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Homogeneous-Dilution Model of Partially Fueled Simplified Pulse Detonation Engines

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A model for estimating the propulsive performance of a partially fueled simplified pulse detonation engine is proposed. The model has two significant advantages: no empirical parameter is required, and the model enables estimation of both the impulse and the duration during which the pressure at the thrust wall remains higher than its initial value. In the model, an objective partially fueled pulse detonation engine is replaced with the equivalent fully fueled pulse detonation engine. The equivalent pulse detonation engine is fully filled with a homogeneous mixture of the detonable and inert gases that separately fill the objective partially fueled pulse detonation engine. The performances of the equivalent fully fueled pulse detonation engine are instead estimated by a previously developed performance-estimation model for a fully fueled pulse detonation engine. The applicability of the model is examined by comparing the results of the model with numerical and experimental results in the cases where hydrogen or ethylene was used as fuel. Further, the applicability limits, which arose from replacement of the objective partially fueled pulse detonation engine with the equivalent fully fueled pulse detonation engine, are described.

Nomenclature

a	=	speed of sound
D_{CJ}	=	Chapman–Jouguet detonation speed
e	=	thermal energy per unit mass
I_{cyc}	=	impulse per unit cross section per cycle
I_{spd}	=	detonable-gas-based specific impulse
I_{spf}	=	fuel-based specific impulse
L	=	length of fully fueled pulse detonation engine tube
L_{PF}	=	length of partially fueled pulse detonation engine tube
M_{CJ}	=	propagation Mach number of Chapman–Jouguet detonation wave; $M_{\mathrm{CJ}} = D_{\mathrm{CJ}}/a_1$
N	=	degree of freedom of a molecule
p	=	pressure
q	=	heat released by combustion per unit mass
T	=	temperature
t_{exhaust}	=	duration during which pressure at thrust wall remains higher than its initial value
u	=	flow velocity
v	=	specific volume; $v = 1/\rho$
Y	=	initial mass fraction of gas in partially fueled pulse detonation engine
α	=	parameter used in empirical formula proposed by Li and Kailasanath
γ	=	specific-heat ratio
ε	=	molar thermal energy
μ	=	molar mass
ρ	=	mass density
τ	=	period of one cycle of pulse detonation engine operation
Φ	=	initial mole fraction of gas in partially fueled pulse detonation engine
Φ_V	=	initial volume fraction of gas in partially fueled pulse detonation engine
ϕ_f	=	initial mass fraction of fuel in detonable gas

Subscripts

d	=	detonable gas in partially fueled pulse detonation engine
n	=	inert gas in partially fueled pulse detonation engine
out	=	outer surface of thrust wall of pulse detonation engine tube
w	=	inner surface of thrust wall of pulse detonation engine tube
1	=	undisturbed initial state
2	=	rear surface of detonation wave

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Introduction

PARTIAL fueling of a propulsive pulse detonation engine (PDE), a manner of fueling in which only a part of the combustor is filled with detonable gas and the remainder is filled with inert gas, such as air, is an interesting technique. Schauer et al. [1] carried out experiments on partial fueling and demonstrated that a decrease in

the volume fraction of the combustor filled with detonable gas resulted in an increase in the fuel-based specific impulse, although with a decrease in impulse per cycle.

This paper proposes a model for estimating the propulsive performances of a partially fueled (P–F) simplified PDE and examines its applicability, where a simplified PDE means a PDE whose combustor is a straight tube with one closed end and one open end. Compared with previously proposed models [2–5] for estimating the propulsive performances of a P–F simplified PDE, the model proposed in this paper has two significant advantages: no empirical parameter is required, and the model enables estimation of both the impulse and the duration (denoted by t_{exhaust} in this paper) during which the pressure at the thrust wall (closed end of the combustor) remains higher than its initial value. The time-averaged thrust of a PDE is the product of the impulse per cycle and the operation frequency. That is, the upper limit of the operation frequency is one of the important performance parameters, as is the impulse per cycle. The upper limit of the operation frequency is the reciprocal of the minimum time required for one cycle, which is the sum of duration required for gas recharge, duration required for detonation initiation, and duration required for combustion and exhaust (t_{exhaust}). The former two durations depend strongly on the individual design of a PDE. Namely, the first depends strongly on the number and performances of valves; Wintenberger and Shepherd [6] recently addressed this issue analytically in consideration of a simplified situation. The second duration depends strongly on the method of detonation initiation, which is, for example, a deflagration-to-detonation transition by obstacles or a quick initiation by a predetonator [7]. Meanwhile, in the case of a simplified PDE the third duration is predominantly determined by one-dimensional gas dynamics in a straight tube and accordingly can be treated as a fundamental performance parameter. However, this duration cannot be estimated by the previously proposed models.

In the proposed model, an objective P–F PDE is replaced with an equivalent fully fueled (F–F) PDE and the performance parameters of the equivalent F–F PDE are instead estimated by a proper performance-estimation model for an F–F PDE. That is, the proposed model solves, rather than the complicated wave dynamics in a P–F PDE, the relatively simple wave dynamics in the equivalent F–F PDE. Because the equivalent F–F PDE is not completely equivalent to the objective P–F PDE, the proposed model has some applicability limits, particularly in the case where the inert gas is light and hot and the fueling fraction is low, and these limits are also examined in this paper. In the following, first, the model is described. Next, the results from the model are compared with those from numerical simulations, and the applicability of the model is examined. Then, the results from the model are compared with published results. Finally, the applicability limits of the model are discussed.

Model

Setup of the Problem

This paper uses the P–F PDE shown in Fig. 1a. The PDE is simplified as a straight tube of length of L_{PF} with a fixed cross section, one end of which is closed and the other open. The P–F PDE is filled with detonable and inert gases with mole fractions of Φ_d and Φ_n, respectively, where $\Phi_n = 1 - \Phi_d$.

