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Exergy Analysis of a Pulse Detonation Power Device

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Abstract. *Recent research has been developed in thermodynamic analysis of pulse detonation engines. However, the focus of contemporary work is on thrust production for propulsion systems. The present work develops an exergy analysis of a pulse detonation power device. The objective of this analysis is to quantify the efficiency, in terms of availability, of a power device operated by detonation. This study considered the fuel availability and the losses in the system. Losses are due to irreversibilities during processes and due to availability transfer. The Second Law or exergetic efficiency was computed based on the fuel availability. The device modeled here embraces a low pressure compressor, a check valve, a detonation chamber, a two stage turbine and a generator. The results are then compared with the exergetic efficiency applied to deflagration systems. Data for detonation and deflagration were obtained from C.E.A. code (McBride and Gordon, 1994), using two different hydrocarbon fuels: methane (CH_4) and propane (C_3H_8). The results of this study show that detonation is a much more energetic process than deflagration, and the exergy analysis makes clear that this device is efficient for power generation.*

keywords: *pulse detonation, exergy analysis, power generation*

1. Introduction

1.1. Deflagration

Deflagration is the most common type of combustion. It is a subsonic combustion process, and the reaction propagates at relatively low speed. The propagation of a deflagration consists in diffusion of unburned gases ahead of the flame and burned gases behind the flame. Deflagration produces small decreases in pressure and can be modeled as a constant pressure process.

1.2. Detonation

Detonation is a supersonic combustion wave. Detonation is a much more energetic process than deflagration and produces large overpressures. A detonation wave compresses a fluid, increasing its pressure, density and temperature. Detonation can be approximated by a constant volume combustion process. A simple planar model for the supersonic detonation shock waves used is the Chapmam Jouguet (C-J) model.

1.3. Pulse Detonation Engines - PDE

Recent efforts on controlling detonation for aerospace propulsion arise from the potential for an increase in performance, and simplicity, compared to deflagrative modes (Kailasanath, 2003). That is because, in principle, detonations are an extremely efficient means of combusting a fuel-oxidizer mixture and releasing its chemical energy content. Research in PDE embraces the development of the basic theory and design concepts (Meyers et al., 2003), as experimental tests in PDE's, the investigation of detonation initiation (Kailasanath and Patnaik, 2000) and numerical simulations applied to the dynamics of detonation processes (Eidelmann and Grossmann, 1992). The focus of some recent review is on performance estimates from various experimental, theoretical and computational studies. Such investigations make use of first law cycle efficiency analysis, gasdynamics of detonation or computational fluid dynamics analysis.

A pulse detonation engine (PDE) is usually modeled by a constant volume, Humphrey cycle (or a closely related "PDE cycle"), as opposed to a constant pressure Brayton cycle for a conventional jet engine (Heiser and Pratt, 2002; Wu et al., 2002).

An ideal Brayton cycle consists of isentropic compression, isobaric combustion, isentropic expansion and return to ambient conditions. In the other hand, Humphrey cycle consists in a constant volume combustion, followed by isentropic expansion and return to ambient conditions.

1.4. Pulse Detonation Power Device - PDPD

Power production systems, using detonation engines, utilize the same principle as the propulsion systems.

In the PDPD, shown schematically in Fig.1, air enters through a low-pressure fan from the left and is mixed with a gaseous hydrocarbon (GHC), such as propane or methane, in the detonation chamber. These GHCs are alternative fuels which are clean, readily available and combine the storage and transportation advantages of a liquid with the fuel advantages of a gas. The PDPD exploits pre-existing methane and propane infrastructure in the U.S. and other parts of the world.

The fuel-air mixture is ignited by a high-energy, high-frequency source within the detonation chamber. The combustion accelerates due to the presence of a Shchelkin spiral and propagates a detonation wave to the right. This detonation wave then enters a plenum, driving a two-stage turbine.

