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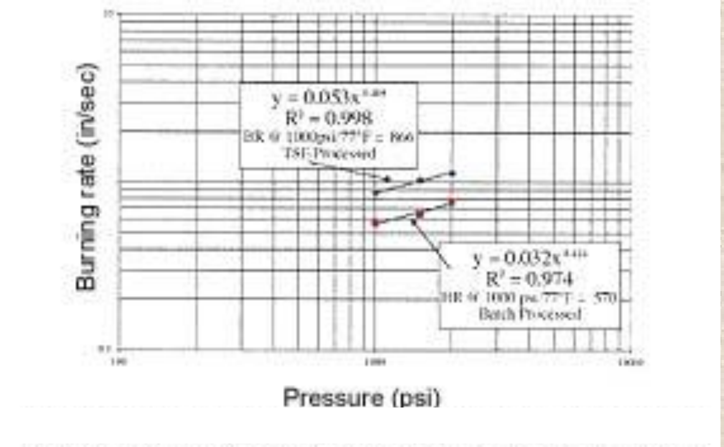
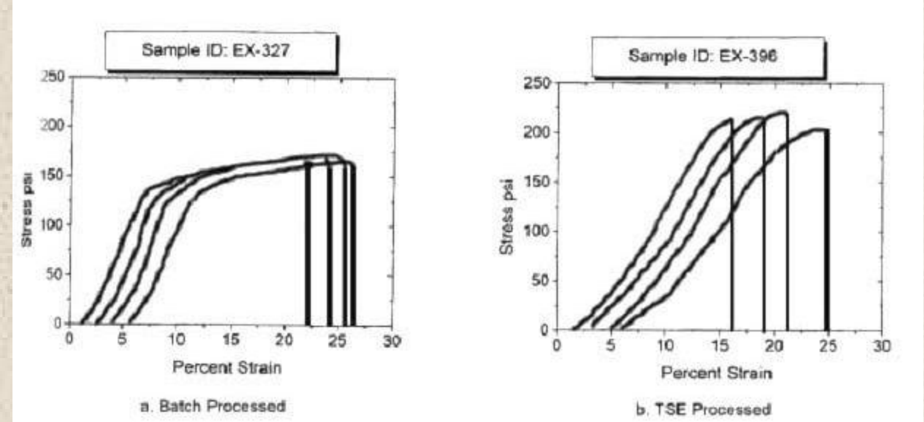
Materials by Design: Simulation-based Development and Manufacturing of Functionally Graded Energetic Materials

Department of Mechanical Engineering

Motivation

- Composite Energetic Materials have been traditionally manufactured using batch processing (*like baking a cake*)
- New continuous manufacturing technology known as Twin Screw Extrusion (TSE) is being used to produce higher quality composite energetic materials with more flexibility and control (*high tech*)
- Current manufacturing of composite energetic materials is simply focused on homogenizing formulations and does not require simulation tools
- The continuous nature of the TSE process is ideally suited for the manufacture of materials by design, such as Functionally Graded Materials (FGMs), using advanced simulation tools