The initial state of the detonable gas in the P–F PDE is characterized as follows. We adopt $p_{1,d}$ and $a_{1,d}$ as independent thermodynamic variables. The species of the detonable gas is specified by $\mu_{1,d}$, $\gamma_{1,d}$, $\gamma_{2,d}$, $M_{\text{CJ},d}$, and $\phi_{f,d}$. That is, the detonable gas and its burned gas in the P–F PDE are assumed to be calorically perfect gases whose specific-heat ratios are $\gamma_{1,d}$ and $\gamma_{2,d}$, respectively. The initial mechanical state of the detonable gas is specified by $u_{1,d}$. The initial state of the inert gas in the P–F PDE is characterized as follows. We adopt $p_{1,n}$ and $a_{1,n}$ as independent thermodynamic variables. The species of the inert gas is specified by μ_n and γ_n. That is, the inert gas in the P–F PDE is assumed to be a calorically perfect gas whose specific-heat ratio is γ_n. The initial mechanical state of the inert gas is specified by $u_{1,n}$. This paper considers only the case where $u_{1,d} = u_{1,n} = 0$, making the model

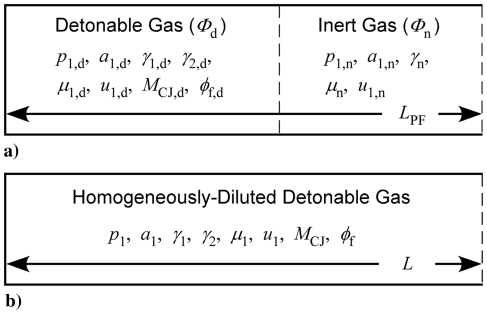

Fig. 1 Initial states of a) the objective P–F PDE and b) the equivalent F–F PDE.

described in this paper applicable to only single-cycle or low-frequency multicycle cases. The influence of gas-flow speed in a detonation tube on impulse was recently discussed by Wintenberger and Shepherd [6].

Homogeneous-Dilution Model of a P–F PDE

To develop a model for estimating the propulsive performances of a P–F simplified PDE, attention is focused on the following phenomenon. According to experiments carried out by Zhdan et al. [8], impulse per cycle of an F–F simplified PDE has low dependence on the location of the detonation initiation, so long as all of the charged detonable gas is burned inside the tube. This experimental observation leads to a hypothesis that every performance parameter obtained by integrating phenomena in one cycle is predominantly determined by only the energy and mass contents in the tube, so long as a detonation wave is properly initiated so that the detonation wave can catch up with any precursor compression waves that push gases toward the open end.

On the basis of this hypothesis, the homogeneous-dilution model of a P–F simplified PDE is proposed. In the model, an objective P–F PDE, as shown in Fig. 1a, is replaced with the equivalent F–F PDE shown in Fig. 1b, which is energetically equivalent to the objective P–F PDE. That is, this equivalent F–F PDE is fully filled with the homogeneous mixture of the detonable and inert gases that separately fill the objective P–F PDE. The homogeneously diluted detonable gas in the equivalent F–F PDE is identical to the gas in the objective P–F PDE in terms of pressure, total internal (thermal) energy, and total mass. In this model, the propulsive performances of the equivalent F–F PDE are instead estimated from the results of the theoretical analysis [9] of an F–F simplified PDE. In the theoretical analysis in [9], the wave dynamics in an F–F PDE were properly solved by analyzing the trajectories of characteristics with some approximations, and the pressure history at the thrust wall could be calculated.

The initial state of the homogeneously diluted detonable gas in the equivalent F–F PDE is characterized as follows, and supplemented in the Appendix. In this paper, the homogeneously diluted detonable gas and its burned gas in the equivalent F–F PDE are assumed to be calorically perfect gases whose specific-heat ratios are γ_1 and γ_2, respectively. First, the following three relations can be derived by considering the boundary conditions at the interface between the detonable and inert gases and the molecular-level ideal mixing.

$$p_1 = p_{1,d} = p_{1,n} \tag{1}$$

$$u_1 = u_{1,d} = u_{1,n} = 0 \tag{2}$$

$$\mu_1 = \Phi_d \mu_{1,d} + \Phi_n \mu_n \tag{3}$$

Equation (3) means that the homogeneous mixture of the detonable and inert gases (homogeneously diluted detonable gas) behaves as a single fluid with molar mass of μ_1.

The specific-heat ratios, γ_1 and γ_2, are formulated as follows. The degree of freedom of a molecule (N) and specific-heat ratio (γ) are related by the following well-known relation for a calorically perfect gas.

$$\gamma = (N+2)/N \tag{4}$$

For the homogeneously diluted detonable gas, the degree of freedom of an averaged molecule N_1 is given by the following formula because perfect gases are considered.

$$N_1 = \Phi_d N_{1,d} + \Phi_n N_n \tag{5}$$

Therefore, the specific-heat ratio γ_1 is formulated as

$$\gamma_1 = 1 + \left(\frac{\Phi_d}{\gamma_{1,d} - 1} + \frac{\Phi_n}{\gamma_n - 1} \right)^{-1} \tag{6}$$

The specific-heat ratio γ_2 is approximated by the following formula, although strict consideration shows that the number of molecules changes by burning.

$$\gamma_2 = 1 + \left(\frac{\Phi_d}{\gamma_{2,d} - 1} + \frac{\Phi_n}{\gamma_n - 1} \right)^{-1} \tag{7}$$

The speed of sound a_1 is formulated as follows. Molar thermal energy (ε) and the speed of sound (a) have the following relationship, which is also a well-known relation for a calorically perfect gas.

$$\varepsilon = \frac{\mu a^2}{\gamma(\gamma - 1)} \tag{8}$$

For the homogeneously diluted detonable gas, the molar thermal energy of averaged molecules ε_1 is given by, in consideration that the total internal (thermal) energy is unchanged by mixing,

$$\varepsilon_1 = \Phi_d \varepsilon_{1,d} + \Phi_n \varepsilon_{1,n} \tag{9}$$

Therefore, the speed of sound a_1 is formulated as

$$a_1 = \sqrt{\frac{\gamma_1(\gamma_1 - 1)}{\mu_1} \left[\frac{\Phi_d \mu_{1,d} a_{1,d}^2}{\gamma_{1,d}(\gamma_{1,d} - 1)} + \frac{\Phi_n \mu_n a_{1,n}^2}{\gamma_n(\gamma_n - 1)} \right]} \tag{10}$$

In consideration of the above results, the mass density of the homogeneously diluted detonable gas ρ_1 is given by

$$\rho_1 = \gamma_1 p_1 / a_1^2 \tag{11}$$

The above equation is consistent with the well-known expression for the speed of sound in an ideal compressible gas and can be derived directly from the latter.

The thermodynamic state of a homogeneous system is uniquely determined from its pressure, total internal (thermal) energy, and total mass. Therefore, in this case the volume of the homogeneously diluted detonable gas is a dependent variable. In this model, the cross-sectional area of the equivalent F–F PDE is assumed to be the same as that of the objective P–F PDE, and the length of the equivalent F–F PDE is formulated as follows.

$$L = \frac{\mu_1 \upsilon_1}{\Phi_d \mu_{1,d} \upsilon_{1,d} + \Phi_n \mu_n \upsilon_{1,n}} L_{\mathrm{PF}} \tag{12}$$

Based upon the above relation, it can be easily shown that $L = L_{\mathrm{PF}}$ in the case where $T_{1,d} = T_{1,n}$.

