AVT-340 Research Workshop on Preparation and Characterization of Energetic Materials

Burning Rate Prediction Through Application Of Machine Learning To Curated Datasets

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HEILMEIER Q&A

Energetic Formulations

What are you trying to do?

Predict composition and particle-size dependent properties (e.g. burn rate) using ML, create ML tools to transition.

How is it done today?

Formulation property estimates via empirical formulas or hydrocode simulations.

What is your approach?

Curate data, augment with controlled experiments. Create ML tools, provide in a modular, convenient package.

Who cares?

Reduce the number of experiments needed to optimize formulations; also suggest novel formulations.

What are the risks?

Data are noisy, sparse, scattered.

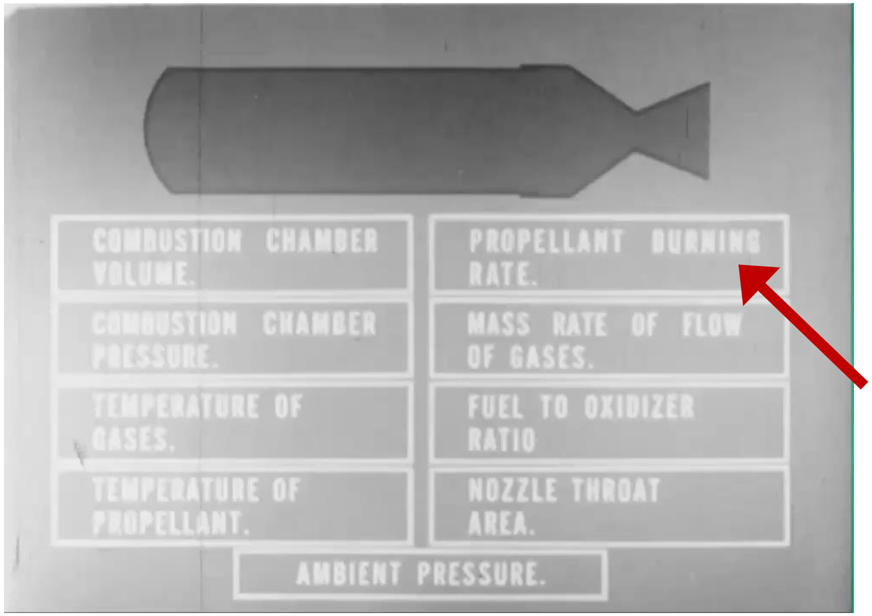
PREDICTING PROPERTIES (BURNING RATE)

Past 30+ years several have stated,“**Exact prediction of the burning rate from the composition has not yet been achieved in a general way**”

Burning rate is tailored for constraints:

- Thrust level
- Thrust duration
- Missile weight
- Critical impact velocity
- Processability

… the list goes on.



Burning rate is a number. Let’s describe a formulation as a set of numbers.

$$\text{Rate} = f(\vec{x})$$

Machine learning provides a route to $f(\vec{x})$ that has not yet been attempted.

