

# Considerations and simulations about Pulse Detonation Engine

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**Abstract.** PDE propulsion can work from a subsonic regime to hypersonic regimes; this type of engine can have higher thermodynamic efficiency compared to other turbojet or turbofan engines due to the removal of rotating construction elements (compressors and turbines) that can reduce the mass and total cost of propulsion system. The PDE experimental researches focused on both the geometric configuration and the thermo-gas-dynamic flow aspects to prevent uncontrolled self-ignition. This article presents a series of numerical simulations on the functioning of PDE with hydrogen at supersonic regimens.

## Acronyms and symbols

PDE	pulse detonation engine
AB PDE	after burner pulse detonation engine
DDT	deflagration-to-detonation transition
PDRE	pulse detonation rocket engine
ZDN	Zel'dovich-von Neumann-Doering
$M_x, M_y$	Mach numbers
$p$	pressure
$v$	volume
$T$	temperature
$\rho$	density
$u_1, u_2$	velocity
$h_1, h_2$	enthalpy
$s_1, s_2$ (S)	entropy
$V_o, V_\infty$	speed

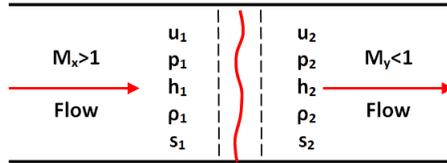
## 1 INTRODUCTION

Detonation is an effective means of burning a fuel mixture and transforming chemical energy into mechanical energy. However, this concept of running the propulsion systems involves difficulties both in rapidly achieving the fuel mixture at high speeds and in initiating and sustaining detonation in a controlled manner.

PDE differs from conventional propulsion systems in two main aspects: it generates an intermittent pulse and produces high pressure increase in the combustion chamber, which also represents a major advantage of a PDE, see Figure 1.

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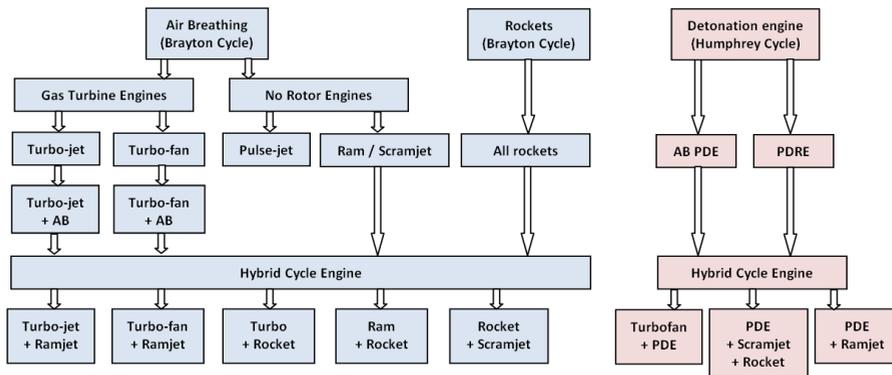


**Fig. 1.** Detonation concept, [3]

This paper will present some benchmarks on the experimental and theoretical research status of PDE. Then there is presented a numerical analysis regarding the functioning of PDE at supersonic speeds having hydrogen as working fluid, analyzes that want a continuation of a previous work where numerical simulations have been performed with methane working fluid, [10].

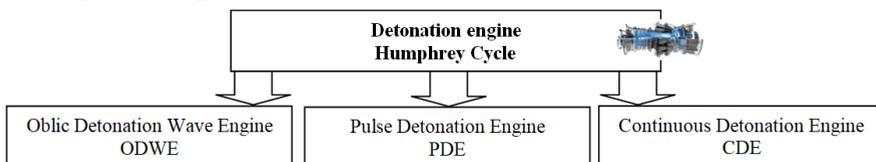
In present known from the analysis of the thermodynamic cycle that a motor based on a constant volume combustion process has a higher thermodynamic efficiency than a constant pressure motor. According to the references, the first work on intermittent detonation is attributed to Hoffman in 1940, based on a mixture of acetylene fuel and benzene, [1-2]. The PDE is one of propulsion systems based on a rapid detonation wave that transforms chemical energy into mechanical energy and generates greater kinetic energy [3-5] compared to deflagration [6] in the context of a repeated detonation firing with unstable increases in pressure and temperature [7-8].

The issues regarding the current stage of the PDE are well documented and structured by Kailasanath in [9], for a positioning of the PDE within the aerospace proposition systems; we highlight a classification in the diagram in Figure 2.