Because the mass fraction of the detonable gas against the entire gas in the P–F PDE is expressed as

$$Y_d = \frac{\Phi_d \mu_{1,d}}{\mu_1} \tag{13}$$

the mass fraction of fuel in the homogeneously diluted detonable gas ϕ_f is given by

$$\phi_f = \frac{\phi_{f,d} \Phi_d \mu_{1,d}}{\mu_1} \tag{14}$$

The propagation Mach number of the Chapman–Jouguet (CJ) detonation wave in the homogeneously diluted detonable gas M_{CJ} is formulated as follows. From the viewpoint of energetics, the heat released by combustion per unit mass of the homogeneously diluted detonable gas q is expressed as

$$q = \frac{q_d \Phi_d \mu_{1,d}}{\mu_1} \tag{15}$$

This means that the heat released by combustion in the equivalent F–F PDE is the same as that in the objective P–F PDE. In this expression, q_d (the heat released by combustion per unit mass of the real detonable gas in the objective P–F PDE) is given, in terms of $M_{\mathrm{CJ},d}$, by

$$q_d = \frac{a_{1,d}^2}{2(\gamma_{2,d}^2 - 1) M_{\mathrm{CJ},d}^2} \times \left\{ \left[M_{\mathrm{CJ},d}^2 - \frac{(\gamma_{2,d}+1)(\gamma_{2,d} - \gamma_{1,d}) + (\gamma_{2,d}-1)(\gamma_{2,d} + \gamma_{1,d})}{2\gamma_{1,d}(\gamma_{1,d} - 1)} \right]^2 - \frac{(\gamma_{2,d}^2 - 1)(\gamma_{2,d}^2 - \gamma_{1,d}^2)}{\gamma_{1,d}^2 (\gamma_{1,d} - 1)^2} \right\} \tag{16}$$

Finally, the propagation Mach number of the CJ detonation wave in the homogeneously diluted detonable gas M_{CJ} is formulated, in terms of q, as

$$M_{\mathrm{CJ}} = \sqrt{\frac{\gamma_2 - 1}{2} \left[(\gamma_2 + 1) \frac{q}{a_1^2} + \frac{\gamma_2 + \gamma_1}{\gamma_1(\gamma_1 - 1)} \right]} + \sqrt{\frac{\gamma_2 + 1}{2} \left[(\gamma_2 - 1) \frac{q}{a_1^2} + \frac{\gamma_2 - \gamma_1}{\gamma_1(\gamma_1 - 1)} \right]} \tag{17}$$

Equations (16) and (17) were obtained from the results in [10]. The CJ detonation speed in the homogeneously diluted detonable gas D_{CJ} is expressed by

$$D_{\mathrm{CJ}} = M_{\mathrm{CJ}} a_1 \tag{18}$$

Summary of the Formulation

When the performances of a P–F simplified PDE are estimated, parameters Φ_d, $\Phi_n (= 1 - \Phi_d)$, L_{PF}, τ, p_{out}, and p_1, and the species and temperatures of the detonable and inert gases are typically given.

First, the parameters shown in Fig. 1a are determined from the given conditions. Given the species of the detonable and inert gases, parameters $\mu_{1,d}$, μ_n and $\phi_{f,d}$ can be calculated immediately. Parameters $p_{1,d}$ and $p_{1,n}$ are determined from p_1 by means of Eq. (1). Once the pressures and temperatures of the initial detonable and inert gases are known, their speeds of sound, $a_{1,d}$ and $a_{1,n}$, can be determined as their frozen speeds of sound. These calculations can be carried out by chemical–thermodynamic software; for example, STANJAN [11]. The specific-heat ratio of the inert gas γ_n is determined from the relation $a_{1,n}^2 = \gamma_n p_{1,n} / \rho_{1,n}$, where $\rho_{1,n}$ is determined from $p_{1,n}$, $T_{1,n}$ and μ_n using the thermal equation of state for a perfect gas. Once the species and thermodynamic state of the initial detonable gas are given, parameters $M_{\mathrm{CJ},d}$, $\gamma_{1,d}$, and $\gamma_{2,d}$ can be calculated. Parameter $M_{\mathrm{CJ},d}$ can be calculated using chemical–thermodynamics software, and parameter $\gamma_{1,d}$ is determined using the relation $a_{1,d}^2 = \gamma_{1,d} p_{1,d} / \rho_{1,d}$, where $\rho_{1,d}$ is determined from $p_{1,d}$, $T_{1,d}$, and $\mu_{1,d}$ using the thermal equation of state for a perfect gas. Parameter $\gamma_{2,d}$ is determined from the relation $a_{2,d}^2 = \gamma_{2,d} p_{2,d} / \rho_{2,d}$, where $a_{2,d}$ is the equilibrium speed of sound of the burned gas at the CJ state [9], and parameters $a_{2,d}$, $p_{2,d}$, and $\rho_{2,d}$ can be calculated using chemical–thermodynamics software. Parameters $u_{1,d}$ and $u_{1,n}$ are given by Eq. (2). Additionally, the initial mass fraction of the detonable gas in the P–F PDE Y_d, which is not shown in Fig. 1a, is given by Eq. (13).

Next, the parameters shown in Fig. 1b are calculated using the parameters shown in Fig. 1a. Parameter p_1 has already been given, u_1 is given by Eq. (2), and μ_1 is determined from Eq. (3). Parameters γ_1 and γ_2 are calculated using Eqs. (6) and (7), respectively; a_1 is calculated using Eq. (10); L is calculated using Eq. (12); and ϕ_f is

calculated using Eq. (14). Parameter M_{CJ} is calculated as follows. First, parameter q_d is calculated using Eq. (16). Next, q is determined from Eq. (15); then parameter M_{CJ} can be calculated using Eq. (17).

Here, formulas suitable for estimating the performance parameters of the equivalent F–F PDE are needed. It should be noted that parameter M_{CJ} is varied within the range $1 < M_{CJ} \leq M_{CJ,d}$ when parameter Φ_d is varied within the range $0 < \Phi_d \leq 1$. Accordingly, the necessary formulas for an F–F PDE should be applicable within the parameter range of $1 < M_{CJ} \leq M_{CJ,d}$ independent of actual detonability, where $M_{CJ,d} \approx 5$–7, corresponding to typical fuel–oxygen mixtures at atmospheric pressure and room temperature. As such formulas, the theoretical analysis results for an F–F simplified PDE described in [9] are used. Using the results in [9], the pressure history at the thrust wall p_w and performance parameters $t_{exhaust}$, I_{cyc}, I_{spf}, I_{spd} of the equivalent F–F PDE can be obtained when parameters γ_1, γ_2, M_{CJ}, D_{CJ}, L, p_1, p_{out}, τ, ρ_1, and ϕ_f are given. Parameters ρ_1 and D_{CJ} are calculated using Eqs. (11) and (18), respectively.