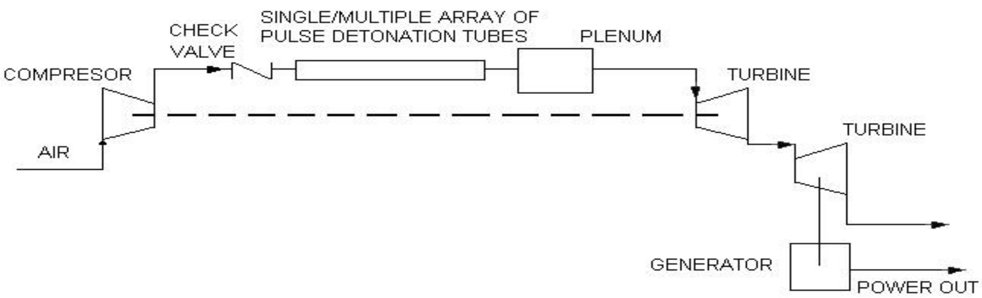

Figure 1. Pulse Detonation Power Device

2. Exergy Analysis

2.1. Conservation Equations

From the First Law of Thermodynamics, the equation for conservation of energy, for open systems, is given by Eq. (1), as follows.

$$\frac{dE}{dt} = \dot{Q} - \dot{W} + \sum_{in} \dot{m}\,(h_0) - \sum_{out} \dot{m}\,(h_0) \tag{1}$$

where $h_0 = h + \frac{u^2}{2}$ is the total enthalpy, $h = \hat{u} + pv$ is the enthalpy and $\hat{u}$ is the internal energy of the system.

For a gas obeying the ideal gas model, the specific heat at constant pressure, c_p, is written according to Eq. (2).

$$c_p(T) = \frac{dh(T)}{dT} \rightarrow dh(T) = c_p(T)dT \tag{2}$$

$$c_p(T) = c_v(T) + R \tag{3}$$

If the gas is calorically perfect, then c_p does not vary with the temperature and the enthalpy change, from state 1 to state 2, follows Eq. (4) and (6) .

$$h(T_2) - h(T_1) = c_p(T_2 - T_1) \tag{4}$$

$$c_pT_0 = c_pT + \frac{u^2}{2} \tag{5}$$

So,

$$h_0(T_{0_2}) - h_0(T_{0_1}) = c_p(T_{0_2} - T_{0_1}) \tag{6}$$

2.2. Second Law of Thermodynamics and Entropy

The second law, through the corollaries of Clausius and Kevin-Plank for a cycle, in combination with the first law stated by Eq. (1), gives Eq. (7)

$$S_2 - S_1 \geq \int_1^2 \frac{\delta Q}{T} \tag{7}$$

which shows that the increase in entropy is greater when internal irreversibilities are present than when they are not. Thus it may be said that when there are internal irreversibilities entropy is produced. The entropy generation, σ, can be defined by Eq. (8), as follows.

$$\sigma = S_2 - S_1 - \int_1^2 \frac{\delta Q}{T} \geq 0 \tag{8}$$

where, S is the entropy, σ is the entropy generation and s is specific entropy.

For open systems, Eq. (8) becomes

$$\dot{\sigma} = \frac{dS}{dt} - \sum_i \frac{\delta \dot{Q}_i}{T_i} + \sum_{out} \dot{m}s - \sum_{in} \dot{m}s \geq 0 \tag{9}$$

where, $\dot{\sigma}$ is the time rate of entropy generation.

For gases obeying the ideal gas model, the entropy change between state 1 and state 2 is given, using Eq. (2) and (3), by

$$s(T_{0_2}, p_{0_2}) - s(T_{0_1}, p_{0_1}) = \int_{T_{0_1}}^{T_{0_2}} \frac{c_p(T)}{T} dT - R \ln \left(\frac{p_{0_2}}{p_{0_1}} \right) \tag{10}$$

where R is the universal gas constant for a specific gas.

2.3. Availability and Exergy Analysis

Exergy or availability is defined as the work that is available in a gas, fluid or mass as a result of its nonequilibrium condition relative to some reference condition. Considering the *dead state* as the sea level, at atmospheric condition, useful work can be obtained from a gas that is not in these conditions.

The exergy method of analysis is a technique of using the second law of thermodynamics in actual system analysis. It states that work can be performed only under conditions that are not in equilibrium with the surrounding environment. Work is performed as the state of conditions returns to equilibrium with the surroundings, as all matter will eventually do. The exergy method is concerned with how well the available work that is generated from the energy resources is used. The exergy method makes extensive use of entropy.

With reference to an open system the first and second law are given as in Eq. (11) and Eq. (12).

$$\frac{dE}{dt} = \sum_i \dot{Q}_i - \dot{W} + \sum_{in} \dot{m}h_0^\circ - \sum_{out} \dot{m}h_0^\circ \tag{11}$$

$$\dot{\sigma} = \frac{dS}{dt} - \sum_i \frac{\dot{Q}_i}{T_i} + \sum_{out} \dot{m}s - \sum_{in} \dot{m}s \geq 0 \tag{12}$$

where h_0° is the total enthalpy at a reference state.

