Steady Deflagration Structure in Two-Phase Granular Propellants

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Envisioned Two-Phase Deflagration



Review of Two-Phase Deflagration

1973--Kuo, Vichnevetsky, and Summerfield, AIAA Journal

1974--Kuo and Summerfield, AIAA Journal

1975--Kuo and Summerfield, 15th Combustion Symposium

1986--Drew, Combustion, Science and Technology

Related Work

1986--Baer and Nunziato, International Journal of Multiphase Flow

1988--Powers, Stewart, and Krier, Dynamics of Explosions, AIAA Progress

1989--Powers, Stewart, and Krier, Journal of Applied Mechanics

1989--Powers, Stewart, and Krier, Combustion and Flame

Model Features

-Representative of a larger class of two-phase models

-Each phase obeys a mass, momentum, and energy evolution equation

-Mixture mass, momentum, and energy conserved

-Volume fraction ($\phi \equiv$ phase volume / total volume) utilized

-PDE's are hyperbolic

-Characteristic wave speeds: $u_1, u_2, u_1 \pm c_1, u_2 \pm c_2$

-Dynamic compaction equation employed for closure

-Number of particles conserved

-Compressible spherical reactive particles

-Simplified drag and convective heat transfer relations

-Virial gas equation of state for inert gas

-Tait equation of state for reactive particles

-Viscosity or heat conduction in gas not considered

-Viscosity or heat conduction in solid not considered

-Radiation not considered

Two-Phase Model Equations

-ordinary differential equations in steady wave frame

 $-\xi$ = distance in steady wave frame $\xi = \xi$ - Dt

-D = steady wave speed

-with additional algebraic equations, the model can be represented by four differential equations in four unknowns

$$\frac{d}{d\xi} \left(\rho_2 \phi_2 v_2 \right) = - \left(\frac{3}{r} \right) \rho_2 \phi_2 \alpha P_1^m H(T_2 - T_{ig}), \qquad \text{particle mass}$$

$$\rho_2 \phi_2 v_2 \frac{dv_2}{d\xi} + \frac{d}{d\xi} \left[P_2 \phi_2 \right] = -\beta \frac{\phi_1 \phi_2}{r} \left[v_2 - v_1 \right], \text{ particle momentum}$$

$$\rho_2 \mathbf{v}_2 \frac{d\mathbf{e}_2}{d\xi} + \mathbf{P}_2 \frac{d\mathbf{v}_2}{d\xi} = -\mathbf{h} \frac{\phi_1}{r^{1/3}} \begin{bmatrix} \mathbf{T}_2 - \mathbf{T}_1 \end{bmatrix}, \qquad \text{particle energy}$$

$$v_2 \frac{d\phi_2}{d\xi} = \frac{\phi_1 \phi_2}{\mu_c} \left(P_2 - P_1 - \frac{P_{20} - P_{10}}{\phi_{20}} \phi_2 \right) - \left(\frac{3}{r} \right) \phi_2 \alpha P_1^m H(T_2 - T_{ig}).$$

dynamic pore collapse

Conservation Relations

-obtained by integrating conservative differential equations -initial conditions specify integration constants

1) Mixture mass, momentum, and energy:

$$\rho_1 \phi_1 v_1 + \rho_2 \phi_2 v_2 = -D \rho_a$$
, mixture mass

 $\rho_1 \phi_1 v_1^2 + P_1 \phi_1 + \rho_2 \phi_2 v_2^2 + P_2 \phi_2 = \rho_a D^2 + P_a, \quad \text{mixture momentum}$

$$\rho_1 \phi_1 v_1 \left[e_1 + v_1^2 / 2 + P_1 / \rho_1 \right] + \rho_2 \phi_2 v_2 \left[e_2 + v_2^2 / 2 + P_2 / \rho_2 \right] = -\rho_a D \left[e_a + D^2 / 2 + P_a / \rho_a \right],$$

mixture energy

- "a" denotes apparent or bulk initial property

$$\rho_{a} = \rho_{10}\phi_{10} + \rho_{20}\phi_{20},$$
 apparent initial density

$$P_{a} = P_{10}\phi_{10} + P_{20}\phi_{20},$$
 apparent initial pressure

$$e_{a} = \frac{\rho_{10}\phi_{10}e_{10} + \rho_{20}\phi_{20}e_{20}}{\rho_{10}\phi_{10} + \rho_{20}\phi_{20}}.$$
 apparent initial energy