At the end of this section, some comments on the extension of the model are given. In some cases, a P–F PDE might be filled with several species of gases. For example, two species of detonable gases might be used, one of which has a higher detonability, such as a stoichiometric ethylene–oxygen gas mixture for quick detonation initiation, whereas the other has a lower detonability, such as a jet-fuel–air gas mixture as the main detonable gas. In other cases, two species of inert or nondetonating gases might be used, where one is air for the separation of the fresh (unburned) detonable gas from the hot burned gas, and the other is the residual hot burned gas from the previous cycle. The proposed model in this paper can be easily extended to such situations. That is, when calculating the initial conditions of the equivalent F–F PDE, we have only to take into account all gas species existing in the objective P–F PDE and mix them while maintaining pressure, total mass, and total internal energy unchanged. The revision of the equations is not complicated.

Comparison with Numerical Simulations, Experiments, and Previous Models

Comparison with Numerical Simulations

Numerical simulations were carried out. The computational domain was axisymmetric and is shown in Fig. 2. The detonable gas was a stoichiometric hydrogen–oxygen gas mixture. The inert gas charged inside the tube was air or helium, which were chosen for examining the influences of the species of the charged inert gas. In all cases, the ambient gas surrounding the tube was air. In the numerical simulations, air was treated as $O_2 + 3.76N_2$. The initial pressure and temperature were 0.101325 MPa (1 atm) and 298.15 K, respectively, in the entire computational domain.

In the hydrodynamic code [4,12], an elementary-reaction model [13] was adopted for calculating the heat release and the chemical composition throughout, where eight chemical species (H_2, O_2, H, O, OH, H_2O, HO_2, and H_2O_2) and 19 elementary reactions were considered, although nitrogen was treated as inert. The governing equations were the Euler equations. The algorithm used for solving the governing equations was Yee's non-MUSCL type total variation diminishing upwind explicit scheme. A chemical reaction source term was treated by a linearly point implicit manner.

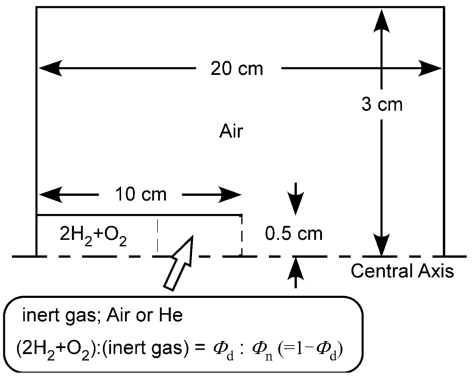

Fig. 2 Geometrical conditions for numerical simulations.

The detonation wave was initiated by setting an artificial high-pressure region, measuring 3 MPa in pressure, 3000 K in temperature, and 0.4 mm in thickness, on the thrust wall. Because of this thin artificial high-pressure region for the detonation initiation, the pressure history at the thrust wall showed a narrow initial peak. The contribution of this initial peak to the detonable-gas-based specific impulse was a few seconds [9]. To shorten the computation time, a one-dimensional (along the axis of the tube) calculation of the flowfield was carried out only in the tube before the shock front broke out the open end of the tube. After that, a two-dimensional (axisymmetric) calculation of the flowfield in the whole domain was conducted. In the following, all of the numerical simulation results are those on the central axis.

Figure 3 shows a comparison between the model and the numerical simulations for performance parameters $t_{exhaust}$, I_{cyc}, and I_{spd}. In the model calculations, $\gamma_{1,d} = 1.397$, $\gamma_{2,d} = 1.129$, $M_{CJ,d} = 5.293$, and $D_{CJ,d} = 2842$ m/s. These values were obtained using the chemical–thermodynamic software STANJAN [11]. Furthermore, $\gamma_n = \frac{7}{5}$ for air and $\gamma_n = \frac{5}{3}$ for helium. Although the maximum disagreement between the results of the model and the numerical simulations was 25% for $t_{exhaust}$ (when the inert gas was air and $\Phi_d = 0.7$) and 31% for I_{spd} (when the inert gas was helium and $\Phi_d = 0.1$), the model reproduced well the entire dependency obtained by the numerical simulations.

Figure 4 shows a comparison between the model and the numerical simulations for the pressure history at the thrust wall. In the case of an F–F PDE, the pressure history at the thrust wall is

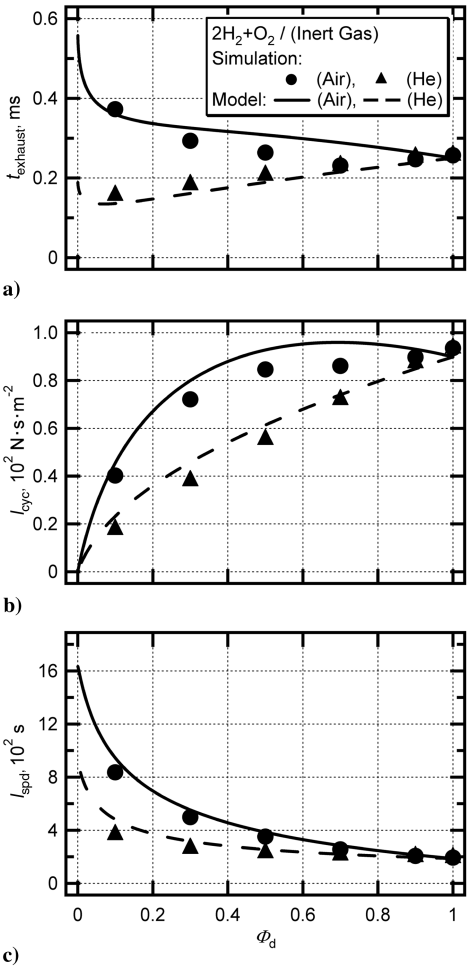

Fig. 3 a) Duration of positive overpressure ($t_{exhaust}$), b) impulse per unit cross section per cycle (I_{cyc}), and c) detonable-gas-based specific impulse (I_{spd}), as functions of initial mole fraction of the detonable gas (Φ_d).

generally composed of a plateau and a following decay, as shown in Fig. 4a. In the theoretical analysis in [9], this pressure history was obtained as follows. The duration of the plateau was accurately calculated by tracing the trajectories of the CJ detonation wave and the front surface of the exhausting rarefaction wave. The following decay is governed by the interference between the exhausting rarefaction wave and its reflection from the thrust wall. This interference was treated by replacing the exhausting rarefaction wave with the self-similar rarefaction wave propagating from the open end toward the thrust wall.