For the purpose of maximizing the work, only the heat interaction with the surroundings, $\dot{Q}_o$, is changed. Then, eliminating $\dot{Q}_o$ between Eq. (11) and Eq. (12), the work transfer rate $\dot{W}$ depends explicitly on the degree of thermodynamic irreversibility of the system $\dot{\sigma}$,

$$\dot{W} = -\frac{d}{dt}(E - T_0 S) + \sum_i \left(1 - \frac{T_0}{T_i}\right) \dot{Q}_i + \sum_{in} \dot{m}(h - T_0 s) - \sum_{out} \dot{m}(h - T_0 s) - T_0 \dot{\sigma} \tag{13}$$

Moreover, considering the second law Eq. (12), the entropy generation rate ought to be non-negative, and so the upper limit for $\dot{W}$ when a system operates reversibly is given by Eq. (14) below.

$$\dot{W}_{rev} = -\frac{d}{dt}(E - T_0 S) + \sum_i \left(1 - \frac{T_0}{T_i}\right) \dot{Q}_i + \sum_{in} \dot{m}(h - T_0 s) - \sum_{out} \dot{m}(h - T_0 s) \tag{14}$$

Summarizing

$$\dot{W}_{rev} - \dot{W} = T_0 \dot{\sigma} \geq 0 \tag{15}$$

Equation (15) is called the lost available work, which is the work destroyed whenever a system operates irreversibly. If the system experiences a change in volume while being resisted or assisted by the atmospheric pressure reservoir the available work reduces to

$$\dot{E}_W = \dot{W} - P_0 \frac{dV}{dt} \tag{16}$$

For steady-flow processes Eq. (14) becomes

$$\dot{W}_{rev} = \sum_i \left(\dot{E}_Q\right)_i + \sum_{in} (\dot{m}b) - \sum_{out} (\dot{m}b) - T_0 \dot{\sigma} \tag{17}$$

where

$$b = h - T_0 s \tag{18}$$

is the flow availability measured at each port.

Hence,

$$\dot{E}_W = \sum_i \left(\dot{E}_Q\right)_i + \sum_{in} \dot{m} e_x - \sum_{out} \dot{m} e_x - T_0 \dot{\sigma} \tag{19}$$

and the new property e_x is the flow exergy given by Eq. (20).

$$e_x = b - b_0 = h - h_0 - T_0 (s - s_0) \tag{20}$$

2.4. Second Law Efficiency

Many of the expressions used to gauge the performance of devices and processes are based on energy. But the measurements of performance that take into account limitations imposed by the second law are also useful. The latter is called the *second law efficiency*.

$$\begin{aligned} \eta &= \frac{\text{Energy out in product}}{\text{Energy in}} \\ &= 1 - \left(\frac{\text{Loss}}{\text{Input}}\right) \end{aligned} \tag{21}$$

$$\begin{aligned} \varepsilon &= \frac{\text{Availability out in product}}{\text{Availability in}} \\ &= 1 - \left(\frac{\text{Loss + destruction}}{\text{Input}}\right) \end{aligned} \tag{22}$$

The large number of expressions for the second law efficiencies has the objective of indicating how effectively availability is used. For the case where power production is the purpose of the system, the second law efficiency is more suitable in the form of Eq. (23).

$$\varepsilon = \frac{\dot{W}}{(\text{Fuel flow rate})\bar{\xi}_{ch}} \tag{23}$$

where, $\bar{\xi}_{ch}$ is the fuel chemical availability in molar bases.

3. Pulse Detonation Theory

Considering the processes that occur behind the incident detonation wave when it reaches the open end of the tube, one can have an understanding of the gas dynamics in one cycle of a pulse detonation. The flow behind the detonation is a subsonic flow which can be assumed to be at a Mach number approximately 0.8 for gaseous hydrocarbon fuels. When the detonation wave reaches the open end of the tube, a reflected wave propagates back into the tube. This reflection wave can be either a shock or an expansion wave. For the detonation case with hydrocarbon fuel in a stoichiometric mixture, the reflected wave is an expansion. So, the detonation shock wave propagates inside the tube followed by the Taylor expansion wave.