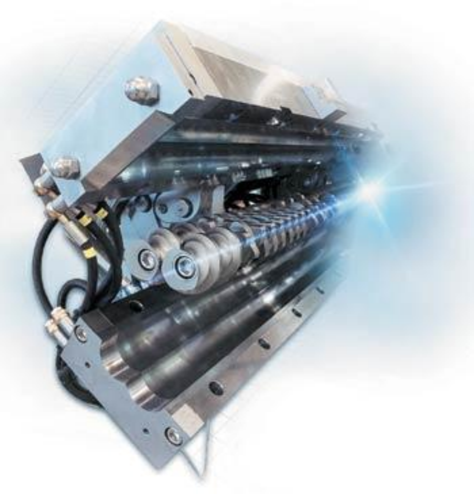




a. Batch Processed

b. TSE Processed

Batch vs. TSE



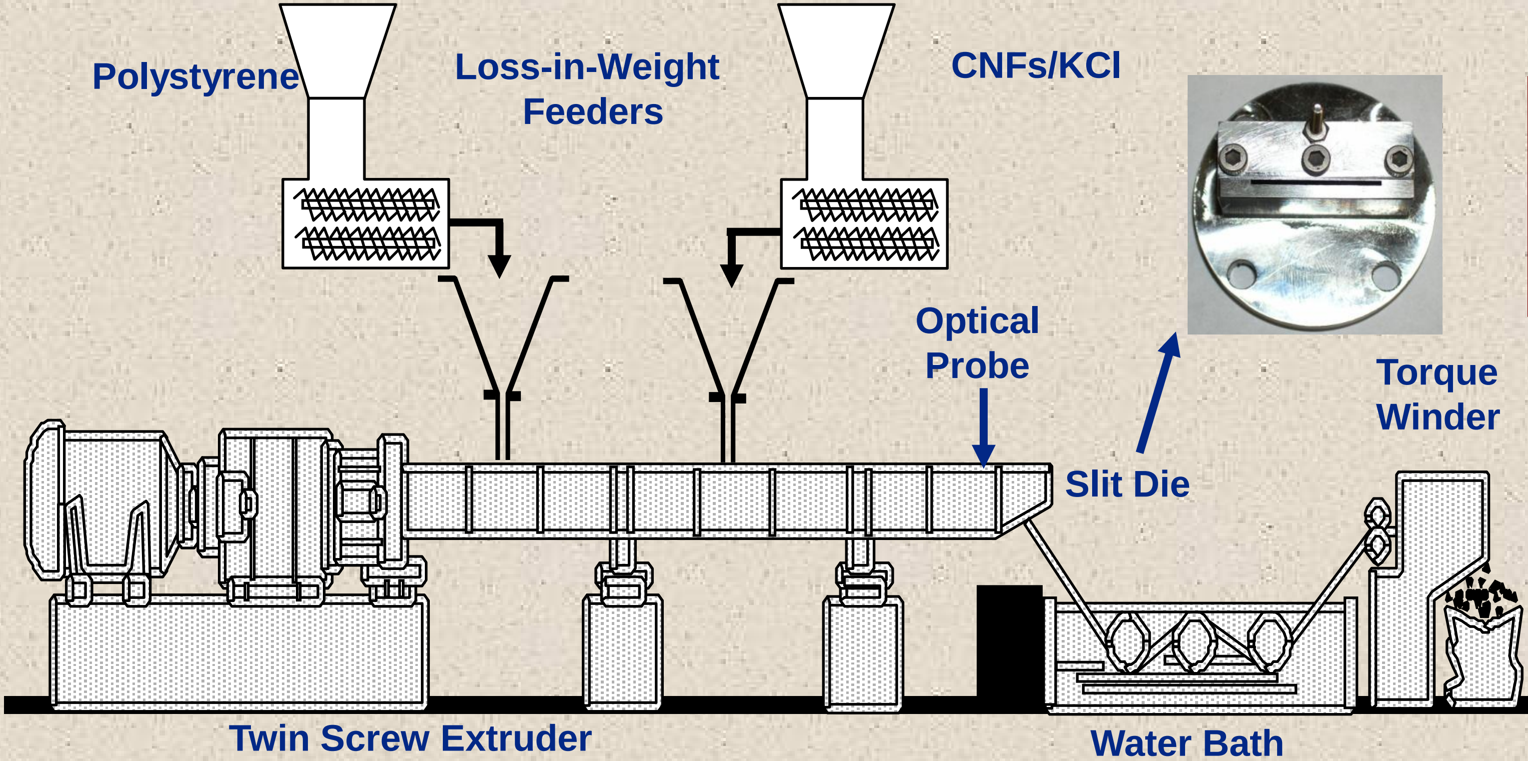
Batch Processing

- Old-fashioned way to make cakes or energetic materials
- High throughput by mixing large quantities of energetic materials can be dangerous
- Only homogenizes materials
- One defect ruins whole batch

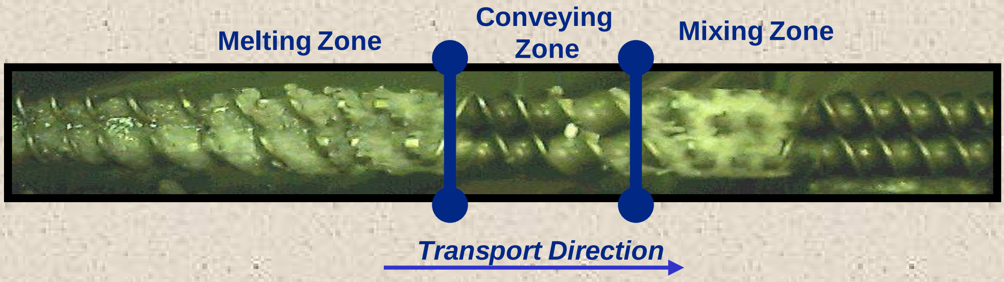
Twin Screw Extrusion

- High Tech 21st century manufacturing of energetic materials at Indian Head
- High throughput by continuous mixing of smaller, safer quantities
- Can vary composition easily
- Defects are not a problem

TSE process



Feed rate
Impulse
Step
Ramp

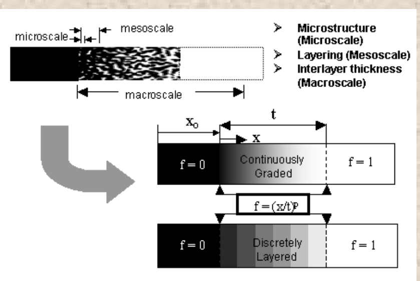


Processing Parameters
Screw Speed
Feed Rate

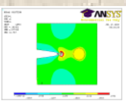
Research Objective

To characterize and model the TSE process and performance of Energetic Materials in FGM architectures for a new “Materials-by-design” simulation-based approach to tailor performance of rocket motors/warheads

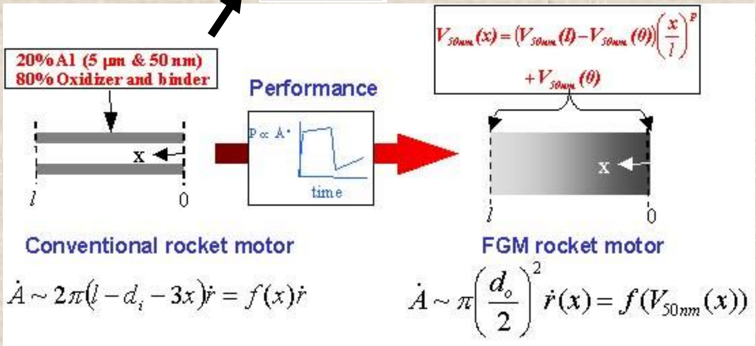
Energetic Material Continuously Extruding from Die of TSE



