Modeling the Electrical Ignition of Energetic Material via Joule Heating and Chemical Reaction

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1 Introduction

The process of producing heat as a result of current flow in a conductor is known as Joule heating. The interaction between the atomic ions that make up the conductor and the flowing electrons that make up the current results in Joule heating. An electric field in an electronic circuit can accelerate charged particles, such as electrons, and cause them to move in a certain direction. However, as these particles collide with ions in the circuit, they can lose kinetic energy and the energy of the ions increases. This transfer of energy between the charged particles and ions is what gives rise to the Joule heating effect. The magnitude of the heating effect depends on the resistance of the material in the circuit, the strength of the electric field, and the flow of current. The Joule heating effect is an important aspect of many electronic and electrical systems and is widely utilized for its efficient and controlled heating capabilities. Through this procedure, ions' increased kinetic or vibrational energy manifests as heat, raising the conductor's temperature, also, by definition temperature is the measure of the average kinetic energy of the particles in motion. The first law of the Joule states that the heat produced is directly proportional to the square of the current and the product of the wire's electrical resistance. In real life, Joule heating is applied in a variety of ways for example, when the filament is heated by Joule heating, incandescent bulbs operate on the principle of emitting light due to heat radiation. An electric fuse melts when sufficient current flows and a circuit breaks. It also serves as a safety measure for numerous pieces of electric machinery. E-cigarettes work on the principle of Joule heating to vaporize propylene glycol and vegetable glycerin. In addition, a wide variety of heating appliances, including electric stoves, electric heaters, soldering irons, cartridge warmers, and kitchen appliances, utilize the Joule heating concept. However, a numerical solver that can comprehend the heat generation induced by Joule heating and the ensuing explosive reaction of reactants must be created to apply the Joule heating phenomenon to electric propulsion fields. For the Joule heating analysis and high energetic-explosive explosion analysis in this work, a proven hydrocode solver [1] capable of analyzing heat generation and explosion events was used. The solver's ability to analyze high-pressure fluids using a Level-set method, MPI processing, and accurate numerical approaches [2], while guaranteeing high accuracy and quick analysis speed, is a benefit. Based on this, this study attempts to simulate heat generation by Joule heating and detonation of Hexolite (RDX) using a validated solver.

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2 Theory and result

2.1 Verification

Verification of the Joule heating phenomenon that has not yet been verified in hydrocode was conducted by comparing it with the results of a previous study [3]. The geometric diagram in Fig. 1 is what was employed in the earlier work to interpret the Joule heating phenomena. The hydrocode domain created with this scale is depicted in Fig. 2. To run the simulation, an energy equation based on Joule heating was added to the energy source term of the Euler equation. It was confirmed that a plausible interpretation of the heating phenomena brought on by Joule heating in hydrocode was supported by the temperature distribution results for the x/L value, which are in close agreement with the experimental and numerical findings of the prior work. In Fig. 3, the verification outcomes are shown and compared.

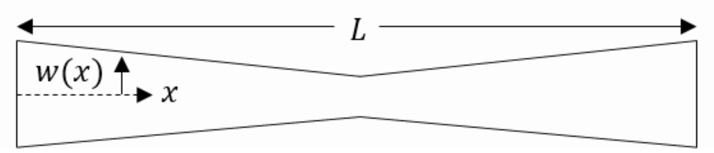

Figure 1: Geometric schematic used to interpret the Joule heating phenomenon in a previous study [3]

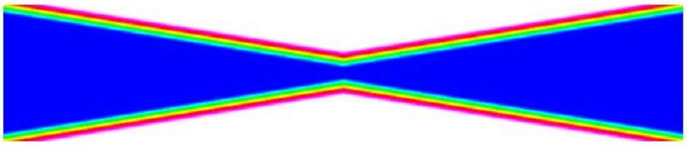

Figure 2: The domain of verification in hydrocode

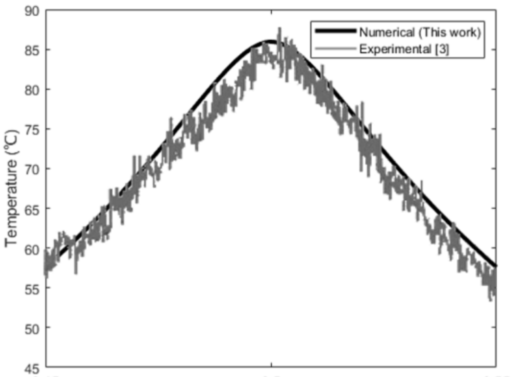

Figure 3: Verification result in this work vs previous study [3]