2) Particle number equation:

$$r = r_0 \sqrt[3]{\frac{-v_2 \phi_2}{D \phi_{20}}}.$$

Gas and Particle State Equations

1) Gas:

$$P_{1} = \rho_{1} RT_{1} (1 + b\rho_{1}), \qquad \text{gas thermal}$$
$$e_{1} = c_{v1}T_{1}. \qquad \text{gas caloric}$$

2) Particle:

 $P_{2} = (\gamma_{2} - 1) c_{v2} \rho_{2} T_{2} - \frac{\rho_{20} \sigma}{\gamma_{2}},$

particle thermal

particle caloric

 $e_2 = c_{v2}T_2 + \frac{\rho_{20}\sigma}{\gamma_2\rho_2} + q.$

Saturation condition:

$$\phi_1 + \phi_2 = 1.$$

Initial Conditions

-Eight independent initial conditions specified for original eight differential equations

-Temperature and density for each phase

-Velocity for each phase

-Initial particle radius

-Initial volume fraction

 $\rho_2 \ = \ \rho_{20}, \quad \varphi_2 \ = \ \varphi_{20}, \quad v_2 \ = \ - \ D, \ T_2 \ = \ T_0.$

 $\rho_1 = \rho_{10}, \quad v_1 = -D, \quad T_1 = T_0, \quad r = r_0.$

-Specified so that initial state is an equilibrium state

-Remaining initial conditions fixed by state equations and saturation condition:

$$P_{10} = \rho_{10} RT_0 (1 + b\rho_{10}), \quad e_{10} = c_{v1} T_0,$$

$$P_{20} = (\gamma_2 - 1) c_{v2} \rho_{20} T_0 - \frac{\rho_{20} \sigma}{\gamma_2}, \quad e_{20} = c_{v2} T_0 + \frac{\sigma}{\gamma_2} + q,$$

$$\phi_{10} = 1 - \phi_{20}.$$

Dimensional Input Parameters

a	[m / (s Pa)]	2.90 x 10 ⁻⁹
ρ ₁₀	[kg / m ³]	$1.00 \ge 10^{0}$
m		$1.00 \ge 10^{0}$
β	[kg / (s m ²)]	1.00 x 10 ⁴
ρ ₂₀	[kg / m ³]	1.90 x 10 ³
h	[J / (s K m ^{8/3})]	1.00 x 10 ⁷
c _{v1}	[J / (kg K)]	2.40×10^3
c _{v2}	[J / (kg K)]	$1.50 \ge 10^3$
R	[J / (kg K)]	8.50 x 10 ²
σ	[(m / s) ²]	7.20 x 10 ⁶
q	[J / kg]	5.84 x 10 ⁶
r ₀	[m]	1.00 x 10 ⁻⁴
b	[m ³ / kg]	1.10 x 10 ⁻³
γ ₂		5.00 x 10 ⁰
μ	[kg / (m s)]	1.25 x 10 ²
T ₀	[K]	$3.00 \ge 10^2$
T _{ig}	[K]	3.00 x 10 ² +