**Fig. 2.** Aerospace propulsion chart, [11]

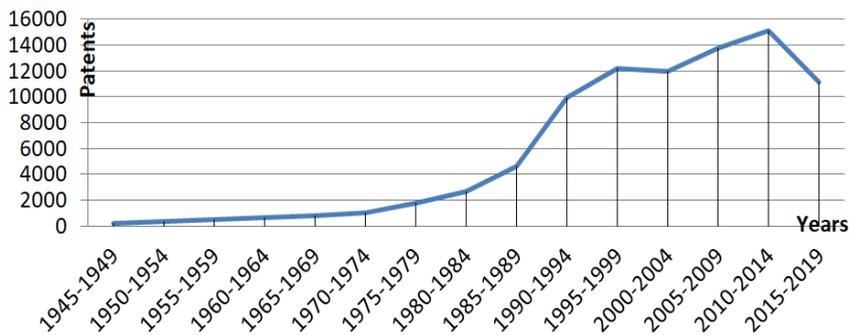
Musielak [11] divides PDE (Humphrey cycle) into three major categories in terms of detonation type, see Figure 3.



**Fig. 3.** PDE classification, [11]

A series of theoretical and practical research on PDE on both design (constructive) and optimization of combustion processes (methods of operation and combustion) have been completed with patented innovations and inventions, a search for inventions published on Google Patents has revealed over 56,000 results, of which more than 37,000 have been submitted since 2000, just over 11,000 have been filed over the past five years, and just over 1,000 patents are for 2018.

A global evolution of patent applications in the PDE field can be seen in Figure 4, [12]. Particular attention is drawn to concerns about the development of the PDE over the period 1985-1995. Theoretical references and numerical simulation will be discussed in the following sections.



**Fig. 4.** Invention patents in 1945-2019

CFD simulations of complex three-dimensional thermo-gas-dynamic processes on PDE operation require global approaches simplified or regional with a high degree of refinement of initial conditions. The challenges of simulating the deflagration-detonation transition (DDT) involve complex turbulence models that often require geometric simplifications or operation (heat transfer, time) to understand how PDE geometry interacts with shock waves and flame structures.

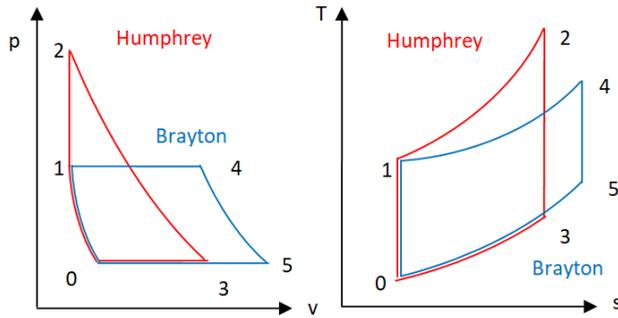
## 2 THEORETICAL ASPECTS

### 2.1 Comparison between deflagration and detonation. Running cycles

The most important aspect is the value of process speed, detonation is a supersonic burning process and deflagration is subsonic. In combustion engines the energy is released by deflagration, the detonation engines use a shock wave that compresses the fuel mixture followed by a sudden increase of pressure together with a rapid release of heat, see Figure 5.

In a conventional Brayton cycle, the heat injection process has a maximum exergy, which depends directly on the pressure supplied by the compressor and the maximum thermodynamic cycle allowance, so the exergy can be increased if the heat injection process follows another path cyclic thermodynamics, [3, 13].

The ideal PDE thermodynamic cycle is similar to the ideal Brayton cycle, while the Humphrey cycle is considered a change in the Brayton cycle where the constant pressure heat-adding process is replaced by a constant volume heat-adding process [14].



**Fig. 5.** Brayton cycle and Humphrey cycle (p-v, T-S)

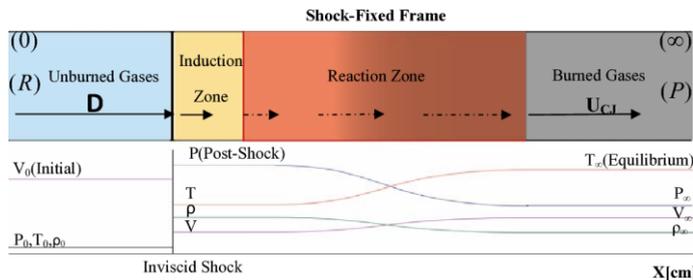
The Humphrey cycle (see Figure 5) is much more effective than the Brayton cycle, where there is a very rapid firing, there is not enough time to balance the pressure, and the whole process is a thermodynamic process to close the gas oxidation process, while the continuous pressure process is unstable of conventional propulsion systems [15]. Generally, the Humphrey cycle consists of four processes: the first is an isentropic compression, taking place before the detonation wave in PDE; the second process is the compression followed by the burning of the constant volume followed by the isentropic process of decomposition of the combustion products at atmospheric pressure and finally the exhaust of the burnt gas.