FGM Architecture



Crack grows at perf



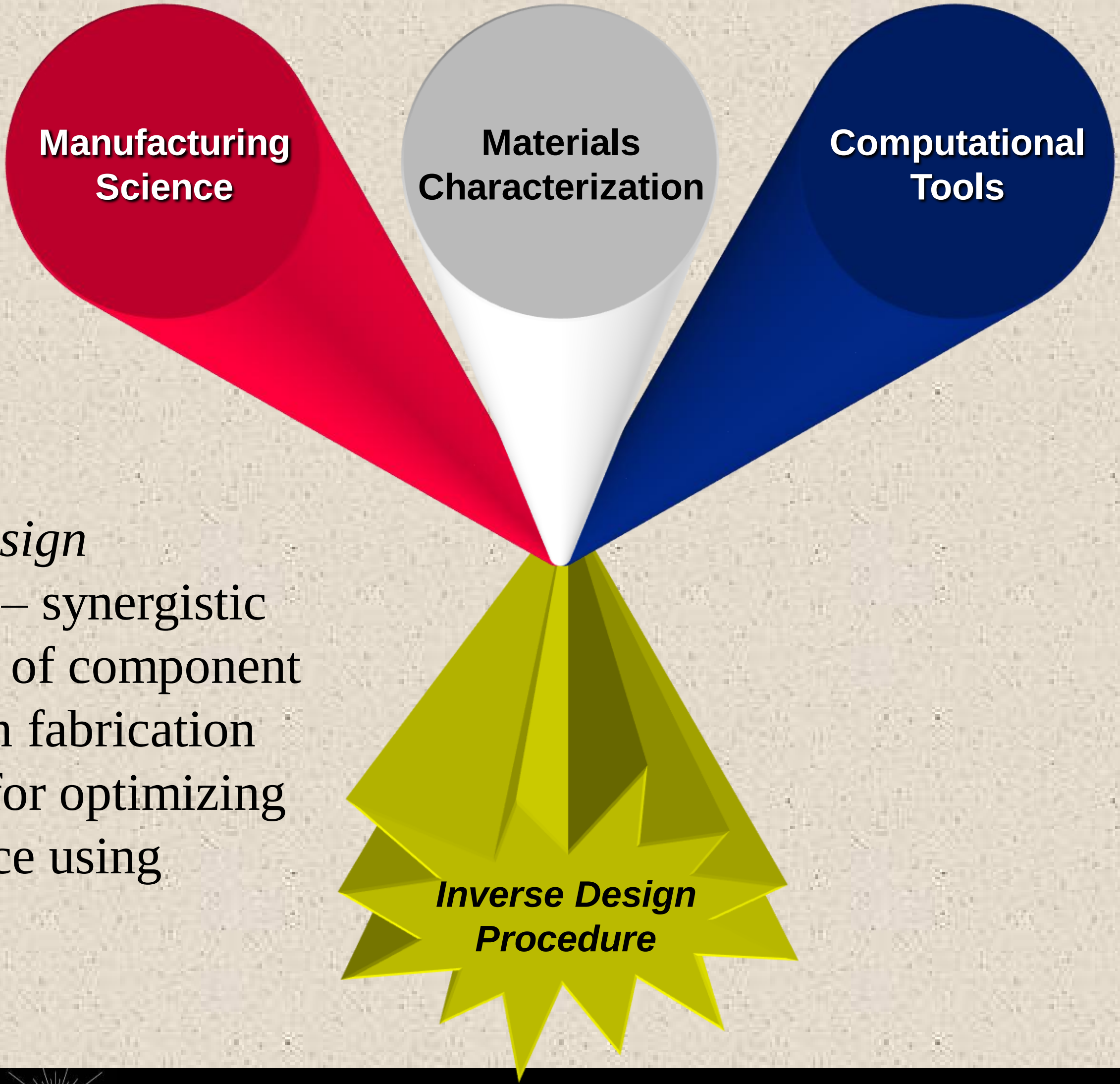
$$V_{50nm}(x) = (V_{50nm}(l) - V_{50nm}(0))\left(\frac{x}{l}\right)^p + V_{50nm}(0)$$

$$\dot{A} \sim 2\pi(l - d_i - 3x)\dot{r} = f(x)\dot{r}$$

$$\dot{A} \sim \pi\left(\frac{d_o}{2}\right)^2 \dot{r}(x) = f(V_{50nm}(x))$$

New Rocket Motor Concept

Simulation Approach

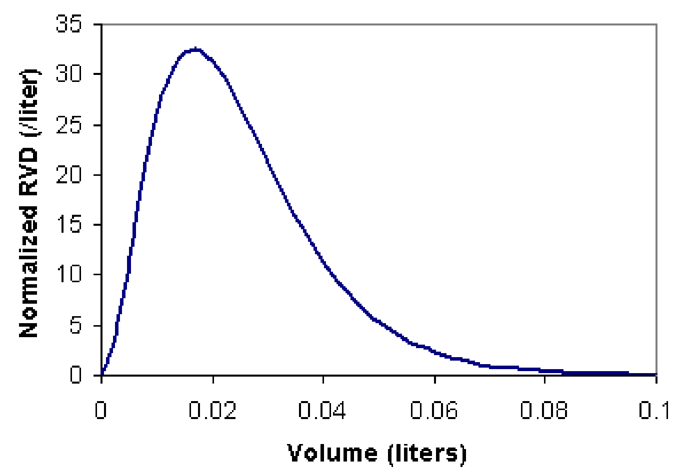


Inverse Design Procedure – synergistic integration of component design with fabrication processes for optimizing performance using FGMs

Modeling of TSE Process

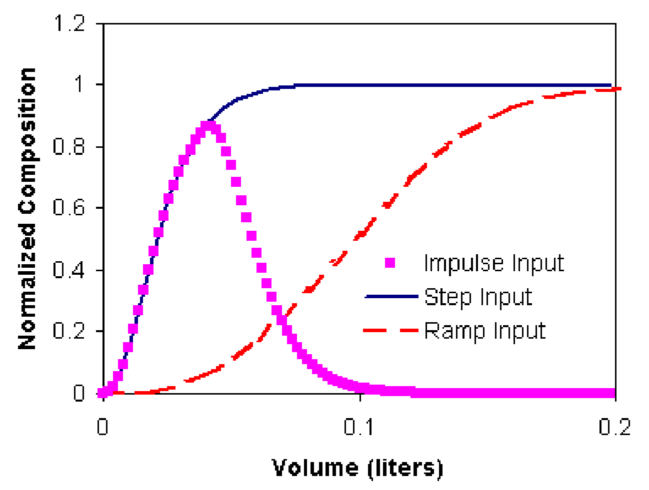
Residence Time Distribution:

$$e(t) = \frac{c(t)}{\int_0^\infty |c(t)| dt}$$



$$f[z(v)] = \int_o^v g(v - v')h(v')dv'$$

Can predict gradient architecture using RVD convolution!