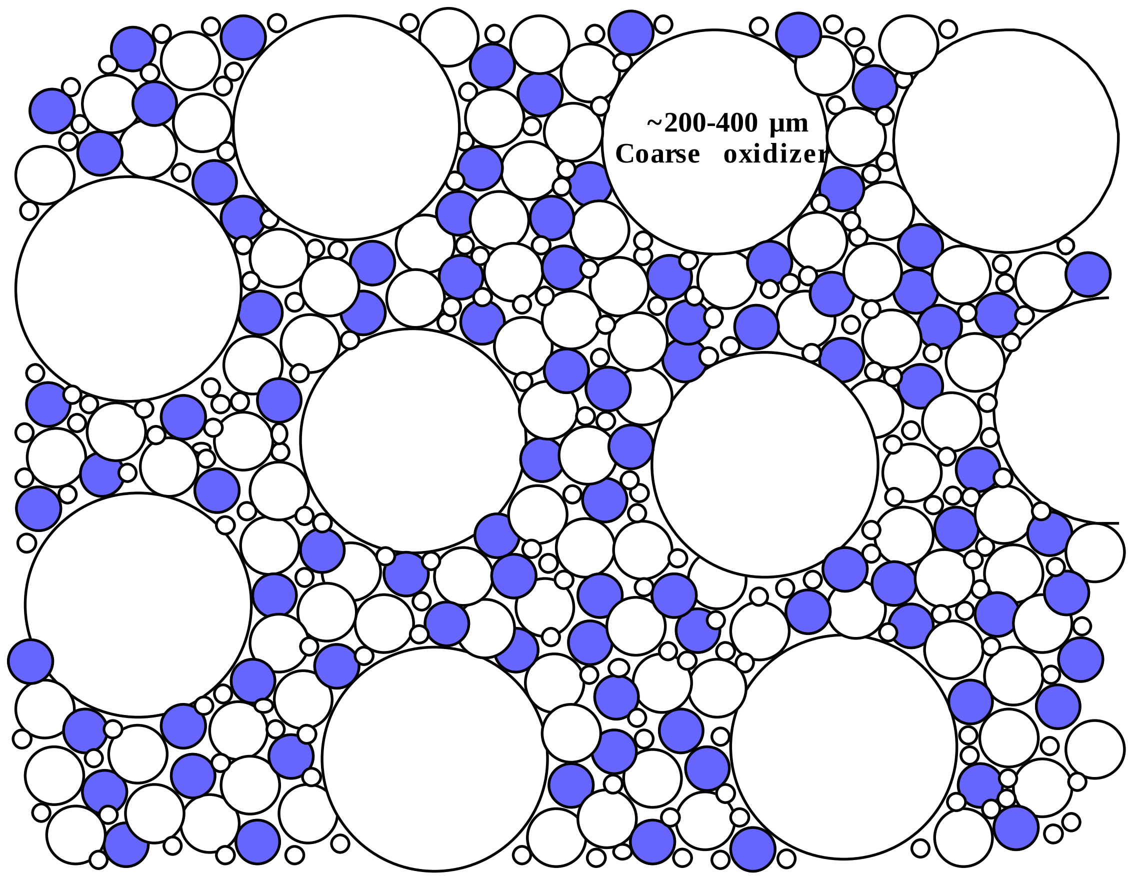
Typical Solid Propellant Mixture

~14% Binder (HTPB)

~16% Aluminum

~70% Oxidizer

- **Fine oxidizer ~1-20 μm (bacteria to talcum powder)**
- **Aluminum ~ 20-50 μm**
- **Medium oxidizer ~ 20-100 μm (white blood cell to hair)**
- **Coarse oxidizer ~ 200-400 μm (fine to medium beach sand)**



- Very heterogeneous burning surface
- Dimensions don't allow direct combustion measurements
- Crystals are not round - irregular shapes

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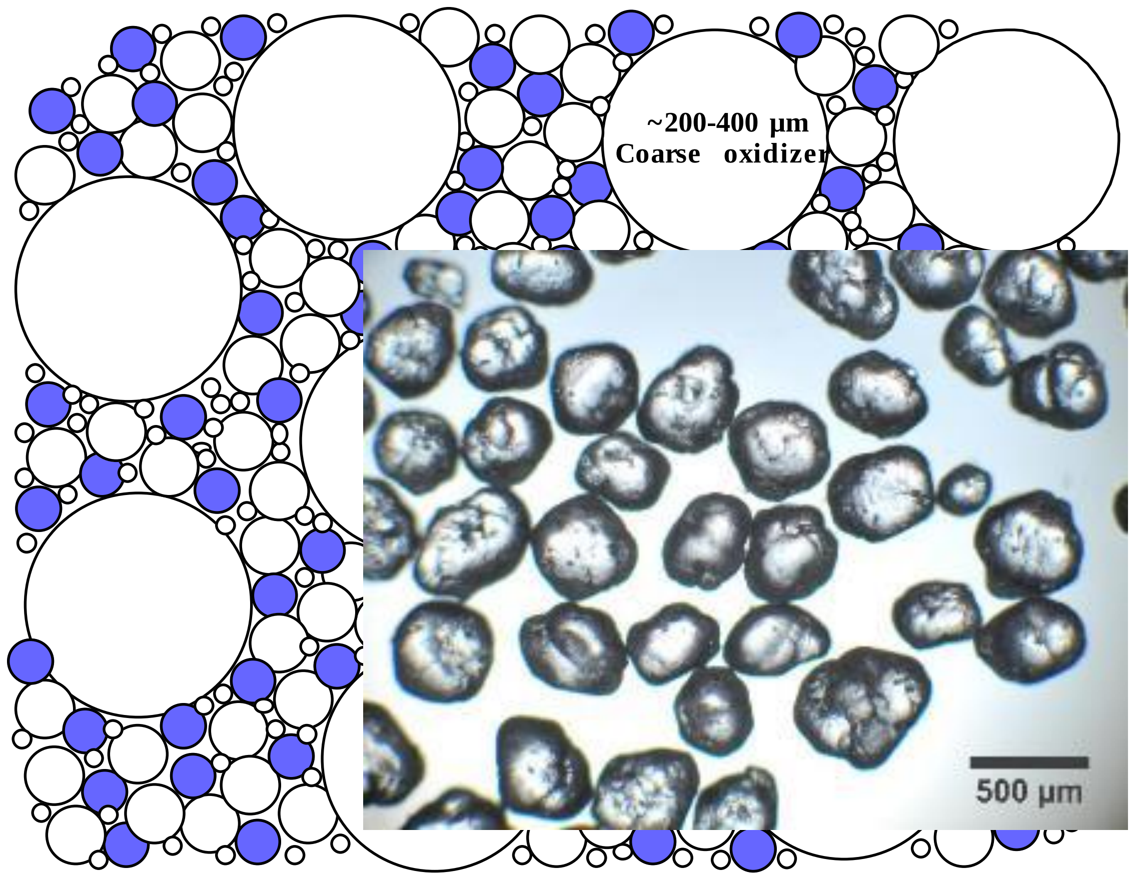