2.2 Problem description

The study's simulation domain is depicted in Fig. 4. x = 0.05 m and y = 0.1 m were set, and each vertical thickness of electrodes was set to 0.025 m. When a voltage of 1200 V was applied, the heat generation caused by Joule heating and the resulting explosion of high energetic-explosive were simulated. RDX is the high energetic-explosive used in this study.

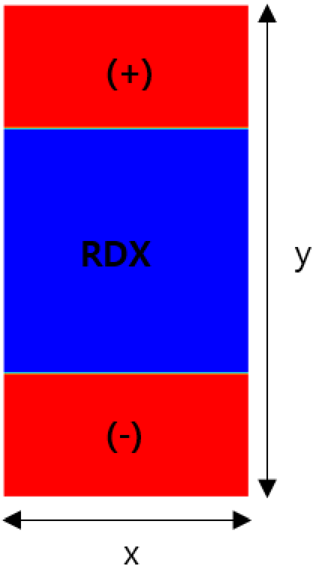

Figure 4: The domain of simulation in this study

2.3 Equations

The total combustion process is interpreted using the Euler Equation, as given in (1)[4].

$$\frac{\partial \vec{U}}{\partial t}+\frac{\partial \vec{E}}{\partial x}+\frac{\partial \vec{F}}{\partial y}=\vec{S}(\vec{U})$$

$$\vec{U}=\begin{pmatrix}\rho\\ \rho u_x\\ \rho u_y\\ \rho E\\ \rho\lambda\end{pmatrix},\vec{E}=\begin{pmatrix}\rho u_x\\ \rho u_x^2+p\\ \rho u_x u_y\\ u_x(\rho E+p)\\ \rho u_x\lambda\end{pmatrix},\vec{F}=\begin{pmatrix}\rho u_y\\ \rho u_y u_x\\ \rho u_y^2+p\\ u_y(\rho E+p)\\ \rho u_y\lambda\end{pmatrix},$$

$$\vec{S}=\begin{pmatrix}-\frac{\rho u_x}{x}\\ -\frac{\rho u_x^2}{x}\\ -\frac{\rho u_x u_y}{x}\\ -\frac{u_x(\rho E+p)}{x}+\rho Q\dot{w}\\ \rho\dot{w}\end{pmatrix} \tag{1}$$

JWL (Jones Wilkins Lee) EOS (2) is the equation of state for calculating the pressure and sound speed of RDX [4].

$$p_{explosive,unreacted}$$
$$=A\left(1-\frac{\omega}{R_1\left(\frac{\rho_0}{\rho}\right)}\right)e^{-R_1\left(\frac{\rho_0}{\rho}\right)}+B\left(1-\frac{\omega}{R_2\left(\frac{\rho_0}{\rho}\right)}\right)e^{-R_2\left(\frac{\rho_0}{\rho}\right)}+\frac{\omega e_0}{\left(\frac{\rho_0}{\rho}\right)}$$

$p_{explosive,reacted}$

$$= Ae^{-R_1\left(\frac{\rho_0}{\rho}\right)} + Be^{-R_2\left(\frac{\rho_0}{\rho}\right)} + \frac{C}{\left(\frac{\rho_0}{\rho}\right)^{\omega+1}}$$

$c^2_{explosive,unreacted}$

$$= -\frac{\rho_0}{\rho^2}\left[A\frac{\omega}{R_1 v^2}e^{-R_1\left(\frac{\rho_0}{\rho}\right)} + B\frac{\omega}{R_2 v^2}e^{-R_2\left(\frac{\rho_0}{\rho}\right)} - \frac{\omega e_0}{\left(\frac{\rho_0}{\rho}\right)} - AR_1\left(1-\frac{\omega}{R_1\left(\frac{\rho_0}{\rho}\right)}\right)e^{-R_1\left(\frac{\rho_0}{\rho}\right)} - \mathrm{B}R_2\left(1-\frac{\omega}{R_2\left(\frac{\rho_0}{\rho}\right)}\right)e^{-R_2\left(\frac{\rho_0}{\rho}\right)}\right]$$

