

# Technical Notes

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## Thermodynamic Cycle Analysis for Propagating Detonations

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### Introduction

**P**ROPAGATING detonations have recently been the focus of extensive work based on their use in pulse detonation engines.<sup>1</sup> The entropy minimum associated with Chapman–Jouguet (CJ) detonations<sup>2</sup> and its potential implications on the thermal efficiency of these systems<sup>3</sup> has been one of the main motivations for these efforts. The notion of applying thermodynamic cycles to detonation was considered first by Zel’dovich,<sup>4</sup> who concluded that the efficiency of the detonation cycle is slightly larger than that of a cycle using constant-volume combustion. More recently, Heiser and Pratt<sup>3</sup> conducted a thermodynamic analysis of the detonation cycle for a perfect gas using a one- $\gamma$  model of detonations. Other studies have used constant-volume combustion as a surrogate for the detonation process.<sup>5</sup> This work presents two main contributions. First, we present an alternative physical model for the detonation cycle handling propagating detonations in a purely thermodynamic fashion. The Fickett–Jacobs (FJ) cycle is a conceptual thermodynamic cycle that can be used to compute an upper bound to the amount of mechanical work that can be obtained from detonating a given mass of explosive. Second, we present computations of the cycle thermal efficiency for a number of fuel-oxygen and fuel-air mixtures using equilibrium chemistry, and we discuss the strong influence of dissociation reactions on the results.

We recognize that the scope of this analysis is limited because the efficiencies computed cannot be used directly to estimate pulse-detonation-engine performance because of the unsteadiness of the exit flow.<sup>6</sup> The performance can only be measured by accounting for the complex gas dynamics of realistic pulse detonation engines.<sup>7–9</sup> Furthermore, our analysis is ideal in the sense that it accounts for entropy generation only during the detonation process. Practical pulse detonation engines will have additional entropy generation caused by shock waves, mixing, unsteady operation, or flow separation.<sup>9</sup> However, we believe that this analysis is relevant to the development of high-level performance strategies and to the identification of key physical phenomena affecting performance such as precompression of the reactants or dissociation reactions in the detonation products.

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### Fickett–Jacobs Cycle

The FJ cycle for propagating detonations is described in Fickett and Davis<sup>10</sup> and is an elaboration of the original ideas of Jacobs.<sup>11</sup> Zel’dovich’s ideas<sup>4</sup> were not known (personal communication from W. C. Davis, April 2003) to Jacobs or Fickett and, until recently, there was no appreciation in the West of this work by Zel’dovich.

The basis of the cycle is the piston-cylinder arrangement of elementary thermodynamics of Fig. 1a. The reactants and explosion products are at all times contained within the cylinder and pistons, which are assumed to be rigid, massless, and adiabatic. The explosive, pistons, and cylinder will be considered as a closed thermodynamic system. The pistons can be independently moved, and there is a work interaction per unit mass  $w$  ( $>0$  for work done by the system) with the surroundings that results from these motions. To have a complete cycle, there will be a heat interaction per unit mass  $q$  ( $>0$  for heat transferred into the system) between the system and the surroundings.