### 2.2 Principle and stages of operation

According to Chapman-Jouguet theory, the detonation wave consists of a shock wave and an initiation flame, the gas is compressed due to the passage of the waveform leading to a rapid chemical reaction that ends at the end of the shock wave boundary.

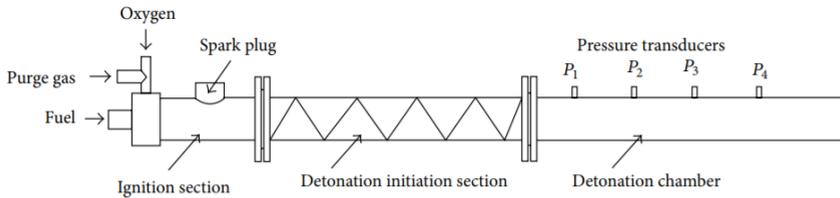
The Zel'dovich-von Neumann-Doering (ZND) theory uses the concept of finite-rate chemical reaction, according to which the detonation wave comprises two fundamental processes: a compression process given a shock wave followed by a deflagration process an induction and reaction front, these being separated by an induction zone, although in reality the detonation wave is not a shock wave 2D but is composed of small cellular shock waves.

According to conventional boundary layer approaches [25-26] and PDE papers [14, 17, 23-24] detonation is modelled as a Zel'dovich-von Neumann-Doering (ZND) normal wavelength, in the fuel-air mixture of a uniform tube, which is almost at rest for combustion inlet conditions, see Figure 6.



**Fig. 6.** Diagram for Zel'dovich-von Neumann-Doering detonation, [17]

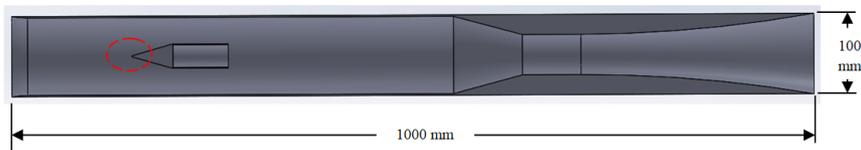
Due to the difficulty of initiating air-fuel mixtures in short tubes and obtaining a constant detonation firing, methods involving deflagrative combustion processes leading to detonation reactions by the placement of optimized obstacles to create turbulent mixtures and to accelerate the gas flow (DDT), as an example, we describe the Shchelkin spiral coil, perforated plates or convergent-divergent jaws, see Figure 7, [18, 19, 20, 21, 22].



**Fig. 7.** Shchelkin spiral, [21]

### 3 NUMERICAL SIMULATION ON PDE PERFORMANCE

Numerical simulations have focused on the study of the dynamics of the intake (axis-symmetrical flow) with a fine grid in the slope of the flow. As a first attempt, the approach was to use a numerical simulation applied to a single tube, single phase and single cycle, see Figure 8, [10].



**Fig. 8.** PDE geometry [10]

#### 3.1 Geometry and analysis conditions

Numerical simulations were tried at Mach 5 and Mach 6, the results being compromised by burning across the entire intake channel, total firing corresponding to the 15° value, which determines a larger angle of impact wave with implications for upstream self-ignition. As in the previous article [10], the initial analysis data is those in Table 1.

**Table 1.** Analysis conditions

Parameters	Values	Parameters	Values
Altitude	10000 m	Fluid	H <sub>2</sub> and air
Admission pressure	26436 Pa	Admission speed	7 Mach
Admission temp.	223.16 K	Cells number/type	quadrilaterals / 33696
Wall type	adiabatic	Ramp angle	15°

For CFD 2D flow analysis, Ansys Fluent 18 [16] and simple geometry of the PDE propulsion system were used with the initial conditions in Table 1 for stoichiometric firing. For stoichiometric burning ( $\lambda=1$ ), see equation 1, on input or imposed following chemical

compositions (molar):  $H_2=0.2958$ ,  $O_2=0.1479$ ,  $N_2=0.5563$ . The quadrilateral cell mesh grid is highlighted in Figure 9.