As shown in Fig. 4a, the pressure history at the thrust wall obtained by the numerical simulation was well reproduced by the model in the case of the F–F PDE. However, as shown in Figs. 4b–4e, the model could not reproduce the pressure histories obtained by the numerical simulations in the cases of the P–F PDEs. This disagreement in the P–F PDE cases originates in the equivalent F–F PDE being not completely equivalent to the objective P–F PDE, because the waves are reflected at the interface between the detonable and inert gases in the objective P–F PDE [2], but no such reflection is present in the equivalent F–F PDE. However, note that the duration of positive overpressure (t_{exhaust}) was appreciably well reproduced by the model, as shown in Fig. 3a. This indicates that the proposed model can be used under some conditions for estimating performance parameters obtained by integrating the phenomena in one cycle. The applicability limits are discussed later.

Comparison with Published Results

Figure 5a shows a comparison for the impulse per unit cross section per cycle between experiments carried out by Schauer et al. [1] and the model. The data shown in Fig. 5a were replotted in Fig. 5b in terms of fuel-based specific impulse. In Fig. 5, the results of the experiments and those of the proposed model in this paper are represented by open circles and solid curves, respectively. The experimental conditions were as follows [1]. The detonable gas was a stoichiometric hydrogen–air gas mixture and the inert gas was air, which were initially at ambient pressure and temperature. The simplified PDE used in the experiments was 915 mm long and had an inner diameter of 50.8 mm. To ensure quick initiation of detonation, Shchelkin's wire spiral, whose length was 305 mm, was set in the vicinity of the thrust wall. In Fig. 5, the length of the Shchelkin's wire spiral is shown as "obstacle," because when the fueling fraction was small the length of the fueled region was comparable with that of the Shchelkin's wire spiral. The experiments were carried out in multicycle operation, where the frequency was 12 or 16 Hz. In the model calculations, $\gamma_{1,d} = 1.394$, $\gamma_{2,d} = 1.167$, $M_{\text{CJ},d} = 4.852$, $D_{\text{CJ},d} = 1979$ m/s, which were calculated using STANJAN [11], and $\gamma_n = \frac{7}{5}$. As shown in Fig. 5, the entire dependency obtained by the experiments was well reproduced by the proposed model in this paper. The disagreement between the experimental and model results was within about 15%. As mentioned in the section "Setup of the Problem," this paper considers only the case where the $u_{1,d} = u_{1,n} = 0$. Accordingly, this good agreement may be due to the low frequency of the multicycle experiments.

To examine the applicability of the proposed model to fuels other than hydrogen, the case of ethylene fuel is now presented. Figure 6 shows the results of the proposed model and those of numerical simulations, from which empirical formulas were derived in [2,4], for the detonable-gas-based specific impulse. The conditions for the comparison were as follows. The detonable gas was a stoichiometric ethylene–oxygen gas mixture and the inert gas was air, both of which were initially at atmospheric pressure and room temperature. In the model calculations, $\gamma_{1,d} = 1.329$, $\gamma_{2,d} = 1.140$, $M_{\text{CJ},d} = 7.267$, $D_{\text{CJ},d} = 2376$ m/s, which were calculated using STANJAN [11], and $\gamma_n = \frac{7}{5}$. In Fig. 6, the results of the proposed model are represented by a solid curve. The simulation results obtained by Li and Kailasanath [2] are plotted as open squares, and those obtained by Sato et al. [4] are plotted as open circles.

As shown in Fig. 6, the simulation results by Sato et al. [4] are higher than those by Li and Kailasanath [2] overall. In particular, the

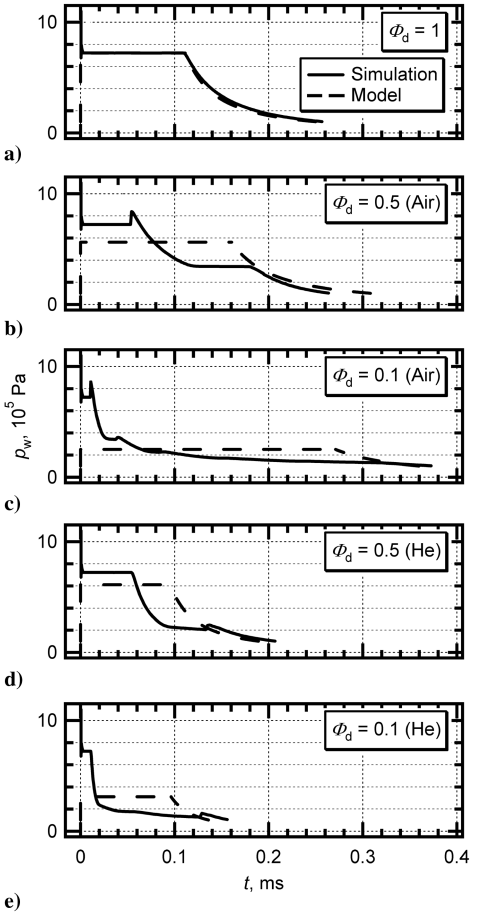

Fig. 4 Pressure histories at the thrust wall in a) the F–F PDE; b–e) the P–F PDE.

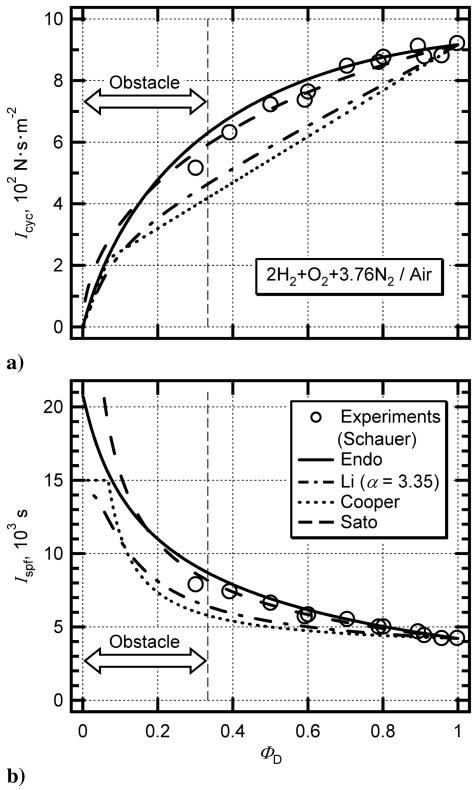

Fig. 5 a) Impulse per unit cross section per cycle (I_{cyc}), and b) fuel-based specific impulse (I_{spf}), as functions of initial mole fraction of the detonable gas (Φ_d).