$c^2_{explosive,reacted}$

$$= \frac{\rho_0}{\rho^2}\left[AR_1e^{-R_1\left(\frac{\rho_0}{\rho}\right)} + \mathrm{B}R_2e^{-R_2\left(\frac{\rho_0}{\rho}\right)} - C\frac{1+\omega}{\left(\frac{\rho_0}{\rho}\right)^{2+\omega}}\right] \tag{2}$$

The Arrhenius equation is used to describe the chemical reaction of RDX as demonstrated in (3).

$$\mathrm{k(T)} = \mathrm{Z}e^{-\frac{E_\alpha}{RT}} \tag{3}$$

The energy expression presented in (4) is added to the energy source part of the Euler Equation to explain the exothermic phenomenon brought on by Joule heating [3].

$$\sigma\left(\frac{\partial\phi}{\partial x}\right)^2 \left(\frac{\partial\phi}{\partial x} = \vec{E} = \frac{\vec{J}}{\sigma}\right) \tag{4}$$

2.4 Result

Heat generation and explosion reaction were analyzed when 1200 V of electricity was applied to RDX. The temperature distributions from the simulation are shown in Fig. 5. Since the exothermic decomposition reaction temperature of RDX is 496.35K, it may be seen that RDX ignites and explodes at about 0.13 seconds. The findings of the change in the values of species are shown in Fig. 6. This indicates that the RDX explosive reaction begins around 0.13 seconds since the species value of RDX starts to shift from 0 to 1 at around that time.

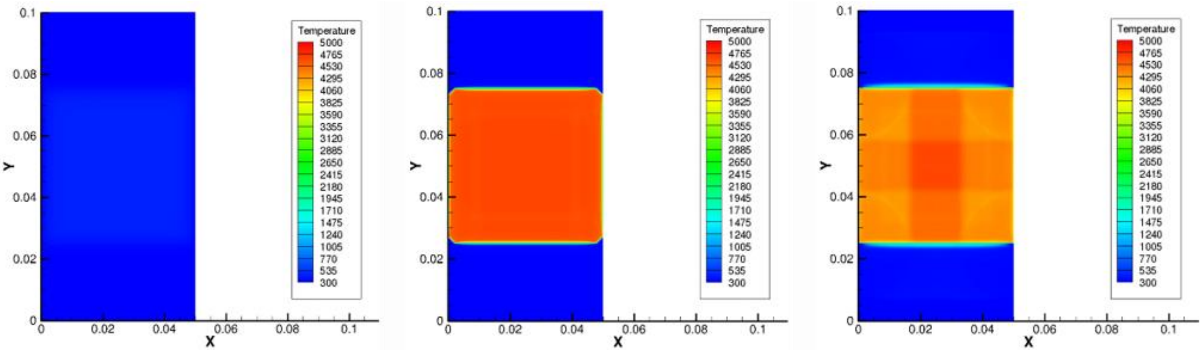

Figure 5. Temperature distribution at t=0.12(before detonation), 0.13(after detonation), 0.130003

