# Numerical Modeling of Sub-Scale Convective Combustion of M1 propellant

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## **Abstract**

A numerical methodology capable of modeling HD 1.3 gun propellant combustion has been developed. The model is based on observations of several tests conducted by NAWCWD which included ignition of propellant pellets packed into cylindrical polycarbonate tubes. The systematic sequence of tests clearly indicated the significant role pellet gasification plays in the accidental ignition of propellants. To enable such modeling new algorithms to evaluate heat transfer from the igniter combustion products to the gun propellant, pellet gasification, propellant pyrolysis and combustion of the generated gasses and the propellant were implemented. Development and validation of these models has been guided by the experimental NAWCWD data.

#### Introduction

The Department of Defense Explosive Safety Board (DDESB) recently began revising the siting methodologies for energetic ordnance other than Hazard Division (HD) 1.1. An investigation indicated that improvements of the predictive modeling of HD 1.3 gun propellant (M1) combustion placed in a confined storage configuration is necessary.

Funded by DDESB, the Naval Air Warfare Center Weapons Division (NAWCWD) has been conducting a series of experiments of bulk HD 1.3 gun propellant combustion within a confined polycarbonate tube in order to gather insight into the transient combustion behavior of a lightly confined porous bed of HD 1.3 gun propellant.

To date, NAWCWD has conducted 3 calibration tests and 6 propellant combustion tests. The calibration tests checked the igniter performance without the propellant bed. Figure 1 shows the configuration of one of the combustion tests. A 5-3/4-inch inner diameter, 6-inch outer diameter polycarbonate cylinder of 13 inches in length was used to house the M1 propellant bed. Figure 2 shows the M1 gun propellant, which had a density of 1.569 g/cc, the outer diameter of 1.0765, the length of 0.5 cm. Each pellet had 7 perforations, each with a nominal diameter of 0.451mm. Red Dot smokeless powder was used as an igniter, filled in a steel igniter basket hanging on the top of the steel lid. Figure 3 shows the pressure history of the calibration test and propellant combustion test, termed here test#1. In both calibration and combustion tests, 20g of Red Dot was used as the igniter. The amount and height of the M1 propellant in test #1 was 7lb and 8.38

inch respectively. The pressure gauges were located on the top and the bottom of the test tube. Significant time delay on the pressure rise was observed in test#1. Figure 4 shows snapshots of flame propagation in test#1. The flame did not reach the lower part of the pellet bed before the case failure.

The objective of this study is to investigate and understand the physical mechanisms controlling pellet ignition, as observed in the NAWCWD experiments, and develop the numerical tools to accurately model these, with the final objective of developing a numerical methodology capable of modeling accidental ignition and combustion of stored gun propellant.

## **Numerical Results**

There have been many studies of gun propellant combustion under high pressure [1-6]. In contrast, very few investigated combustion under ambient conditions. Correspondingly, the burning rate of Red Dot was determined based on the engineering tool book [7] and then modified based on the calibration test result.

Figure 5 shows the numerical configuration of the model. To save computational time, a scaled diameter of the test tube was modeled, where the tube and igniter conditions were the same as in the experiment. The original M1 pellet shape is cylindrical with 7 perforations as shown in Fig. 2, however, the modeled pellet is star shaped with the exact same surface area as the pellet, to avoid the difficulty of numerically modeling the 0.45 mm perforation in the computational domain. Proper resolution of such a cavity will enforce a very small computational integration time step and unattainable computational resource requirements.

The first step in the validation process modeled the calibration test. The simulation modeled the tube without the M1 propellant bed, as shown in Fig. 5a. The burning surface (heat releasing surface) was defined on the top of the tube. Figure 6 shows a comparison of experimental and numerically predicted pressure time histories at the chamber top. The pressure histories agreed well until the pressure reached 400 psi. In the experiments, the polycarbonate cylinder failed when the pressure reached 400-450 psi. Hence any data after that time cannot be used for analysis.

The experiment data demonstrated a 50-60ms time gap between the pressure rise of the empty tube (the calibration test) and the M1 propellant bed test (test #1), as shown Fig. 3. Since the pressure did not start increasing immediately (as occurred in the empty tube), it indicates that a considerable amount of energy from the igniter was absorbed by the propellant bed. After detailed study of experimental video and previous analysis and research [8-10], we concluded that the heat transfer between the hot gas products and heating, non-burning propellant pellets was not enough to absorb such energy at such short time, meaning advection of the gasses and heat conduction within the pellets cannot account for such a high rate of energy absorption. Gasification under high temperature, on the other hand, is a process that can absorb rapidly significant amounts of energy [10]. Thus, accurate modeling of propellant ignition required not

only modeling the heat transfer between the gas and pellets, but also the nitrocellulose gasification and later, reaction modeling of the gasses. Reference 10 provided the reaction rate of M10 gun propellant, which is a single-base propellant and has a similar character to M1 propellant. Based on the data in ref. 10, a pellet gasification model was developed. Modeling of the gaseous combustion at later time is based on the induced model, which is a simple and robust one equation model [11]. Table 1 shows the coefficients for pyrolysis and regression [7, 10]. Flammability limit of nitrocellulose is between 1.9-48% [12], hence, the model allows the gasified material to burn when the mass reached the lower limit.