Two-Phase Deflagration End States

-arbitrarily assume complete reaction

-mixture equations define two-phase Rayleigh line and Hugoniot equations

 $P_{1} = P_{a} + \rho_{a}^{2} D^{2} \left(\frac{1}{\rho_{a}} - \frac{1}{\rho_{1}} \right), \qquad \text{Rayleigh line}$ $\frac{(P_{a} + P_{1})(1/\rho_{1} - 1/\rho_{a})}{2} + \frac{c_{v1}P_{1}}{R\rho_{1}(b\rho_{1} + 1)} - e_{a} = 0. \qquad \text{Hugoniot}$

-In general, two physical deflagration solutions for a given wave speed D

Low pressure, supersonic, strong solution
 High pressure, weak, subsonic solution

-Maximum deflagration wave speed at CJ condition, sonic solution



Complete Reaction End State

-assume exhaust pressure can be controlled

-deflagration wave speed and all gas phase properties then known as functions of exhaust pressure



-CJ state can be determined numerically

-Simple analytic expression in two limits

1) ideal gas b = 02) $P_a/(\rho_a e_a) \rightarrow 0$

$$\begin{split} \mathrm{D}_{\mathrm{CJ}} &\cong \sqrt{\frac{\gamma_{1}^{2} \mathrm{e}_{\mathrm{a}}}{2(\gamma_{1}^{2} - 1)}} \left(\frac{\mathrm{P}_{\mathrm{a}}}{\mathrm{p}_{\mathrm{a}} \mathrm{e}_{\mathrm{a}}}\right), \\ \mathrm{P}_{\mathrm{CJ}} &\cong \frac{1}{\gamma_{1} + 1} \mathrm{P}_{\mathrm{a}}, \\ \mathrm{p}_{\mathrm{CJ}} &\cong \frac{\gamma_{1}}{2(\gamma_{1} - 1)} \left(\frac{\mathrm{P}_{\mathrm{a}}}{\mathrm{p}_{\mathrm{a}} \mathrm{e}_{\mathrm{a}}}\right) \mathrm{p}_{\mathrm{a}}, \\ \mathrm{T}_{\mathrm{CJ}} &\cong \frac{2}{\gamma_{1} (\gamma_{1} + 1)} \frac{\mathrm{e}_{\mathrm{a}}}{\mathrm{e}_{\mathrm{vl}}}, \\ \mathrm{e}_{\mathrm{CJ}} &\cong \frac{2}{\gamma_{1} (\gamma_{1} + 1)} \mathrm{e}_{\mathrm{a}}, \\ \mathrm{v}_{\mathrm{CJ}} &\cong \mathrm{u}_{\mathrm{CJ}} &\cong -\sqrt{\left(\frac{2(\gamma_{1} - 1)}{\gamma_{1} + 1} \mathrm{e}_{\mathrm{a}}\right)} \end{split}$$

Two-Phase Deflagration Structure

-Ordinary differential equations integrated for D = 100 m/s

-Arbitrarily assumed that no shocks exist in structure or no sonic points

-With this assumption the end state is weak subsonic end state

-exhaust pressure ~ 400 MPa

-Extreme deflagration exhaust conditions because some parameters arbitrarily chosen so that a numerically resolved structure could be presented

-No two-phase steady deflagration structure going to complete reaction was found



Figure 7 Solid Volume Fraction Structure, $\phi_{20} = 0.70$, D = 100 m/s



Figure 8 Gas and Solid Lab Velocity Structure, $\phi_{20} = 0.70$, D = 100 m/s



Figure 9 Gas and Solid Pressure Structure, $\phi_{20} = 0.70$, D = 100 m/s







Figure 11 Gas and Solid Mach Number Squared, $\phi_{20} = 0.70$, D = 100 m/s

Conclusions

-Possible to predict gas phase deflagration end state and wave speed as function of exhaust pressure and initial conditions

-For the region of parameter space studied, no steady two-phase deflagration structure exists

-Processes that support detonation are not sufficient to support a two-phase deflagration

-It may be necessary to include heat conduction and radiation to model twophase deflagrations

-Combustion of granulated propellants could possible accelerate into steady, self-propagating two-phase detonation