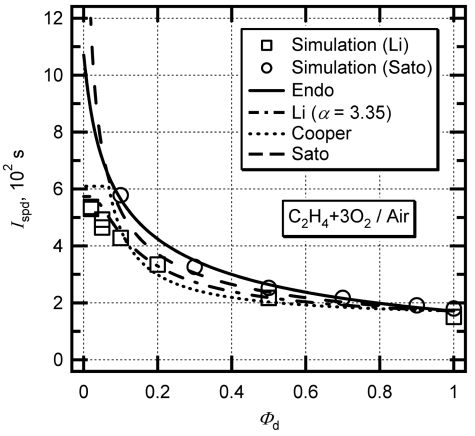

Fig. 6 Detonable-gas-based specific impulse (I_{spd}) as a function of initial mole fraction of the detonable gas (Φ_d).

disagreement is remarkable in cases where Φ_d is small. This disagreement probably originated primarily in the different manners the simulations adopted for the detonation initiation. For the detonation initiation, an artificial high-pressure region of 0.4053 MPa (4 atm) was set on the thrust wall in [2]. On the other hand, an artificial high-pressure region of 3 MPa was set on the thrust wall for the detonation initiation in [4], which was closer to the direct initiation. The theory used in this paper to determine the performance parameters of the equivalent F–F simplified PDE addressed the situation in which the detonation wave was initiated at the thrust wall at the instant of ignition with no delay and the pressure history at the thrust wall showed a plateau from the very beginning; namely, the idealized situation [9]. This situation was similar to the situation in [4] rather than that in [2]. In the simulations in [2], the pressure history at the thrust wall took a good amount of time to begin to show a plateau, and further, the pressure history at the thrust wall showed no plateau in small-Φ_d cases. Because of this difference in the startup phase, the simulation results in [2] are lower than those in [4] overall, and their disagreement was particularly remarkable in small-Φ_d cases. This difference in the startup phase is the primary reason why the results of the proposed model agreed better with the simulation results in [4] (within 7%) than with those in [2].

Figures 5 and 6 also show the results of the empirical formulas proposed thus far [2–4]. The empirical formula proposed by Li and Kailasanath is as follows [2].

$$\frac{I_{spf}}{I_{spf}|_{\Phi_d=1}} = \frac{I_{spd}}{I_{spd}|_{\Phi_d=1}} = \alpha - \frac{\alpha - 1}{\exp[(\Phi_d^{-1} - 1)/8]} \tag{19}$$

where

$$\alpha = \frac{I_{spf}|_{\Phi_d\to 0}}{I_{spf}|_{\Phi_d=1}} = \frac{I_{spd}|_{\Phi_d\to 0}}{I_{spd}|_{\Phi_d=1}} \tag{20}$$

In [2], Li and Kailasanath state that $\alpha = 3.2$–3.5. The empirical formula proposed by Cooper et al. is as follows [3]:

$$\frac{I_{spf}}{I_{spf}|_{\Phi_d=1}} = \frac{I_{spd}}{I_{spd}|_{\Phi_d=1}} = \begin{cases} 0.814 + 0.186\Phi_d^{-1} & (\text{for } 0.0676 \le \Phi_d \le 1) \\ 3.560 & (\text{for } 0 < \Phi_d < 0.0676) \end{cases} \tag{21}$$

This empirical formula was obtained using experimental and numerical results for cases where the detonable gases were ethylene–oxygen or acetylene–oxygen gas mixtures. The empirical formula proposed by Sato et al. is as follows [4]:

$$\frac{I_{spf}}{I_{spf}|_{\Phi_d=1}} = \frac{I_{spd}}{I_{spd}|_{\Phi_d=1}} = \frac{1}{\sqrt{Y_d}} \tag{22}$$

The empirical formulas proposed by Li and Kailasanath [2] and by Cooper et al. [3] are applicable to the ethylene-fuel case but inapplicable to the hydrogen-fuel case. The empirical formula proposed by Sato et al. [4] is applicable to both of the ethylene-fuel and hydrogen-fuel cases, but the predicted specific impulse diverges to infinity as the fueling fraction approaches zero. The proposed model in this paper is applicable to both the ethylene-fuel and hydrogen-fuel cases and the predicted specific impulse is finite even when the fueling fraction approaches zero, although the prediction accuracy in small-Φ_d cases has not yet been examined in detail, because the behavior of the specific impulse when the fueling fraction approaches zero is very difficult to investigate numerically or experimentally. The issue of the specific impulse for the limit that the fueling fraction approaches zero was recently addressed by Cooper in [5] by developing the "bubble model." Table 1 shows a comparison of the estimated values of the specific impulse for the limit that the fueling fraction approaches zero ($I_{spd}|_{\Phi_d\to 0}$) between the proposed model in this paper and Cooper's bubble model. In this comparison, the inert gas is air, and the initial pressure and temperature of the gases are 0.101325 MPa (1 atm) and 300 K, respectively. In the proposed model in this paper, the values of $I_{spd}|_{\Phi_d\to 0}$ were estimated by setting Φ_d as 10^{-4}. Also the values of α, whose definition is given by Eq. (20), estimated by the proposed model in this paper are shown in Table 1. Although the correct values of $I_{spd}|_{\Phi_d\to 0}$ have not yet been determined, it is noteworthy that the predictions by these two independent models agreed within a factor of about 2.

Table 1 Estimated values of $I_{spd}|_{\Phi_d\to 0}$ and α

	$I_{spd}\|_{\Phi_d\to 0}$, s	
Detonable gas	Endo	Cooper
$C_2H_4 + 3O_2$	1071 ($\alpha = 6.25$)	556
$C_2H_2 + 2.5O_2$	1015 ($\alpha = 5.87$)	551
$C_2H_4 + 3(O_2 + 3.76N_2)$	517 ($\alpha = 4.47$)	320
$C_2H_2 + 2.5(O_2 + 3.76N_2)$	555 ($\alpha = 4.63$)	334
$2H_2 + O_2$	1627 ($\alpha = 8.73$)	771

Applicability Limits of the Model

Although the proposed model in this paper is applicable to many cases, as shown in the previous section, the applicability of the model must be limited, because in some cases not only energy and mass contents in the tube but also wave dynamics in the tube, which were not properly solved in the model, are important to the performances of a simplified PDE. This section discusses the applicability limits of the model by comparing its results with the results of numerical simulations in somewhat extreme cases.

Numerical simulations were carried out under geometrical conditions similar to those shown in Fig. 2. In the numerical simulations in this section, the radii of the detonation tube and the entire computational domain are 0.25 and 1.64 cm, respectively. The detonable gas is a stoichiometric hydrogen–oxygen gas mixture whose initial pressure and temperature are 0.101325 MPa (1 atm) and 298.15 K, respectively. The inert gas charged in the detonation tube is helium or argon ($\gamma_n = \frac{5}{3}$) whose initial pressure is the same as that of the detonable gas and whose initial temperature is 1000 or 2000 K. The species of the ambient gas surrounding the tube is the same as that of the inert gas charged in the detonation tube, with an initial pressure and temperature of 0.101325 MPa (1 atm) and 298.15 K, respectively. The other conditions are the same as those for the numerical simulations described in the section "Comparison with Numerical Simulations."