A detonation propagates at a very large velocity, and produces very high pressures. The leading part of a detonation front is a strong shock wave propagating into the unburned gas mixture. This shock heats the gas mixture to a very high temperature by compressing it. Chemical reactions are triggered by the shock heating, and proceed violently. The energy from the chemical reactions supports the traveling shock wave in turn, and a balance is attained to form a self-sustaining detonation wave. This stable end state for self-sustaining detonation waves is the *Chapman-Jouguet* (C-J) condition for detonation. Due to the high speed, detonation closely approximates a constant volume process (Bussing and Pappas, 1994; Bussing and Pappas, 1996).

The pressure increase across the leading shock of the detonation wave can be expressed from Eq. (24).

$$\frac{p_s}{p_1} = 1 + \frac{2\gamma_1}{\gamma_1 + 1}\left({M_1}^2 - 1\right) \tag{24}$$

Where, γ_1 is the specific heat of the unburned gases and M_1 is the Mach number of the detonation wave relative to the unburned gas.

Across the *C-J* detonation wave, Eq. (25) and Eq. (26) express the pressure and temperature relations.

$$\frac{p_2}{p_1} = \frac{1 + \gamma_1 {M_1}^2}{1 + \gamma_2} \tag{25}$$

$$\frac{T_2}{T_1} = \frac{m_2}{m_1}\frac{\gamma_2}{\gamma_1}\frac{1}{{M_1}^2}\left(\frac{1 + \gamma_1 {M_1}^2}{1 + \gamma_2}\right)^2 \tag{26}$$

An important parameter is the Mach number of the burned gas relative to the walls of the detonation chamber, as follows.

$$M_{2C} = (M_0 + M_1)\sqrt{\frac{m_2}{m_1}\frac{\gamma_1}{\gamma_2}\frac{T_1}{T_2}} - 1 \tag{27}$$

Where,

M_{2C} is the Mach number of burned gas with respect to the detonation chamber wall,
M_0 is the Mach number of unburned gas with respect to the detonation chamber wall and
M_1 is the Mach number of detonation wave with respect to the unburned gas.

4. Results and Discussion

This present work develops an exergetic preliminary analysis to quantify the performance of a power production device that has pulse detonation as a combustion mode. Such device utilizes a stoichiometric mixture of hydrocarbon fuels such as methane (CH_4) and propane (C_3H_8) with air. The fuel-air mixture is supplied at high pressure to the combustion chamber (3.0×10^5 Pa). Research was made to guarantee that the fuel were in gaseous phase for the temperature and pressure specified.

The losses caused by the processes occurred before the combustion can be neglected, such conclusion was made after calculations for the compressor and valve losses. The results obtained provide the work necessary to run the compressor which is driven by the first stage of the turbine.

All calculations make use of ideal gas approximations and isentropic relations. The losses are introduced by the isentropic efficiencies for the turbine.

For comparison, two combustion modes are object of this study: detonation and deflagration. Data for combustion are obtained from *C.E.A.* code (McBride and Gordon, 1994), which gives the exit state properties, as well as the data for the burned gas mixture.

For detonation, *C.E.A.* code (McBride and Gordon, 1994) gives the C-J properties. So, due to the unsteadiness of the detonation process and to the decay of pressure (Bussing et al., 1997), temperature and density (Kim, 2000) during a detonation cycle, an average approximation for the related properties was adopted. Inside the detonation tube, the detonation wave propagates at C-J velocity followed by Taylor expansion waves. The average thermodynamic properties, are then related to those waves and its interaction with the reflected waves.

The detonation tube is taken as 1.0 meter and the frequency of detonation is 100 Hertz, so that the period of the detonation cycle is 0.01 seconds, not including the fuelling time, only the time after ignition (Wintenberger et al., 2001), even though, the fuelling time is an important parameter for future design optimization.

Applying the analytical model given in previous reference work (Wintenberger et al., 2001), an equivalent pressure multiplied by its related equivalent time can be time averaged, using the period of a detonation cycle. The equivalent pressure can be calculate using isentropic relations across the Taylor expansion waves. Because the density behavior is similar to the pressure (Kim, 2000), the same approach is used. The equivalent density is computed across Taylor expansion waves, and the time average is taken over the period. As the temperature during the cycle does not drop significantly alike the pressure, the procedure for the average temperature is slightly distinct. Average temperature is taken as 80% of the temperature across the Taylor waves.

The velocity at the tube exit can be specified assuming that the Mach number at the exit is 0.4, and assuming that the sonic velocity is the velocity for the average properties.

The total or stagnation properties can, then, be calculated.

The first stage of the turbine drives the compressor. Losses are introduced by assuming the turbine isentropic efficiency as being 85%.