The steps in the cycle are shown in Fig. 1. The cycle starts with the system at the initial state 1. The reactants are isentropically compressed to state 2 (step b) with a compression ratio  $\pi_c = P_2/P_1$ , where  $P$  denotes pressure. The application of external work to move the piston on the left at velocity  $u_p$  instantaneously initiates a detonation front at the piston surface (step c). The detonation propagates to the right and the detonation products following the wave are in a uniform state at a velocity  $u_p$ . The velocity  $U_{CJ}$  of the detonation wave is determined from the mass, momentum, and energy conservation equations given the velocity  $u_p$  of the detonation products. When the detonation reaches the right piston, the piston instantaneously accelerates to velocity  $u_p$ , and the entire piston-cylinder arrangement moves at constant velocity  $u_p$  (step d). The system is then at state 3. The energy of this mechanical motion is converted to external work (step e) by adiabatically and reversibly bringing the detonation products to rest at state 4, maintaining the distance between the two pistons. Then the products are isentropically expanded to the initial pressure (step f) to reach state 5. Heat is extracted by reversibly cooling the products at constant pressure (step g) to the initial temperature (state 6). Finally, the cycle is completed by converting products (state 6) to reactants (state 1) at constant temperature and pressure (step h). The sequence of equilibrium states taken by the system is represented in the pressure-specific volume plane of Fig. 2. The paths drawn between the numbered states consist of the series of equilibrium states occupied by the system during each process except during the detonation process, between states 2 and 3. Although the system is temporarily nonuniform during the detonation process, it is spatially uniform at the beginning and at the end of the process. The dash-dot line drawn between states 2 and 3 does not represent an actual thermodynamic path but is simply an artifice to form a closed cycle, similar to what other researchers have used for detonation or constant-volume combustion.<sup>3,5</sup> This artificial representation bears no influence on the subsequent calculation of the work done, which depends only on the thermodynamic equilibrium states.

The net work done by the system is equal to the sum of the work done during each step. For all steps in the cycle, the first law of thermodynamics yields  $\Delta(e + u^2/2) = q - w$ , where  $e + u^2/2$  is the total energy in the system per unit mass, composed of the internal  $e$  and kinetic  $u^2/2$  energies. The only heat exchange between the system and the surroundings occurs between states 5 and 1. Hence, the work done between states 1 and