RVD Model:

$$g(v) = \frac{a^3}{2}(v - v_d)^2 e^{-a(v - v_d)}$$

$$v_d = A - \frac{3}{C} + B\frac{Q}{N}$$

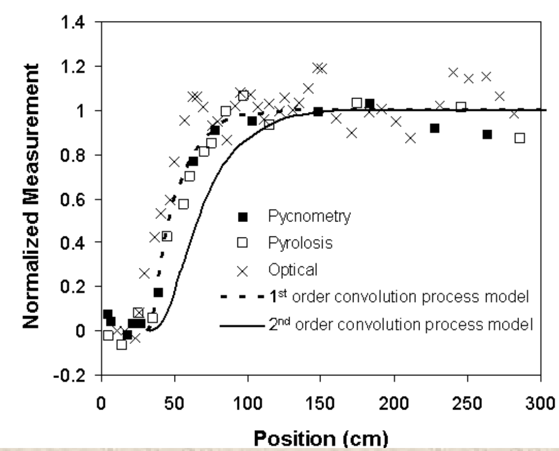
$$A = A_f L_m + V_p$$

$$B = \frac{2 A_f L_c}{(2i - 1)\pi D \cos\theta WHF_d}$$

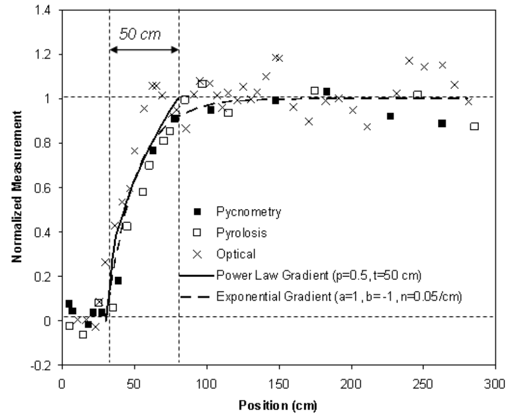
$$a = C$$

TSE parameters

Comparison of Measured and Simulated Composition Gradients



Measured and Modeled Gradient



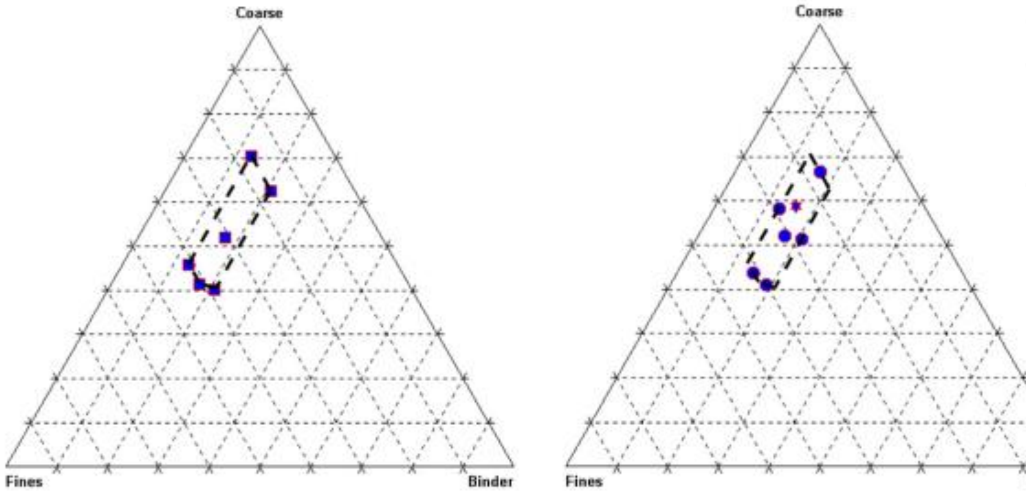
Gradient Description

Graded Polymer Composites

Gradient architecture measured using optical techniques *in situ*, and pycnometry/pyrolosis *a posteriori* to compare with convolution model

Burning Rate Properties: *Design of Experiments*

- Utilize Reduced Mixtures DOE approach developed with Indian Head to minimize number of specimens needed to characterize burning rate



(a) Combinations Made at 45 rpm

(b) Combinations Made at 85 rpm

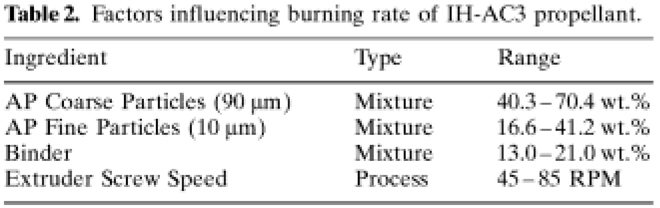
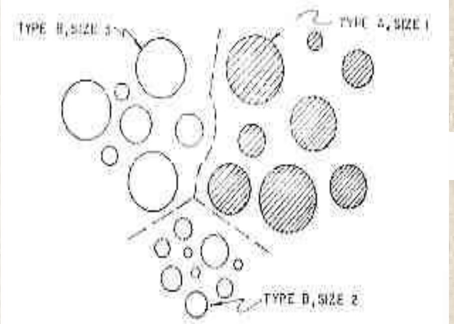


Table 2. Factors influencing burning rate of IH-AC3 propellant.

Ingredient	Type	Range
AP Coarse Particles (90 μm)	Mixture	40.3 – 70.4 wt.%
AP Fine Particles (10 μm)	Mixture	16.6 – 41.2 wt.%
Binder	Mixture	13.0 – 21.0 wt.%
Extruder Screw Speed	Process	45 – 85 RPM

Modeling Burning Rate: *Petite Ensemble Model*

- Statistically-based combustion model
- Combines Beckstead, Derr, and Price (BDP) model with Glick's statistical formalism
- Models composite propellant as a random arrangement of polydispersed pseudopropellants