The implementation of the numerical model is follows:

- -Check the surface faces
- -If proper material/pyrolysis possible
  - -Compute temperature and pressure
  - -Compute reaction/pyrolysis rate
  - -Compute regression velocity
  - -Multiply by time-step: amount of mass pyrolysized
  - -Obtain energy required for pyrolysis
  - -Add mass pyrolysized to gas density
  - -Subtract energy required from flow energy

Figure 7 shows the gas density, velocity, temperature, pressure, and mass fraction of gasified propellant. The hot gas was released from the top of the computational domain at a temperature of about 3200K. The pressure was low, about 2atm, even at late time, as energy is absorbed by the pellet pyrolysis. Temperature rise and gasification of lower-placed material (far from ignition point) were also slow due to the same reason. The low pressure agrees nicely with the experiment as shown in Fig. 3, demonstrating that we have captured the essential physical processes.

## **Conclusions**

A numerical methodology capable of modeling HD 1.3 gun propellant combustion has been developed. The model is based on observations of several tests conducted by NAWCWD which included ignition of propellant pellets packed into cylindrical polycarbonate tubes. The systematic sequence of tests clearly indicated the significant role pellet gasification plays in the accidental ignition of propellants. To enable such modeling new algorithms were implemented to account for heat transfer from the igniter combustion products to the gun propellant, pellet

gasification, propellant pyrolysis and combustion of the generated gasses and the propellant. Development and validation of these models has been guided by the experimental NAWCWD data. Numerical simulations of several tests demonstrated that the model accurately predicts the Red Dot ignition under ambient conditions, and that pellet gasification under high temperature flux will absorb enough energy to prevent pressure rise in a closed chamber.

Future work will focus on modeling of the flame propagation in the tested configuration, and the modeling of ignited propellant barrels in the Kasun facility [13].



Fig. 1. Experimental setup. (6" diameter, 13" height polycarbonate tube filled with 7lb M1 gun propellant. 20g of Red Dot smokeless powder was filled in the steel basket on the steel lid).

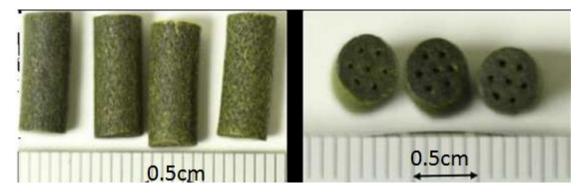


Fig. 2. M1 gun propellant, density=1.569 g/cc, Length=1.0765cm, outer diameter=0.5cm, 7 perforations, each with a nominal diameter of 0.0451 cm.