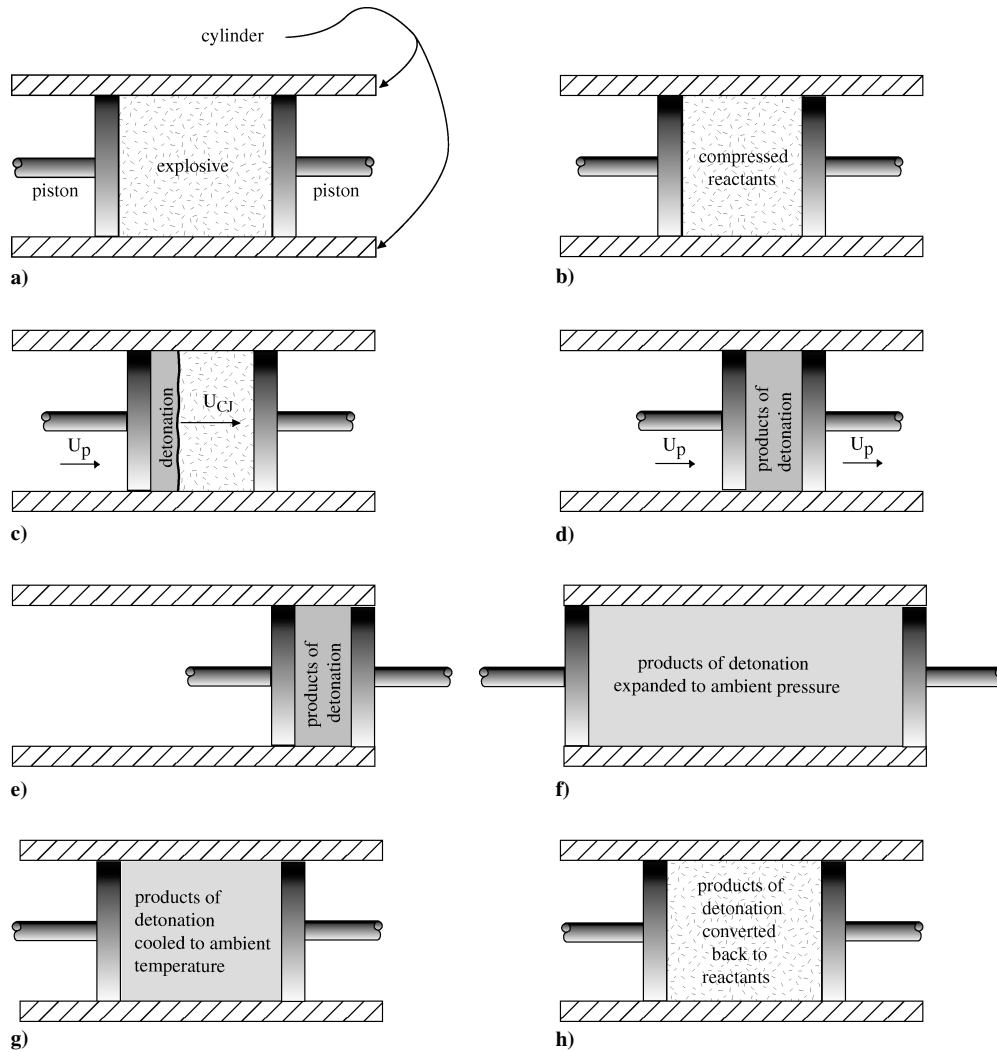


Fig. 1 Physical steps that make up the Fickett–Jacobs cycle.

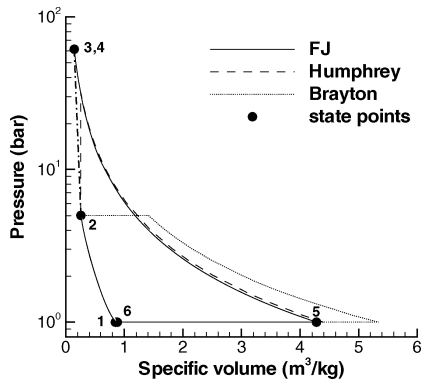


Fig. 2 Pressure-specific volume diagram showing the sequence of states and connecting paths that make up the FJ cycle (with  $\pi_c = 5$ ) for a stoichiometric propane-air mixture at 300 K and 1 bar initial conditions.

5 is  $w_{15} = e_1 - e_5$ , and the work done between states 5 and 1 is  $w_{51} = P_1(v_1 - v_5)$ . The net work done by the system over the FJ cycle is  $w_{net} = e_1 - e_5 + P_1(v_1 - v_5) = h_1 - h_5$ , where  $h$  is the enthalpy per unit mass. (Note that the velocity at states 1 and 5 is zero,  $u = 0$ , so that enthalpy and total enthalpy are equal.) This result is identical to that obtained by Zel'dovich.<sup>4</sup> Because all processes other than the detonation are reversible, the work computed is an upper bound to what can be obtained by any cyclic process using a propagating detonation for the combustion step. Fickett and Davis<sup>10</sup> do not account for the work interaction during the process 5–1 in

their definition of the net work. They do not consider steps g) and h) to be significant for their application to unconfined explosives because the detonation products just mix with the surroundings, and the work generated between states 5 and 1 is “lost.” (Our first effort<sup>12</sup> to apply the FJ cycle to modeling impulse from detonation tubes used Fickett and Davis’ interpretation of the available work rather than the approach taken here. As a consequence, the numerical values of the efficiencies given in Cooper and Shepherd<sup>12</sup> are different than given here.) However, these interactions have to be included for consistency with the first law of thermodynamics for a cyclic process.

An alternative way to compute the net work done by the system consists in computing the work done during each individual process. The sum of these individual contributions was computed with the help of the detonation jump conditions and is found to yield the same result as just quoted for the net work done during the cycle.<sup>13</sup> The agreement between this detailed energy balance and the thermodynamic system approach demonstrates the self-consistency of our formulation of the FJ detonation cycle.

### Thermal Efficiency

The FJ cycle can be used to define an upper bound on the efficiency of devices using a propagating detonation as the combustion step. The thermal efficiency for the conversion of chemical energy into mechanical work is the ratio of the net work done to the specific heat of combustion of the mixture. From the preceding discussion, for FJ cycle this is