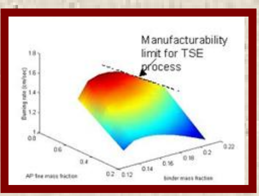
Polydispersed pseudopropellants

$$F_d = \frac{1}{(2\pi \ln \sigma)^{1/2}} \exp\left[-\frac{1}{2} \left(\frac{\ln D_o - \ln \bar{D}_o}{\ln \sigma} \right)^2 \right]$$

$$\bar{r} = \int_{D_o} \frac{r_d F_d}{\alpha_d} d(\ln D_o)$$

$$R_p = \frac{1}{\bar{r}} \int_{D_o} \frac{R_{p,d} r_d F_d}{\alpha_d} d(\ln D_o)$$

$$R_v = \frac{1}{\bar{r}} \int_{D_o} \frac{R_{v,d} r_d F_d}{\alpha_d} d(\ln D_o)$$



Burn rate variation w/ composition

$$\bar{r} = m_{ox}^{p} / \rho_p$$

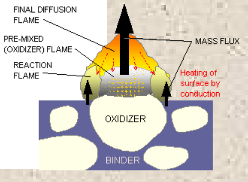
$$m_{ox}^{p} = m_{ox}^{T} \left[3\left(\frac{h}{D_o}\right)_+^2 + 3\left(\frac{h}{D_o}\right)_- + 1 \right]$$

$$m_{ox}^{T} = A_{ox} \exp\left[-\frac{E_{ox}}{RT_{s,ox}} \right]$$

$$\left(\frac{h}{D_o}\right)_{\pm} = f(r_{ox}, \tau_{ign}, D_o)$$

$$r_{ox} = m_{ox}^{T} / \rho_{ox}$$

$$\tau_{ign} = \frac{C_{ign} D_o^{\delta_D + 1}}{p \delta_p}$$

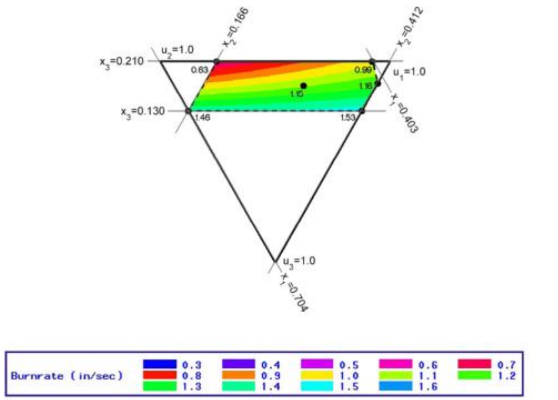


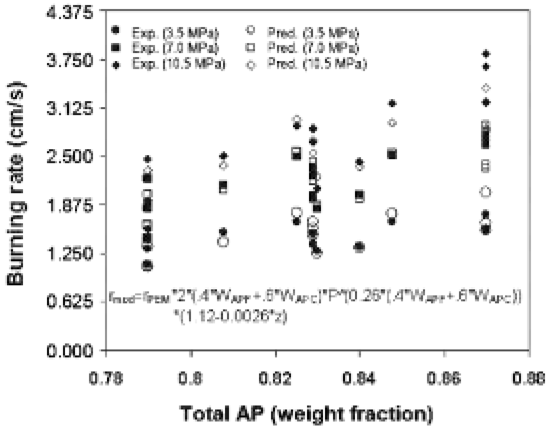
Combustion model

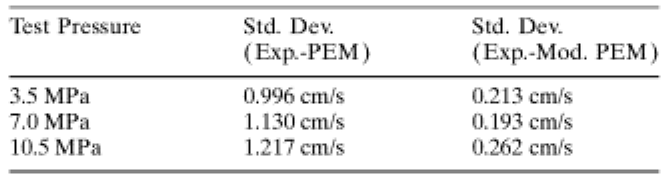
Burning Rate Response Surface Analysis

Modified PEM:

$$r_{mod}=r_{PEM}[\alpha(\beta V_{APF}+(1-\beta)V_{APC)}P\hat{}(\gamma(\beta V_{APF}+(1-\beta)V_{APC}))]*(c_1+c_2 z)$$



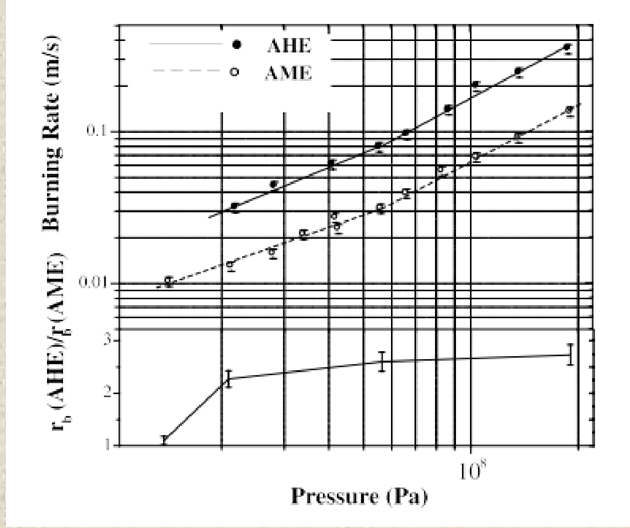




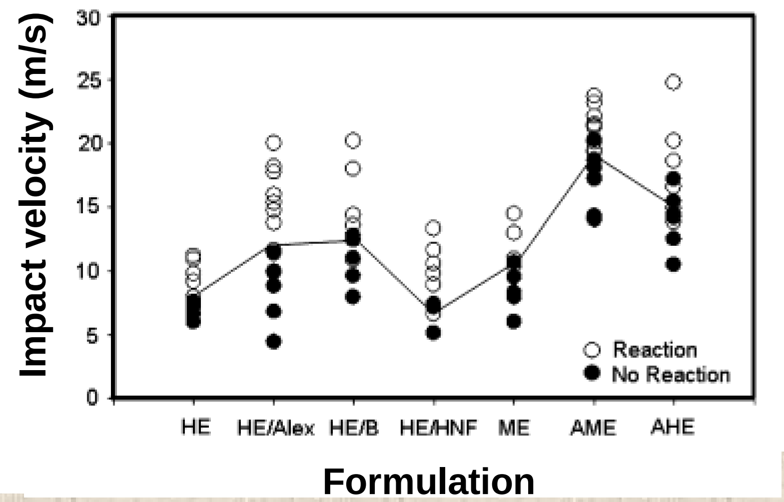
Test Pressure	Std. Dev. (Exp.-PEM)	Std. Dev. (Exp.-Mod. PEM)
3.5 MPa	0.996 cm/s	0.213 cm/s
7.0 MPa	1.130 cm/s	0.193 cm/s
10.5 MPa	1.217 cm/s	0.262 cm/s