Figure 7 shows the results of the numerical simulations and the model. The horizontal axis denotes the volume fraction of the detonable gas in the tube, and the vertical axes denote the performance parameters of the P–F PDEs normalized by those of the F–F PDE. When the inert gas is argon, the results of the model agree fairly well with those of the numerical simulations. However, when the inert gas is helium, the results of the model do not agree well with those of the numerical simulations, especially for smaller fueling

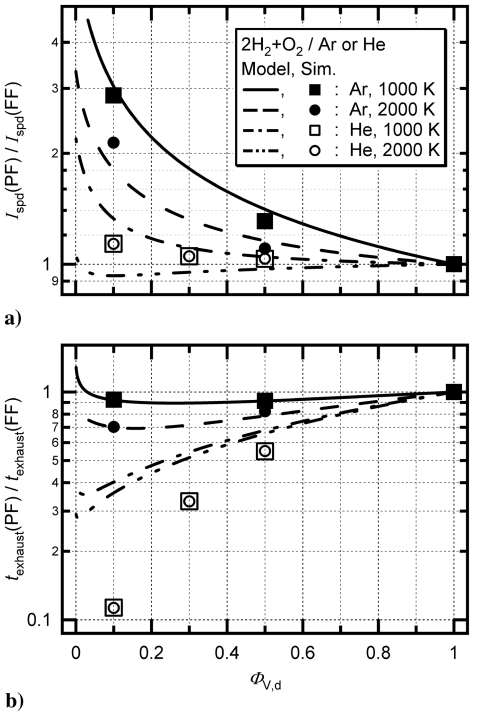

Fig. 7 a) Detonable-gas-based specific impulse, and b) duration of positive overpressure, normalized by those of the fully fueled case, as functions of initial volume fraction of the detonable gas ($\Phi_{V,d}$).

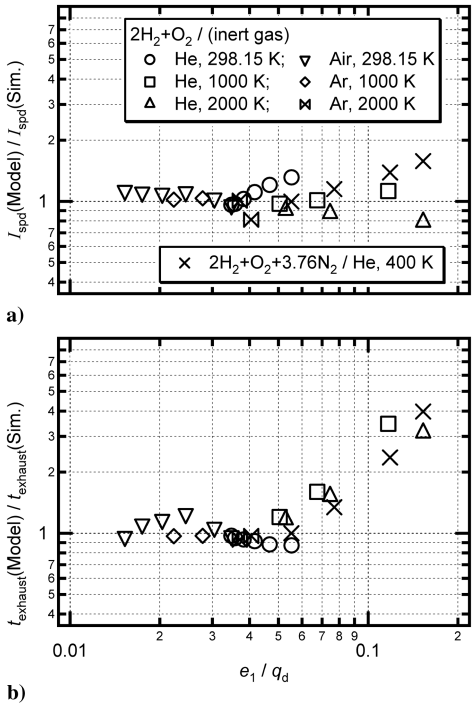

Fig. 8 Ratios of the results of the model to those of the numerical simulations in a) detonable-gas-based specific impulse, and b) duration of positive overpressure, as functions of nondimensional quantity e_1/q_d.

fractions. Here it should be noted that the results of the model agreed well with those of numerical simulations, as shown in Fig. 3, when the initial temperature of the inert gas is 298.15 K, even when the inert gas is helium. These comparisons qualitatively show that the model is not applicable when 1) the initial temperature of the inert gas is high, 2) the molar mass of the inert gas is small, and 3) the filling fraction of the detonable gas is low.

To discuss the applicability limits of the model quantitatively, the internal (thermal) energy per unit mass of the homogeneously diluted detonable gas is used as a governing parameter for the applicability of the model. This quantity is given by

$$e_1 = \frac{\varepsilon_1}{\mu_1} = \frac{a_1^2}{\gamma_1(\gamma_1 - 1)} \tag{23}$$

and is large when the above three conditions for the inapplicability of the model are satisfied. Furthermore, a nondimensional quantity e_1/q_d is examined as the predominant governing parameter for the applicability limits of the model for taking into account the differences in the detonable gas.

For the quantitative study of the applicability limits of the model in terms of the nondimensional quantity e_1/q_d, some additional numerical simulations were carried out in which the stoichiometric hydrogen–air gas mixture ($2H_2 + O_2 + 3.76N_2$) was used as the detonable gas. In these numerical simulations, the detonation wave was initiated by setting an artificial high-pressure region, which was 4 MPa in pressure, 4000 K in temperature, and 0.4 mm in thickness, on the thrust wall. The inert gas charged in the detonation tube was helium with an initial temperature of 400 K. The other conditions for the numerical simulations were the same as those for the numerical simulations whose results are shown in Fig. 7. In the model calculations, $\gamma_{1,d} = 1.394$, $\gamma_{2,d} = 1.167$, $M_{\mathrm{CJ},d} = 4.868$, and $D_{\mathrm{CJ},d} = 1979$ m/s.

Figure 8 shows the ratios of the results of the model to those of the numerical simulations as functions of nondimensional quantity e_1/q_d. Regarding the results of the additional numerical simulations for the hydrogen–air cases, the influence of the artificial high-pressure region for the detonation initiation on the specific impulse was not negligible. Therefore, this influence; namely, the initial narrow peak in the pressure history on the thrust wall, was carefully removed when the results were plotted in Fig. 8. Defining the applicability limits of the model as a 30% disagreement with the numerical simulations, the model is applicable to calculating the specific impulse when $e_1/q_d < 0.1$ approximately, and applicable to calculating the duration during which the pressure at the thrust wall remains higher than its initial value when $e_1/q_d < 0.06$ approximately.

Conclusions

A performance-estimation model for a P–F simplified PDE is proposed. This model requires no empirical parameter and predicts both the impulse and the duration during which the pressure at the thrust wall remains higher than its initial value. In the model, not the propulsive performances of an objective P–F PDE but those of the equivalent fully fueled (F–F) PDE are estimated using a previously developed performance-estimation model for an F–F PDE. The equivalent PDE is fully filled with a homogeneous mixture of the detonable and inert gases that separately fill the objective P–F PDE. The applicability of the model was examined by comparing the results of the model with those of numerical simulations and other published results for the cases of hydrogen and ethylene fuels. Further, by considering rather extreme cases, the applicability limits were described in terms of a nondimensional parameter. Defining the applicability limits of the model as a 30% disagreement with the numerical simulations, the model is applicable to calculating the specific impulse when $e_1/q_d < 0.1$ approximately, and applicable to calculating the duration during which the pressure at the thrust wall remains higher than its initial value when $e_1/q_d < 0.06$ approximately, where e_1 denotes the internal (thermal) energy per unit mass of the homogeneously diluted detonable gas filling the equivalent F–F PDE and q_d denotes the heat released by combustion per unit mass of the real detonable gas in the objective P–F PDE.