$$\eta_{th} = w_{net}/q_c = (h_1 - h_5)/q_c \quad (1)$$

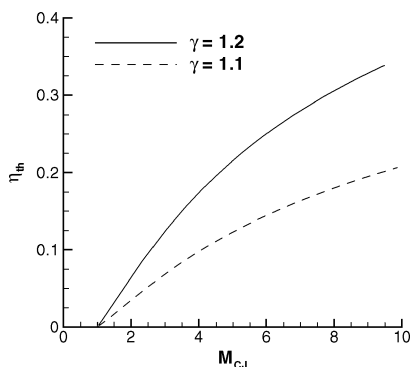


Fig. 3 Thermal efficiency for the FJ cycle as a function of CJ Mach number for the one- $\gamma$  model of detonation for two values of  $\gamma$  representative of fuel-oxygen ( $\gamma = 1.1$ ) and fuel-air ( $\gamma = 1.2$ ) detonations.

The specific heat of combustion  $q_c$  is computed as the enthalpy difference between the reactants and the products at initial pressure and temperature:  $q_c = h_1 - h_6$ .

We first investigate the values of the thermal efficiency for a perfect-gas model by representing the detonation process using the one- $\gamma$  model of detonation,<sup>14</sup> which relates the CJ Mach number to the specific heat of combustion.

$$M_{CJ} = \sqrt{\mathcal{H} + 1} + \sqrt{\mathcal{H}} \quad \text{where} \quad \mathcal{H} = \frac{(\gamma^2 - 1)q_c}{2\gamma RT_2} \quad (2)$$

$$\eta_{th} = 1 - \frac{C_p T_1}{q_c} \left[ \frac{1}{M_{CJ}^2} \left( \frac{1 + \gamma M_{CJ}^2}{1 + \gamma} \right)^{(\gamma+1)/\gamma} - 1 \right] \quad (3)$$

The thermal efficiency is represented in Fig. 3 as a function of the CJ Mach number for two values of the specific heat ratio  $\gamma$  representative of the products of fuel-oxygen and fuel-air detonations. The thermal efficiency increases with increasing CJ Mach number, which increases<sup>14</sup> with the specific heat of combustion  $q_c$ . A higher heat of combustion increases the pressure ratio through the detonation wave significantly more than the temperature ratio. This means that the detonation products undergo a stronger expansion between states 4 and 5, which reduces the temperature at state 5. Thus, less heat is rejected during process 5–1 and the efficiency is higher. Figure 3 also shows that the variation of the thermal efficiency depends strongly on the value chosen for  $\gamma$ . At constant CJ Mach number, a lower value of  $\gamma$  in the detonation products yields a lower efficiency. The parameter  $\gamma - 1$  controls the slope of the isentrope 4–5 in the pressure-temperature plane. Although the pressure ratio  $P_4/P_5$  varies with  $\gamma$ , the main effect of decreasing  $\gamma$  is to increase the temperature at state 5 so that more heat is rejected during process 5–1. The result of Eq. (3) is identical to the result obtained by Heiser and Pratt,<sup>3</sup> who computed the thermal efficiency by calculating the entropy increments associated with each process in the detonation cycle. However, the numerical values we obtain are lower than those given in Heiser and Pratt<sup>3</sup> because they used a value of  $\gamma = 1.4$  corresponding to the reactants, whereas we use values of  $\gamma$  equal to 1.1 or 1.2 more representative of the detonation products. A more realistic cycle analysis for a perfect gas involves using the two- $\gamma$  model of detonations,<sup>14</sup> which was applied by Wu et al.<sup>8</sup>

In reality, one- or two- $\gamma$  models of these cycles cannot correctly capture all of the features of dissociation-recombination equilibria and temperature-dependent properties. The thermal efficiency was calculated based on Eq. (1) using realistic thermochemistry<sup>15</sup> for hydrogen, ethylene, propane, and JP10 fuels with oxygen and air, assuming all chemical states involving combustion products are in equilibrium. The results are significantly influenced by the variation of the specific heat capacity with temperature in the detonation products and the dissociation and recombination processes.