Effects of nano-sized energetic ingredients

- Characterized effects of adding small concentrations (5-10 wt. %) nanoparticles (diameter ~ 150 nm) of Boron and Aluminum for tailoring burn rates, impetus, and impact sensitivity of High Energy (HE) and Medium Energy (ME) propellants



Burn rate comparison



Impact Sensitivity

Can modify the burn rate by 170% at high pressures and decrease impact sensitivity by 30%

Ballistic Modeling of Graded Motor

1-D numerical model developed at Indian Head

Governing Equation:

$$\frac{dP_c}{dt} = \frac{R_g T_c}{V_c}\left(\dot m_g - \dot m_e\right) - \frac{P_c}{V_c}\frac{\dot m_g}{\rho_p} + \frac{P_c}{T_c}\frac{dT_c}{dt} + \frac{P_c}{R_g}\frac{dR_g}{dt}$$

Where chamber pressure is solved incrementally by:

$$P_{c_{i+1}} = P_{c_i} + \frac{dP_c}{dt}\Delta t$$

The time step, Δt, is represented by:

$$\Delta t = \frac{1}{5} = \frac{P_c V_c}{(1-n)(R_g T_c \dot m_e)}$$

The thrust of the rocket motor, F, is calculated in the following manner:

$$F = C_f P_c A_t \qquad (29)$$

where:

$$C_f = \sqrt{\frac{2\gamma^2}{\gamma-1}\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{\gamma-1}}\left[1-\left(\frac{P_e}{P_c}\right)^{\frac{\gamma-1}{\gamma}}\right]} + \frac{P_e - P_a}{P_c}\varepsilon$$

and:

$$\varepsilon = \frac{A_e}{A_t} = \frac{\left(\frac{P_c}{P_e}\right)^{\frac{1}{\gamma}}\left(\frac{2}{\gamma+1}\right)^{\frac{1}{\gamma-1}}}{\sqrt{\left[1-\left(\frac{P_e}{P_c}\right)^{\frac{\gamma-1}{\gamma}}\right]\left(\frac{\gamma+1}{\gamma-1}\right)}}$$

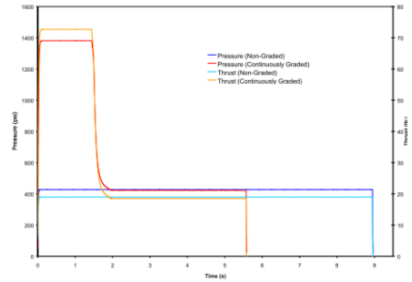


Figure 8. Comparison of simulated pressure and thrust profiles for a non-graded and continuously graded end-burning rocket motor [17].

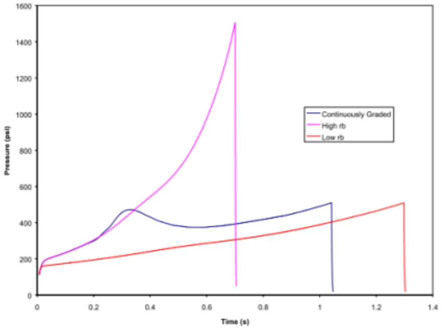
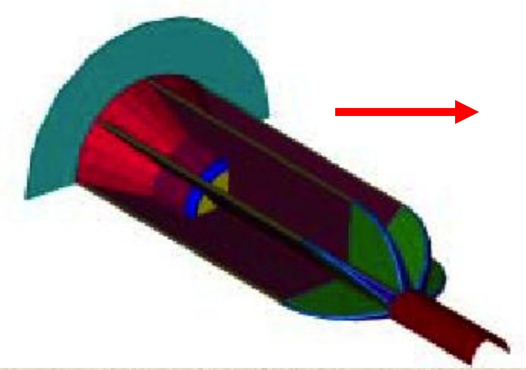


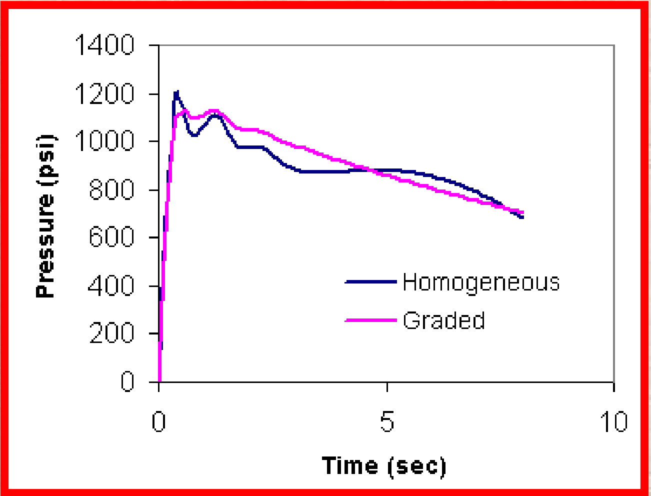
Figure 9. A simulated pressure profile for a continuously graded rocket motor in a center-perforated configuration compared with the high and low burning rate performance [17].