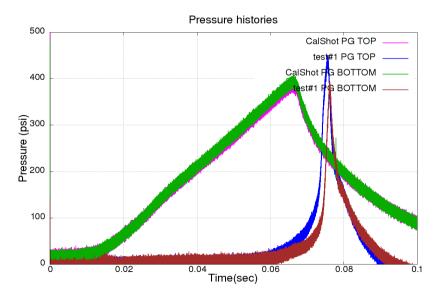


Fig.3 Pressure histories in calibration test and test #1

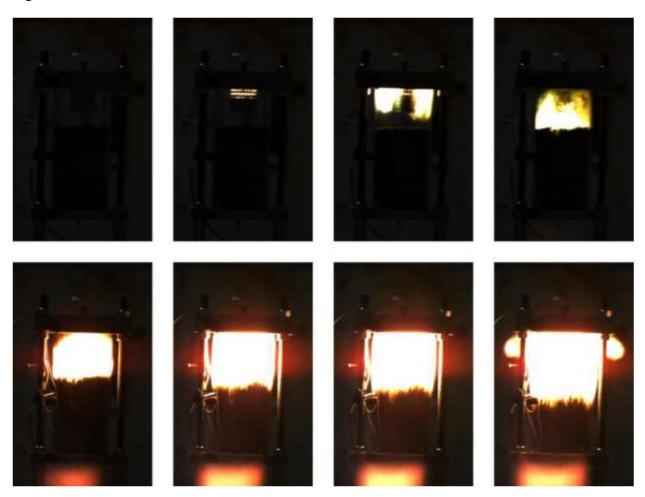


Fig. 4 Snapshots of flame propagation in the experiment



Fig. 5 Numerical configuration of (a) scaled tube and (b) modeled M1 pellet bed

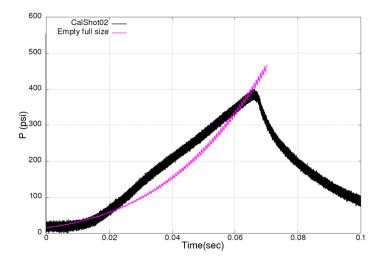
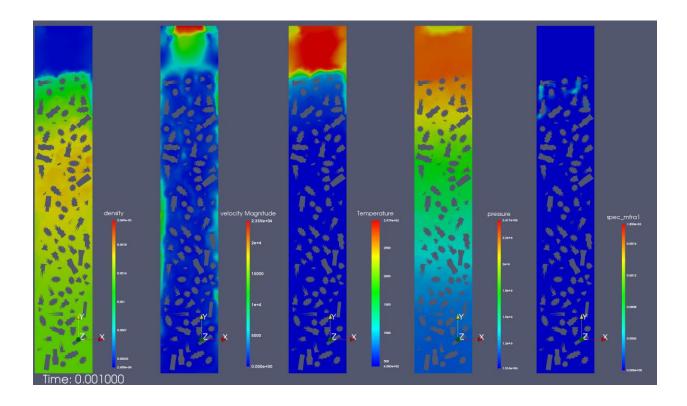
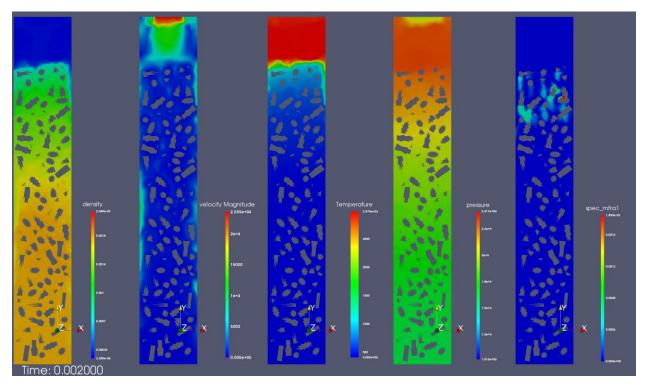


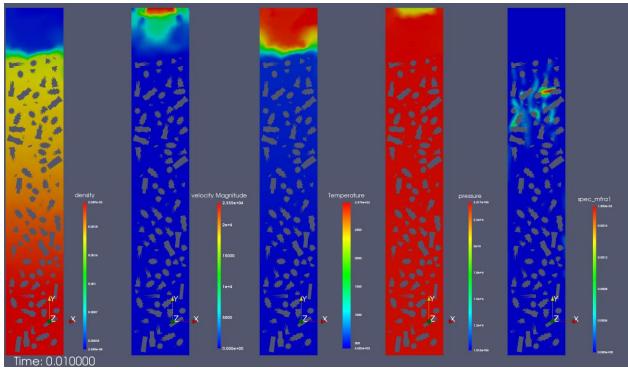
Fig. 6. Pressure history comparison between the measured and computation (The gauge on the top)

Table 1. Coefficient for pyrolysis and regression of single base propellant

Pyrolysis rate: r=Aexp(-E/RT)	A=2.72e27 [1/sec]	E=49.80 [kcal/mol]	Enthalpy H=2.23e9 [erg/g]
Regression rate: v=v0(P/P0) <sup>n</sup>	V0=0.0356 [cm/sec]	n=0.7	







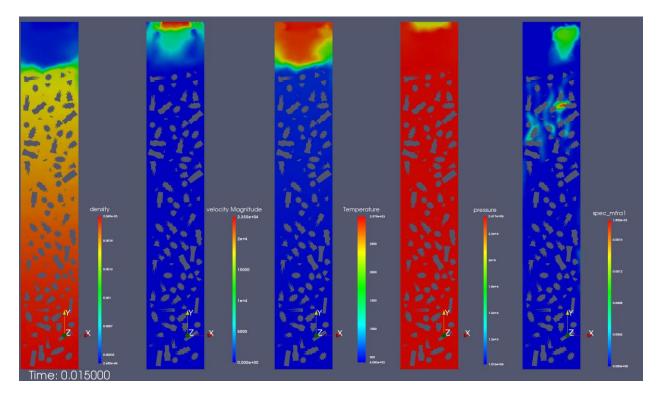


Fig. 7 Gas density, velocity, temperature, pressure, and gasified propellant distributions at 1, 2, 10, and 15 ms.

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