The influence of equivalence ratio on the thermal efficiency is shown in Fig. 4. The thermal efficiency for fuel-air mixtures is

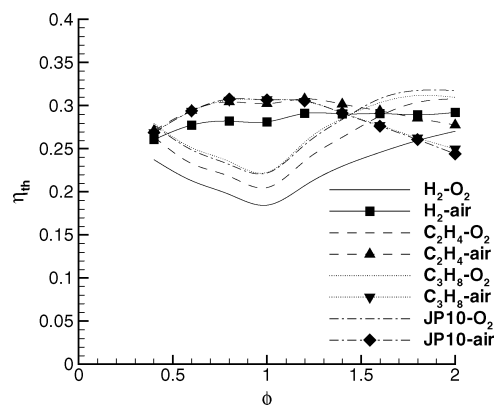


Fig. 4 Thermal efficiency for the FJ cycle as a function of equivalence ratio at 300 K and 1 bar initial conditions for hydrogen, ethylene, propane, and JP10 with no precompression ( $\pi_c = 1$ ).

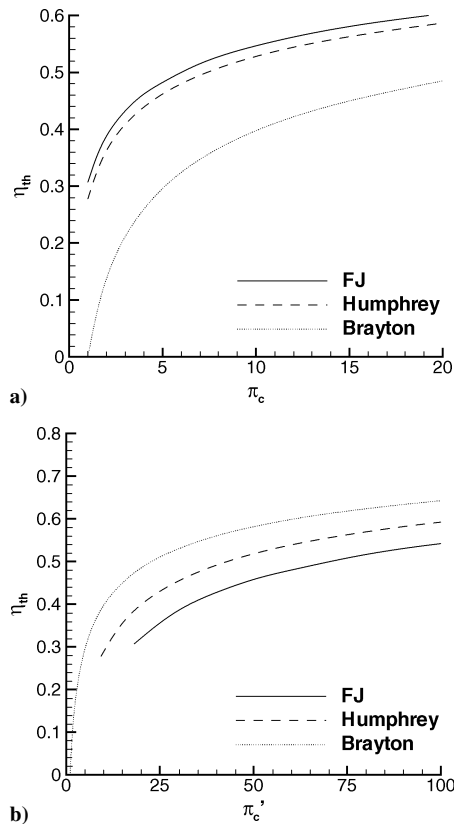
maximum at stoichiometry, whereas it is minimum for fuel-oxygen mixtures. Fuel-air mixtures generate much lower CJ temperatures than fuel-oxygen mixtures. Because of their low extent of dissociation, fuel-air mixtures follow the same trends as the perfect gas and yield a maximum efficiency when the energy release is maximized near stoichiometry. On the other hand, fuel-oxygen mixtures are characterized by high CJ temperatures (in particular near stoichiometry), which promote endothermic dissociation reactions. Although the radicals created by the dissociation reactions start recombining during the subsequent expansion process, the temperature in the detonation products of fuel-oxygen mixtures remains high, and only partial recombination occurs. The energy stored in the partially dissociated products at state 5 is proportionally higher for fuel-oxygen than for fuel-air mixtures, which reduces the thermal efficiency of fuel-oxygen mixtures relative to fuel-air mixtures. This effect increases with increasing CJ temperature and was confirmed by investigations of the influence of nitrogen dilution,<sup>13</sup> which showed that the thermal efficiency increases with increasing nitrogen dilution. The thermal efficiency is also found to decrease with decreasing pressure<sup>13</sup> because of the increasing importance of dissociation at low pressures, and with increasing initial temperature<sup>13</sup> because of the associated decrease in initial mixture density and CJ Mach number.

Although stoichiometric fuel-oxygen mixtures have a higher specific heat of combustion than fuel-air mixtures, Fig. 4 shows that fuel-air mixtures have a higher thermal efficiency. This is attributed mainly to dissociation phenomena, but also to the higher value of the effective ratio of specific heats  $\gamma$  in the detonation products of fuel-air mixtures.<sup>13</sup> Note that fuel-oxygen mixtures still generate two to four times as much work per unit mass of mixture as fuel-air mixtures because of their larger specific heat of combustion.