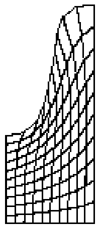
Young, Bruck, et al, *Proceedings of 39th JANNAF Comb.Sub.* (2003)

3-D FEA Simulation of Rocket Motor

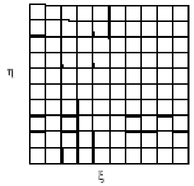
SPP 02 (3-D Euler CFD code)







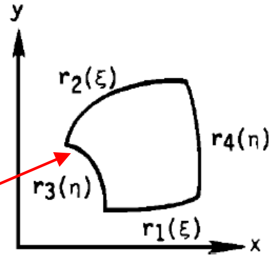
b) Grid in Physical Space, r-θ Coordinates



c) Grid in Transformed Space, ξ-η Coordinates

Graded elements

$$\mathbf{r}(\xi,\eta)=(1-\eta)\mathbf{r}_1(\xi)+\eta\mathbf{r}_2(\xi)+(1-\xi)[\mathbf{r}_2(\eta)-(1-\eta)\mathbf{r}_1(0)-\eta r_2(0)]+\xi[\mathbf{r}_4(\eta)-(1-\eta)\mathbf{r}_1(1)-\eta\mathbf{r}_2(1)] \quad (1)$$



Transfinite Interpolation

$$\xi_{xx}+\xi_{yy}=P(\xi,\eta)$$
$$\eta_{xx}+\eta_{yy}=Q(\xi,\eta) \quad (2)$$

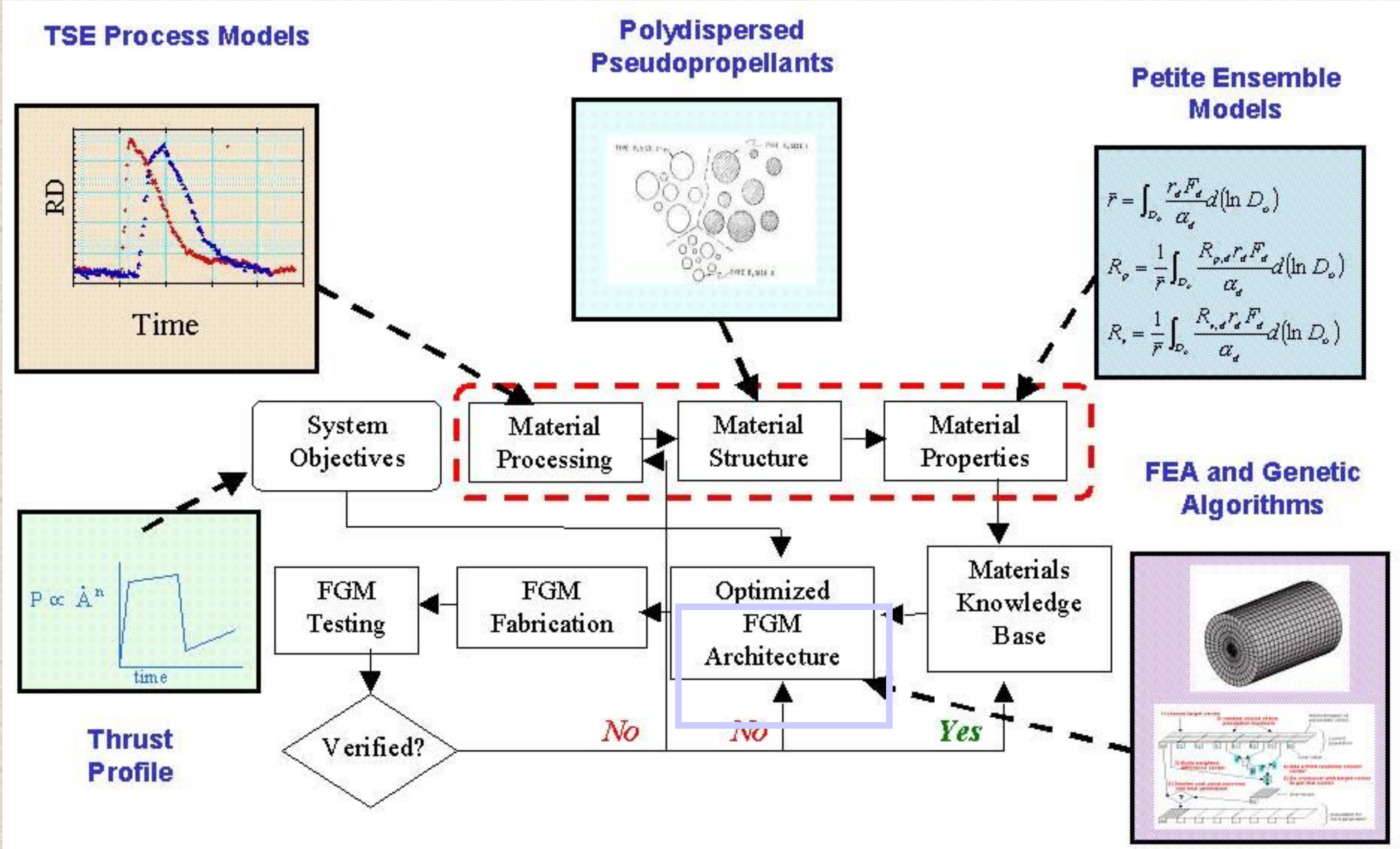
$$\alpha x_{\xi\xi}-2\beta x_{\xi\eta}+\gamma x_{\eta\eta}=-J^2\left(Px_\xi+Qx_\eta\right)$$
$$\alpha y_{\xi\xi}-2\beta y_{\xi\eta}+\gamma y_{\eta\eta}=-J^2\left(Py_\xi+Qy_\eta\right) \quad (3)$$

where

$$\alpha=x_\eta^2+y_\eta^2$$
$$\beta=x_\xi x_\eta+y_\xi y_\eta$$
$$\gamma=x_\xi^2+y_\xi^2 \quad (4)$$
$$J=\frac{\partial(x,y)}{\partial(\xi,\eta)}=x_\xi y_\eta-x_\eta y_\xi$$

Partial Differential Equation

Inverse Design Procedure for FGEMs



TSE Process Models

Polydispersed Pseudopropellants

Petite Ensemble Models

$$\bar{r} = \int_{D_o} \frac{r_d F_d}{\alpha_d} d(\ln D_o)$$

$$R_p = \frac{1}{\bar{r}} \int_{D_o} \frac{R_{p,d} r_d F_d}{\alpha_d} d(\ln D_o)$$

$$R_r = \frac{1}{\bar{r}} \int_{D_o} \frac{R_{r,d} r_d F_d}{\alpha_d} d(\ln D_o)$$

System Objectives

Material Processing

Material Structure

Material Properties

FEA and Genetic Algorithms

Materials Knowledge Base

Optimized FGM Architecture

FGM Fabrication

FGM Testing

Verified?