The exit area of each stage of the turbine is presupposed to be three time the inlet area. And the velocity drop in the second stage of the turbine is taken as being 50%.

The pressure condition at the turbine outlet is the ambient pressure. The work developed by the second stage is the output power available for power generation. The fuel availabilities are given by the *C.E.A.* code (McBride and Gordon, 1994) as being 74599.999 kJ/kg-mol for methane (CH_4) and 104680.000 kJ/kg-mol for propane (C_3H_8).

For deflagration mode, constant pressure combustion was used in *C.E.A.* code. The velocities, for this case are very small, therefore kinetic energy can be neglected. The same approach described before is used here, although making use of static properties and classical thermodynamics relations.

The results shown on Tab. (1) and Tab. (3) for methane and Tab. (2) and Tab. (4) for propane are obtained for an isentropic efficiency for the turbine of $\eta_t = 85\%$ and flow rate $Q = 1.0\ m^3$/sec.

Table 1. Methane CH_4 - Detonation

Point	C-J	After Combustion - Average	After 1^{st} stage	After 2^{nd} stage
T (K)	2838.87	1960.17	1953.13	1627.04
P (Pa)	5231100	451129	429845	100000
h (kJ/kg)	0.883×10^6	4.847×10^6	4.830×10^6	4.024×10^6
T_0 (K)	-	1987.97	1956.33	1627.85
P_0 (Pa)	-	492659	434548	100784
h_0 (kJ/kg)	-	4.916×10^6	4.838×10^6	4.026×10^6

Table 2. Propane C_3H_8 - Detonation

Point	C-J	After Combustion - Average	After 1^{st} stage	After 2^{nd} stage
T (K)	2885.93	1995.76	1989.05	1648.24
P (Pa)	5561300	479630	458555	100000
h (kJ/kg)	0.996×10^6	5.002×10^6	4.985×10^6	4.131×10^6
T_0 (K)	-	2023.60	1992.38	1649.07
P_0 (Pa)	-	524623	463744	100865
h_0 (kJ/kg)	-	5.072×10^6	4.993×10^6	4.133×10^6

Table 3. Methane CH_4 - Deflagration

Point	After Combustion	After 1^{st} stage	After 2^{nd} stage
T (K)	2247.60	2208.89	1931.11
P (bar)	300000	264872	100000
h (kJ/kg)	4.54×10^6	4.46×10^6	3.90×10^6

Table 4. Propane C_3H_8 - Deflagration

Point	After Combustion	After 1^{st} stage	After 2^{nd} stage
T (K)	2292.29	2254.68	1978.51
P (bar)	300000	265469	100000
h (kJ/kg)	4.77×10^6	4.69×10^6	4.12×10^6

Table (5) introduces the results for the power developed for each one of the cases studied.

Table 5. Power Developed (MJ/sec)

	CH_4	C_3H_8
deflagration	1.35	1.38
detonation	1.95	2.06

Finally, Tab. (6) represents the second law efficiencies obtained by this analysis.

Table 6. Second law efficiency

	CH_4	C_3H_8
deflagration	27.5%	55.0%
detonation	38.3%	79.1%

5. Conclusion

The present work is a preliminarily study of a pulse detonation power device, and its purpose is to establish that detonation is a more efficient combustion mode as well to address the critical points that should be taken into account in a future design and optimization project.

The exergy analysis in this work helps to determine which parameters might be of interest when realizing a design optimization of the pulse detonation power device.

Because the scope of this study is to analyze the system performance and not to develop a model for pulse detonation, many assumptions were made.

All calculations used ideal gas model and isentropic relations, as mentioned before. Were only considered losses due to the turbine operation.

Assumptions for the average thermodynamic properties used the model developed in Wintenberger et al., 2001. The latter model describes the behavior of pressure only, the density behavior was assumed similar to the pressure, and the average temperature was only based on the same model considering that the temperature drop is less than the one for pressure and density. In this model the fuelling time was not considered although this might be an important factor in design.

The results provided by this work show that pulse detonation is a efficient combustion mode for power production. The second law efficiency, ε, also makes clear that, for the same purpose, pulse detonation is much more efficient than deflagration. For methane, the second law efficiency is $\varepsilon = 38.3\%$ for detonation and $\varepsilon = 27.5\%$ for deflagration. And for propane, $\varepsilon = 79.1\%$ for detonation and $\varepsilon = 55.0\%$ for deflagration.

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