transient process at the very low partially filled case in both the experimental and numerical results. Therefore, we specify the applicable range $0.05 < Z < 1.0$ of the proposed formula. Furthermore, we do not insist on the advantage of a PDRE of high specific impulse. What we want to show is that the heat of combustion is more efficiently utilized when the filling fraction of the detonable gas is smaller.

Figure 14 shows the comparison between the proposed empirical formula and experimental[6,7] and numerical[11] results reported previously. Although the proposed formula gave slightly higher results than those previously reported, especially in the cases of $Z < 0.1$, the proposed formula reproduced the previously reported results very well as a whole.

Finally, we discuss the physical meaning of the aforementioned empirical formula. Because the proposed empirical formula is very simple compared to the formulas proposed by Li and Kailasanath[11] or Cooper and Shepherd,[4] we believe that the qualitative explanation of the formula is possible and informative.

When the thermal efficiency is denoted by η, the kinetic energies of the exhausted gases in fully and partially filled cases are given, respectively, by

$$Q_F \eta_{\mathrm{th}} = \tfrac{1}{2} m_F v_F^2 \tag{1}$$

$$Q_P \eta_{\mathrm{th}} = \tfrac{1}{2} m_P v_P^2 \tag{2}$$

where v is the characteristic exhaust velocity of the gas in the tube. If the dependency of the thermal efficiency on Z is negligibly weak, namely,

$$\eta_F \cong \eta_p \tag{3}$$

the following relation can be derived:

$$v_P / v_F \cong \sqrt{Z} \tag{4}$$

where we used the relation $Z = (Q_P/m_P)/(Q_F/m_F)$, which was explained earlier. When the contribution of the static pressure at the exit to the impulse is negligibly small compared to that of the dynamic impulse, we can write the following relations:

$$I_{\mathrm{sp,full}} = (m_F v_F)/(m_F g) = v_F/g \tag{5}$$

$$I_{\mathrm{sp}} = (m_P v_P)/(Z m_P g) = v_P/(Zg) \tag{6}$$

To be exact, the characteristic velocities v_F and v_P in Eqs. (5) and (6) are not necessarily the same as those in Eqs. (1), (2), and (4). However, here we consider them the same because our objective is to show the physical meaning of the empirical formula only qualitatively. In this case, we obtain the following relation from Eqs. (4–6):

$$I_{\mathrm{sp}}/I_{\mathrm{sp,full}} = (v_P/v_F)(1/Z) \cong \sqrt{Z}(1/Z) = 1\big/\sqrt{Z} \tag{7}$$

The point is that the specific kinetic energy of the exhausted gas is determined by v^2, which is determined by the heat released by combustion per unit mass of the gas in the tube, although the momentum is determined by v. Indeed, we used some assumptions that are unrealistic in the case of a detonation tube in the preceding derivation. However, those assumptions might be valid in some optimized PDRE systems.

Conclusions

Performances of a single-pulse, single-tube PDRE were numerically investigated. For the effect of initiation position, I_{sp} is of almost the same level regardless of initiation position, so that I_{sp} only depends on the initial energy in the tube. The present simulation results were compared and agreed well with those of several previous studies, and the reliability was confirmed. Based on the simulation results, we proposed a new, simple empirical formula for predicting normalized I_{sp}, formulated using the initial mass fraction of detonable gas only. We indicated the physical meaning of the proposed empirical formula qualitatively under the assumption of constant thermal efficiency. The proposed formula is based on a number of simulation results that involves the change of a number of parameters. The model is efficient for performance prediction of single-tube and single-pulse PDRE.

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