No

No

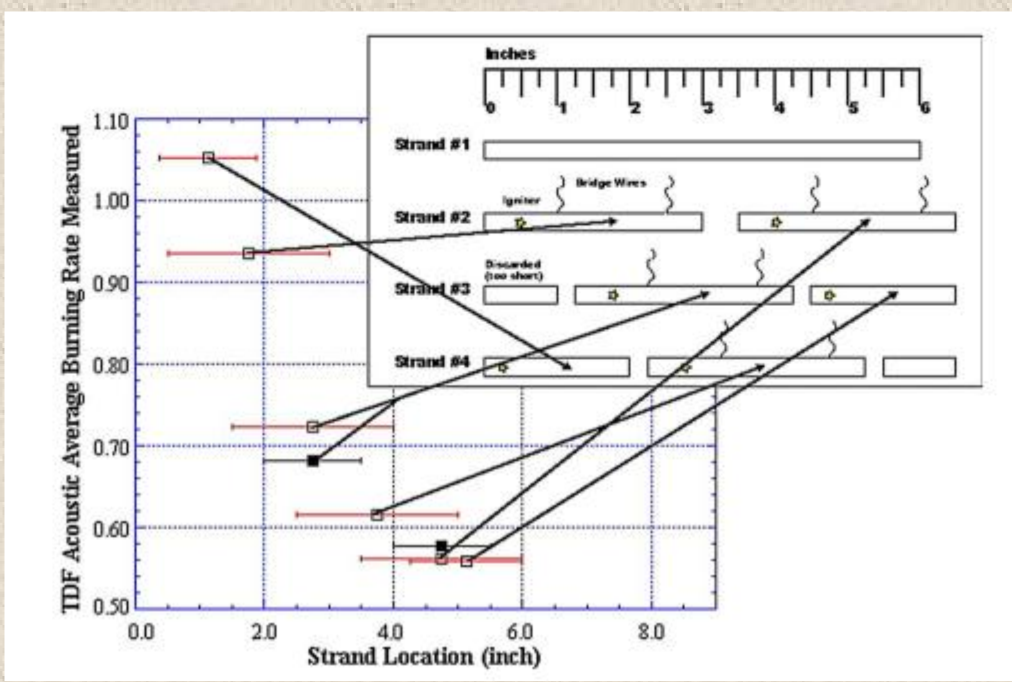
Yes

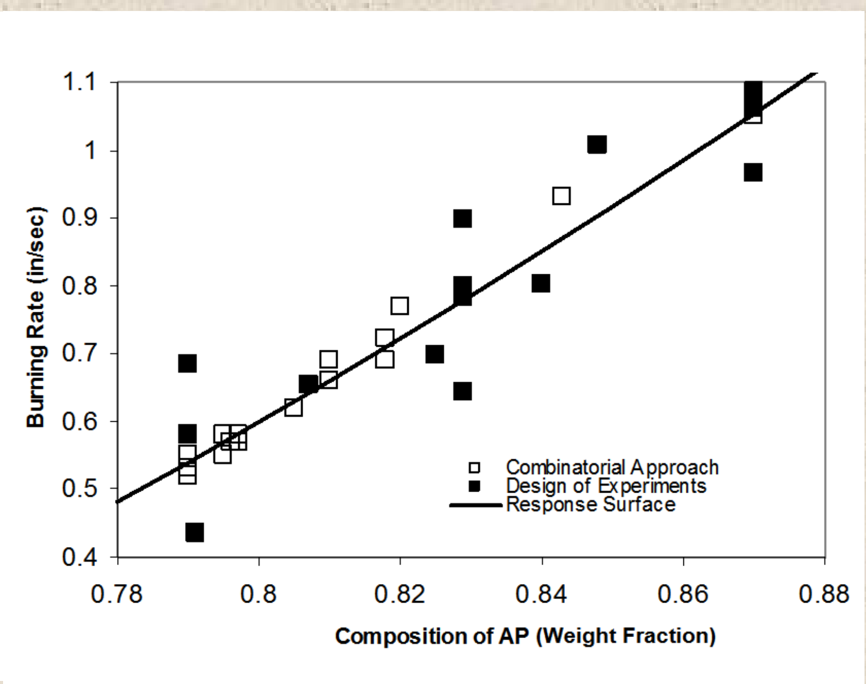
Thrust Profile

Advanced Formulation of EMs: *Combinatorial Materials Science*

- Current process for formulation EMs is “*mix and match*” approach involving slight changes to formulations in many different batch mixing runs in order to determine variation in properties with composition and processing
- Requires making time-consuming multiple batch runs of same fomulation in order to determine statistical “*batch-to-batch*” variation in properties
- New *combinatorial materials science* approach based on the materials by design simulation tools and TSE continuous mixing process provides a much **more rapid, less expensive, and accurate** formulation of new EMs

Combinatorial Materials Science vs. Batch





Combinatorial Materials Science approach using TSE is clearly better at determining the effects of AP composition on burning rates of propellants

Conclusions

- Advanced energetics are being developed and manufactured at Indian Head based on *21st century simulation tools*
- Twin Screw Extrusion (TSE) process has led to a new energetics concept: *Functionally Graded Energetic Materials (FGEMs)*
- Gradient architectures simulated using *new Residence Distribution (RD) Model* of TSE in *convolution process model.*
- New *reduced mixtures DOE* and *modified PEM* simulations have been developed for prediction composition effects on burning rates
- A new *1-D graded rocket motor ballistic analysis* has been developed for simulating performance
- A new *Inverse Design Procedure* has been developed that integrates RD, PEM, and FEA models with GAs for TSE processing of FGEMs
- A new *combinatorial materials science* approach to formulation has been developed based on the simulation tools and TSE process