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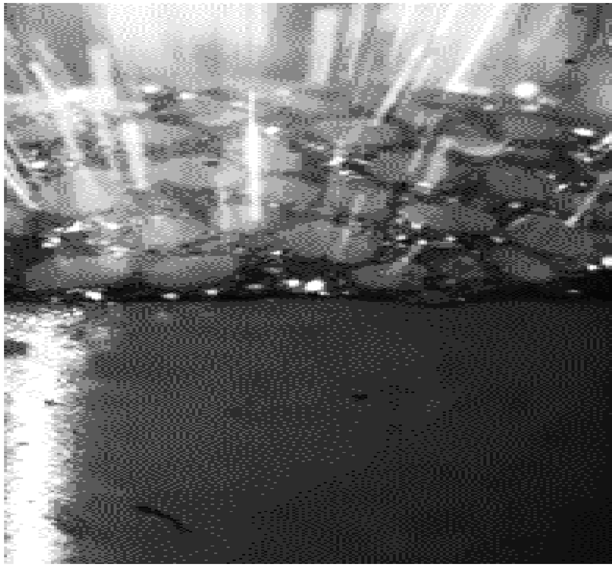
Propellant Formulation

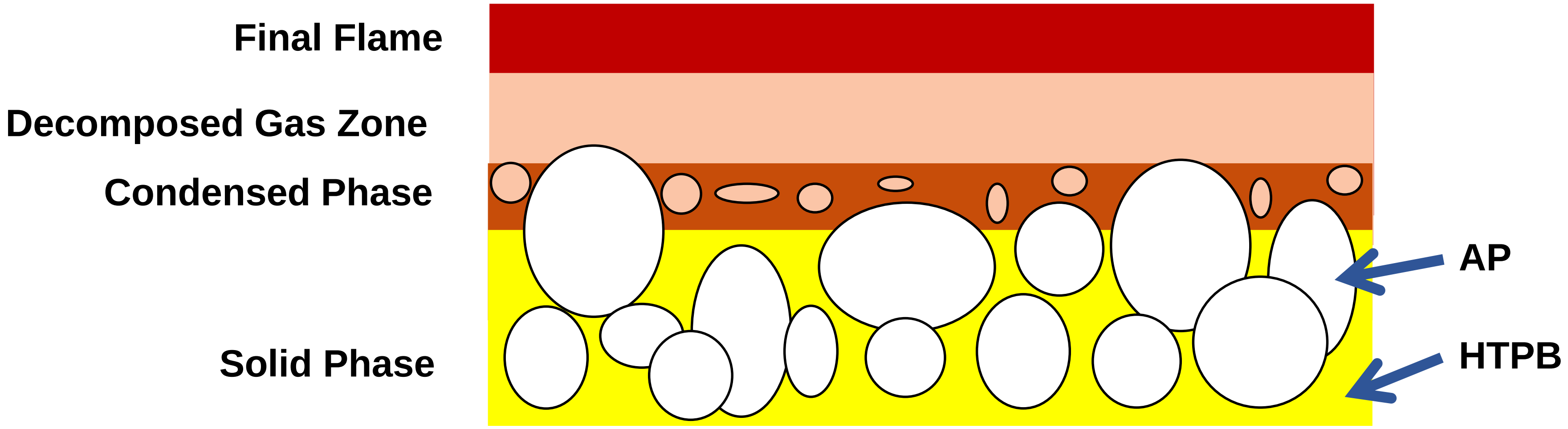
- New propellant development is costly
  - Trial and error process to meet desired requirements
  - Hard to predict based on previous formulations
    - Multiple variables changed between each mix
    - Systematic studies not often performed
    - Don’t report intermediate mixes
  - Few theoretical tools to aid initial design
  - Sometimes call an “Art”
    - Experienced formulators rely on intuition
    - Capabilities often leave with employee
- We need to develop a tool set