### 3.2 CFD 2D analysis

CFD analysis presents the results of a stationary, non-heat transfer case using  $H_2$  as working fluid, see the following graphs.

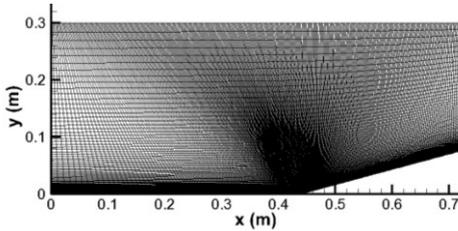


Fig. 9. Mesh 2D domain

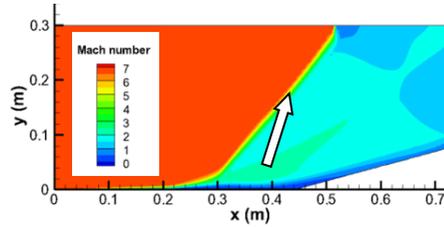


Fig. 10. Mach number, Tecplot

Figure 10 shows the variation of the Mach number, the working fluid braking being placed upstream after a steep slope. Figure 11 shows the distribution of the molar fraction  $H_2$  by the distance to the wall  $y(m)$ .

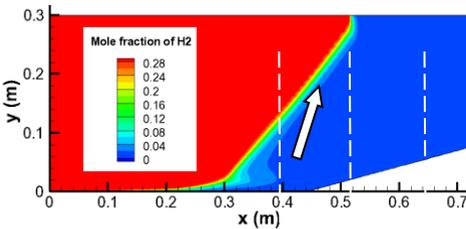


Fig. 11. Molar fraction  $H_2$ , Tecplot

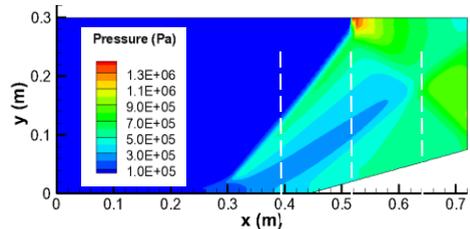


Fig. 12. Pressure, Tecplot

Figure 12 shows the variation of the pressure gradient at  $x=0,45 \div 0,5$  m and in Figure 13 we have a sudden change in temperature after the oblique shock wave with a maximum in the slope area due to the friction effect.

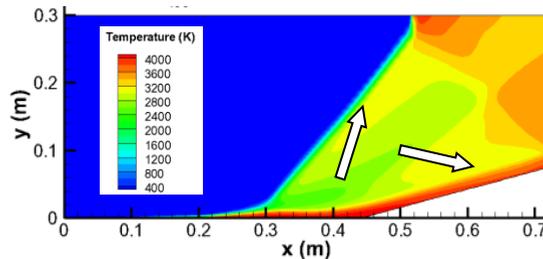
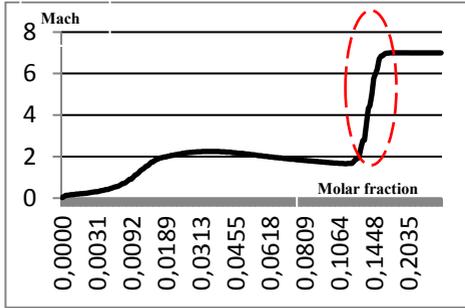


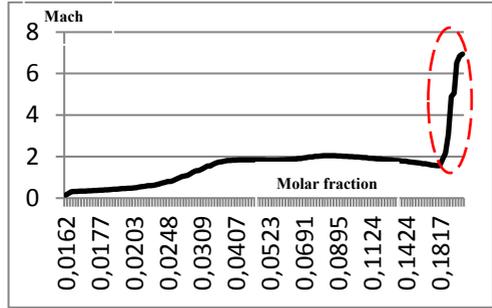
Fig. 13. Temperature, Tecplot

### 3.3 Results analysis

To better understand the 2D behaviour of the mixture, we extracted the values of the Mach number and the molar fraction to the corresponding vertical  $x=0,40$  m and  $x=0,50$  m.