The values obtained for the FJ cycle efficiency with no precompression are quite low, generally between 0.2 and 0.3 for the range of mixtures investigated. For a fixed specific heat of combustion, isentropically increasing the combustion pressure decreases the CJ Mach number [Eq. (2)], which reduces the total entropy rise and results in an increased thermal efficiency (Fig. 5). In terms of net work, precompressing the reactants increases the work done during the expansion process (state 4 to 5). The expansion of the hot gases generates more work than is absorbed by the cold gases during the precompression stage, so that precompression increases the thermal efficiency.

### Comparison with Brayton and Humphrey Cycles

The thermal efficiency of the FJ cycle is compared in Fig. 5 with that of the Brayton and Humphrey cycles. These cycles are plotted with the FJ cycle in the pressure-specific volume diagram of Fig. 2. In comparing different combustion modes, the question of which of the various pressures produced during the combustion event should be considered.<sup>16</sup> Two possibilities are explored here, based on the



**Fig. 5 Thermal efficiency as a function of a) compression ratio and b) combustion pressure ratio for FJ, Humphrey, and Brayton cycles for a stoichiometric propane-air mixture at 300 K and 1 bar initial conditions.**

pressure before combustion, corresponding to propulsion systems with the same feed system, and based on the peak combustion pressure, which corresponds to propulsion systems operating at the same level of material stresses.

The cycle efficiencies are shown in Fig. 5 as a function of the compression ratio  $\pi_c = P_2/P_1$  and the combustion pressure ratio  $\pi_c' = P_3/P_1$ . For a given compression ratio, the FJ cycle yields the highest thermal efficiency, closely followed by the Humphrey cycle and, finally, the Brayton cycle. This result can be directly related to the lower entropy rise associated with CJ detonations in the conventional Hugoniot analysis.<sup>13</sup> The FJ and Humphrey cycles yield very similar efficiencies because of the similarities between detonation and constant-volume combustion.<sup>13</sup> However, when the thermal efficiency is shown as a function of the combustion pressure ratio, the trend is inverted, and the Brayton cycle yields the highest efficiency, followed by the Humphrey and FJ cycles. The lower efficiency of the FJ cycle shown in Fig. 5b is caused by the lower precompression required for the FJ cycle given a fixed combustion pressure ratio. Although these efficiencies cannot be precisely translated into specific performance parameters,<sup>6</sup> these general results agree with the observations of Talley and Coy<sup>16</sup> based on specific impulse calculations using a gas dynamic model of constant-volume combustion propulsion.

This work clarifies the potential for doing work with an idealized cycle using propagating detonations. If we fix the initial state ahead of the combustion wave, in agreement with other analyses, detonations have the potential to generate slightly more mechanical work than a constant-volume combustion process and substantially more than the constant-pressure process. On the other hand, for a given peak pressure in the combustion process the situation is reversed with constant-pressure processes being more efficient than constant-volume or detonation processes. For the case of a fixed thermodynamic state upstream of the combustor and a variable combustion wave speed, detonation appears to be the most efficient combustion process. Although this might seem paradoxical because of the addi-

tional entropy generation of the leading shock wave implicit in the detonation process, in fact under the situation described by Fig. 2 the smallest entropy generation for the combustion step is indeed generated by detonation because the equivalent energy addition is at the highest temperature<sup>3</sup> of the three combustion processes considered. This is a straightforward consequence of the properties<sup>17</sup> of the locus of states (Hugoniot) for idealized combustion processes starting from a fixed initial thermodynamic state (state 3 of Fig. 2) that is at rest. Very different conclusions are reached when state 3 is in motion and the stagnation state upstream of the combustion wave is held constant. For this case, detonation is the least favorable choice for the combustion process, as discussed by Wintenberger and Shepherd.<sup>17</sup>

Another important conclusion is that dissociation processes have a strong influence on the value of the thermal efficiency in real gaseous mixtures. However, as pointed out earlier, pulse-detonation-engine performance cannot be estimated directly from the thermal efficiency.<sup>6</sup> The conversion of thermal energy to impulse in unsteady systems requires detailed consideration of the gas dynamic processes<sup>7-9</sup> within the engine.

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