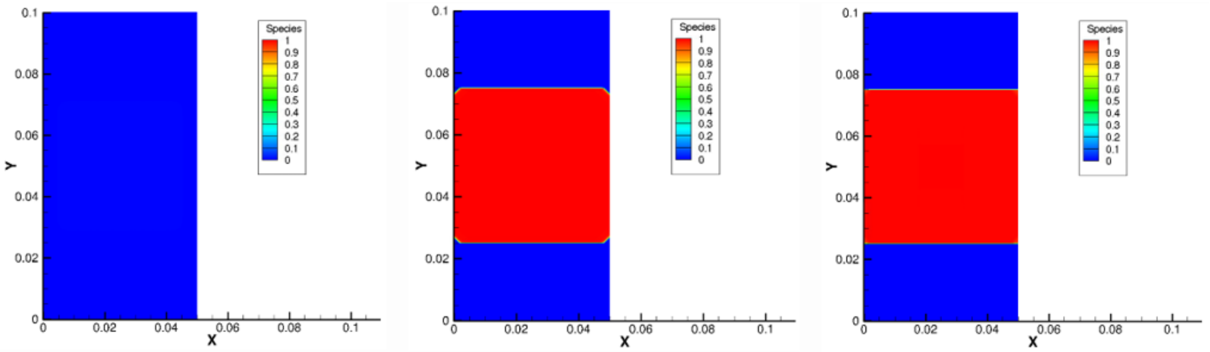

Figure 6. Species at t=0.12(before detonation), 0.13(after detonation), 0.130003

An experiment was conducted to verify whether the solver used for verification and simulation in this study could analyze the performance of ECSP (Electrically Controlled Solid Propellant) [5], which is the final goal of the study. The experimental output from tracking ECSP combustion through time is shown in Fig. 7. In future work, the idea and combustion principle of ECSP will be covered. The study is now underway with the ultimate objective of validating the current solver by using the same domain and properties as the experimental settings and comparing and evaluating the experimental data. Figure 8 shows that the domain of the same scale as the domain used in the experiment is applied to the code, and Table 1 shows the representative properties of ECSP extracted from the experiment. After the verification is finished, it is anticipated that the verified solver will allow for the simulation of diverse electric propulsion fields.

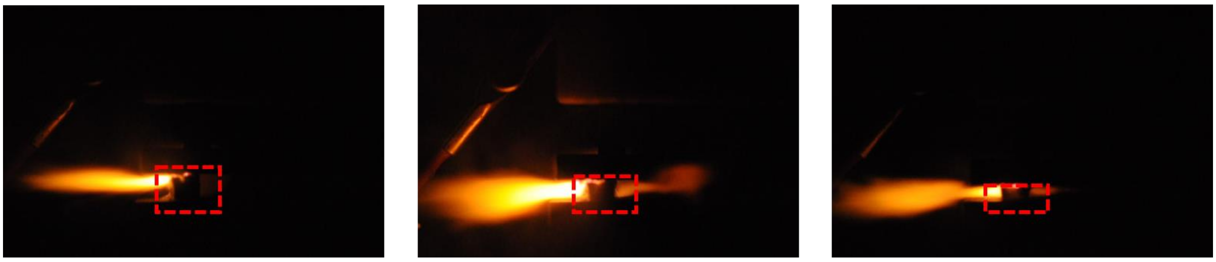

Figure 7. The experimental output from tracking ECSP combustion through time

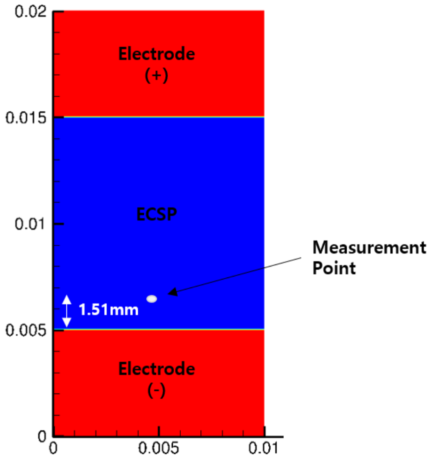

Figure 8. Domain of the same scale as the domain used in the experiment\

H_2O(wt%)	LP(wt%)	PVA(wt%)	Glycerol(wt%)	H_3BO_3(wt%)	Heat of reaction(J/g)	Activation energy(kJ/mol)
53.88	29.12	10	5	2	1162±200	162±26

Table 1: Representative properties of ECSP extracted from the experiment

3 Conclusion

This work examined the generation of heat caused by Joule heating and high-explosive explosion. The total combustion process was explained by the Euler Equation. The Arrhenius equation was used to understand the chemical reaction of high energetic-explosive. The equation of state for high energetic-explosive was the JWL EOS. The Runge-Kutta and CENO (Central Essentially Non-Oscillatory) methods were utilized to understand the differential equation, and the level set approach was used to trace the interface between materials for effective simulation. When electricity is applied to energetic material, the Joule heating effect produces heat, and when the internal temperature of the energetic material reaches a reaction temperature due to heat generation, the high energetic-explosive will detonate. RDX was employed in this study, and 1200 V was used as the applied voltage. The internal temperature increased up to the exothermic decomposition reaction temperature of RDX which happens approximately at 0.13 seconds after the voltage was applied, confirming the RDX explosion. Changes in the species value could be used to determine whether or not RDX detonates. The ability to interpret the electrically powered reaction system was established through this research.

4 References

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