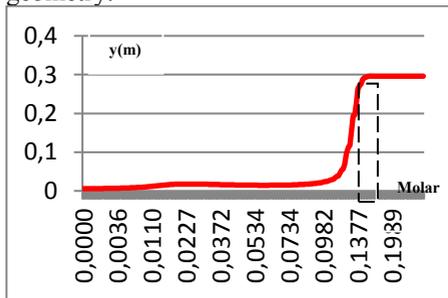


**Fig. 14.** Mach number at  $x=0,4$ m

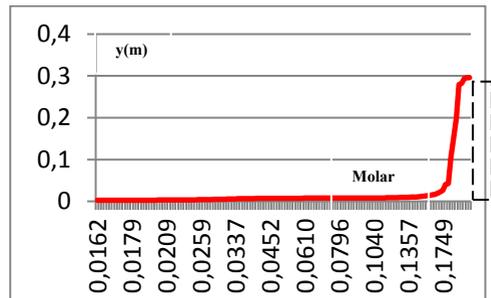


**Fig.15.** Mach number at  $x=0,5$ m

In Figure 14 and Figure 15, both a different kinetic behaviour of the mixture before the slope inflection and a Mach number jump at an ordinate value that reveals the slope of the shock wave are observed. In Figures 16 and 17 we compare, the variation of the variation of the molar fraction  $H_2$  on the minimum slope interval is associated with the shock wave geometry.

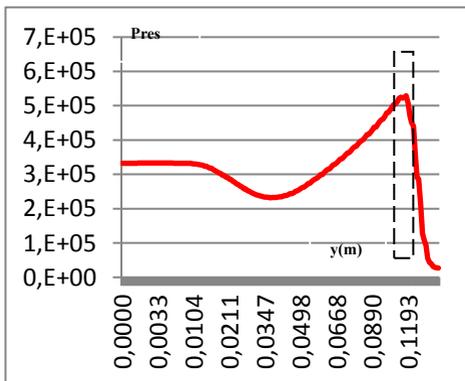


**Fig. 16.** Molar fraction  $H_2$  at  $x=0,4$ m

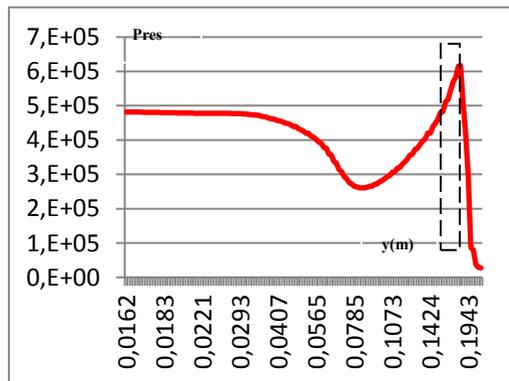


**Fig.17.** Molar fraction  $H_2$  at  $x=0,5$ m

In Figures 18 and 19, static pressure differences are observed at the ordinate values of 0.4m and 0.5m.



**Fig. 18.** Pressure at  $x=0,4$ m



**Fig.19.** Pressure at  $x=0,5$ m

It can be seen in Figures 18 and 19 the correlation of the pressure inflection value with the sudden variation of the molar fraction (figures 16 and 17). According to the numerical data the maximum value of the pressure is  $p=5.29 \times 10^5 \text{ Pa}$  at  $y = 0.11 \text{ m}$  for  $x = 0.4$  and  $1.6$  Mach; and  $p=8.66 \times 10^4$  at  $y=0.20 \text{ m}$  and  $4.8$  Mach for  $x=0.5 \text{ m}$ , decreasing value due to the friction effect.

## 4 CONCLUSIONS

One of the factors that affect the practical implementation of PDE motors is the difficulty of obtaining successive and consistent detonations within the combustion chamber.

Simulation and modelling of detonation processes are essential for understanding the combustion phenomenon under constant heat transfer conditions and supersonic wave bursts, detonation processes requiring kinetic and thermo-chemical limit conditions with direct effects on combustion performance. Numerical simulations can address aspects of the transition of subsonic deflagration coupled with supersonic detonation by: geometric, kinetic and thermo-chemical optimization.

The numerical simulation was focused on the angle of the central body ramp ( $15^\circ$ ) at a Mach high enough to ensure detonation of the working agent (hydrogen) without taking into account the three-dimensional finite effects and thermal transfer effects.

CFD simulation (2D symmetric-axial) using fixed single-cycle geometry is sufficient to predict flow properties with a reasonable degree of confidence.

Future CFD simulations take into account both higher hypersonic speed flow approaches with comparative aspects of various work fluids ( $\text{CH}_4$ ,  $\text{H}_2$ ) and optimized geometries involving thermal transfer and friction.

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