Appendix: Thermodynamic Variables of Ideal Mixture of Ideal Gases

Let n_A moles of gas A, whose molar mass and specific-heat ratio are, respectively, μ_A and γ_A, at a pressure p_A and a sound speed a_A (pressure and sound speed are adopted as two independent

thermodynamic variables) be mixed with n_B moles of gas B, whose molar mass and specific-heat ratio are, respectively, μ_B and γ_B, at the same pressure $p_B\,(=p_A)$ and a sound speed a_B. This mixture is assumed to be an ideal mixture of ideal gases. This means that two calorically perfect gases (gases A and B) are completely mixed in the molecular level, and the mixture behaves as a single calorically perfect gas. According to the fundamental principle of thermodynamics, we can specify two thermodynamic variables of the mixture. First, the pressure of the mixture (p) is specified so as to be the same as the initial pressures of gases A and B before mixing, that is, $p = p_A = p_B$. Next, the internal energy of the mixture is specified so as to be the sum of those of gases A and B before mixing. Under this situation, thermodynamic variables of the mixture are calculated as follows.

By using the well-known formula for the sound speed of a calorically perfect gas, the mass densities of gases A and B (ρ_A and ρ_B) and the temperatures of them (T_A and T_B) before mixing are written as

$$\rho_A = \frac{1}{\upsilon_A} = \frac{\gamma_A p_A}{a_A^2}, \qquad \rho_B = \frac{1}{\upsilon_B} = \frac{\gamma_B p_B}{a_B^2}, \qquad T_A = \frac{\mu_A a_A^2}{\gamma_A R_u}, \qquad T_B = \frac{\mu_B a_B^2}{\gamma_B R_u} \tag{A1}$$

where υ_A and υ_B are the specific volumes of gases A and B before mixing, respectively, and R_u is the universal gas constant. Denoting the volume, mass density, and temperature of the mixture by V, ρ, and T, respectively, the pressure of the mixture is written, adopting the Dalton's partial-pressure model, as

$$p = \frac{n_A R_u T}{V} + \frac{n_B R_u T}{V} = \frac{n_A + n_B}{V} R_u T = \frac{\mu_A n_A + \mu_B n_B}{V} \frac{R_u T}{\frac{\mu_A n_A + \mu_B n_B}{n_A + n_B}} = \rho \frac{R_u T}{\Phi_A \mu_A + \Phi_B \mu_B} \tag{A2}$$

where $\Phi_A = n_A/(n_A + n_B)$ and $\Phi_B = n_B/(n_A + n_B)$ are the mole fractions of gases A and B, respectively. The above equation represents that the mixture behaves as $n = n_A + n_B$ moles of a thermally perfect gas whose molar mass is $\mu = \Phi_A \mu_A + \Phi_B \mu_B$.

The molar specific heats at constant volume and constant pressure of gas A are expressed as $C_{\upsilon A} = N_A R_u/2$ and $C_{pA} = C_{\upsilon A} + R_u$, respectively, where N_A is the degree of freedom of a molecule of gas A. Therefore, N_A is expressed as $N_A = 2/(\gamma_A - 1)$ in terms of the specific-heat ratio of gas A: $\gamma_A = C_{pA}/C_{\upsilon A} = (N_A + 2)/N_A$. Similarly, the degree of freedom of a molecule of gas B (N_B) is expressed as $N_B = 2/(\gamma_B - 1)$ in terms of the specific-heat ratio of gas B (γ_B). Because we consider an ideal mixture of ideal gases, we can write a relation on the degrees of freedom of molecules as $nN = n_A N_A + n_B N_B$ where N denotes the degree of freedom of an averaged molecule of the mixture. Accordingly, N is written as $N = \Phi_A N_A + \Phi_B N_B$. Therefore, the specific-heat ratio of the mixture (γ) is written as follows.

$$\gamma = \frac{N+2}{N} = 1 + \left(\frac{\Phi_A}{\gamma_A - 1} + \frac{\Phi_B}{\gamma_B - 1} \right)^{-1} \tag{A3}$$

By using the formulas for N_A and N_B in terms of the specific-heat ratios and Eq. (A1), the molar internal (thermal) energies of gases A and B (ε_A and ε_B) before mixing are written as follows.

$$\varepsilon_A = \frac{N_A}{2} R_u T_A = \frac{\mu_A a_A^2}{\gamma_A(\gamma_A - 1)}, \qquad \varepsilon_B = \frac{N_B}{2} R_u T_B = \frac{\mu_B a_B^2}{\gamma_B(\gamma_B - 1)} \tag{A4}$$

Because the internal energy of the mixture is the same as the sum of those of gases A and B before mixing, we can write a relation on the internal energies as $n\varepsilon = n_A \varepsilon_A + n_B \varepsilon_B$, where ε denotes the molar internal (thermal) energy of the mixture. From this relation, ε is written as follows.

$$\varepsilon = \Phi_A \varepsilon_A + \Phi_B \varepsilon_B = \frac{\Phi_A \mu_A a_A^2}{\gamma_A(\gamma_A - 1)} + \frac{\Phi_B \mu_B a_B^2}{\gamma_B(\gamma_B - 1)} \tag{A5}$$

Because ϵ is expressed, similarly to Eq. (A4), as $\varepsilon = \mu a^2/[\gamma(\gamma - 1)]$ where a is the sound speed of the mixture, we can express a as follows.

$$a = \sqrt{\frac{\gamma(\gamma-1)}{\mu} \left[\frac{\Phi_A \mu_A a_A^2}{\gamma_A(\gamma_A - 1)} + \frac{\Phi_B \mu_B a_B^2}{\gamma_B(\gamma_B - 1)} \right]} \tag{A6}$$

Similarly to Eq. (A1), the mass density and specific volume of the mixture (ρ and υ) are written as follows.

$$\rho = \frac{1}{\upsilon} = \frac{\gamma p}{a^2} \tag{A7}$$

Because the total volume of gases A and B before mixing ($V_A + V_B$) can be expressed, in terms of n, as $V_A + V_B = n_A \mu_A \upsilon_A + n_B \mu_B \upsilon_B = n(\Phi_A \mu_A \upsilon_A + \Phi_B \mu_B \upsilon_B)$, n can be written as $n = (V_A + V_B)/(\Phi_A \mu_A \upsilon_A + \Phi_B \mu_B \upsilon_B)$. Therefore, the volume of the mixture (V) is written as follows.

$$V = n\mu\upsilon = \frac{\mu\upsilon}{\Phi_A \mu_A \upsilon_A + \Phi_B \mu_B \upsilon_B} (V_A + V_B) \tag{A8}$$

This equation corresponds to Eq. (12).

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