AP/HTPB Propellant Combustion

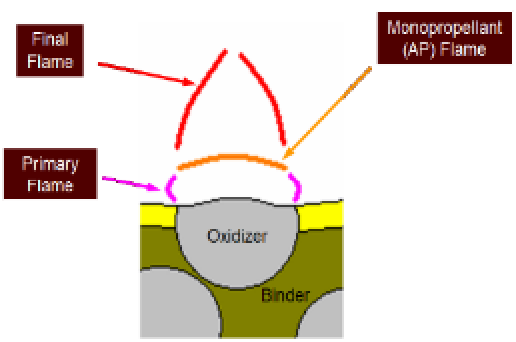
Complex AP Decomposition Process

- AP decomposes to perchloric acid and ammonia
  - React exothermically together -> monopropellant behavior
  - Premixed flamelets
- Excess oxidizer reacts with fuel products from HTPB pyrolysis
  - Diffusion flamelets
- Oxidizer particle size distributions and quantity play significant role
  - Testing a wide range or propellants may result in poor mechanical properties

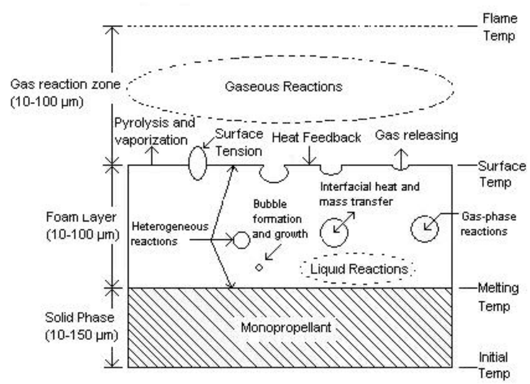


Modeling Efforts

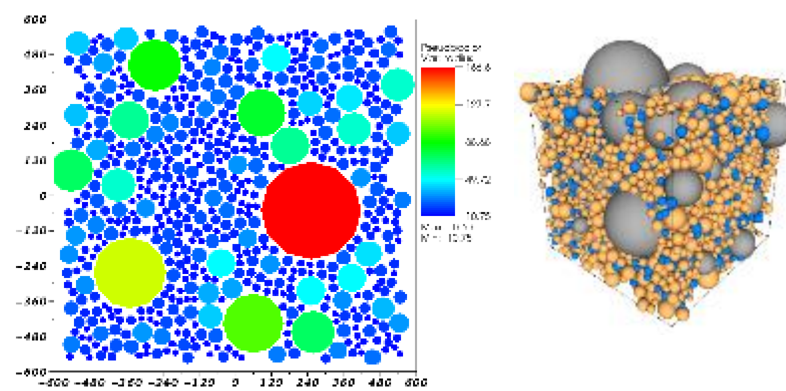
- Propellant models have been around for a long time
  - 3-Flame Structure over single AP crystal from BDP 1970
  - Evolved to sandwich or laminate model (Strahle et al. 1972, Price et al. 1986, Hegab et al. 2000, and others)
  - Rocfire 3D simulation by Jackson et al. 2000, Particle Packing Knott et al. 2001
  - Gallier et al 2006 model for ignition of propellant pack
  - Simulation of diffusion flame by Gross et al 2008-2015
  - Lack the predictive aspect



BDP 1970



Flame structure Gross 2008



Jackson et al. 2000 and Knott et al. 2001

Correlation Efforts

- Correlations based on empirical data to predict particle size effects in both open lit Summerfield 1961
  - Host of others attempting to model the AP size dependence

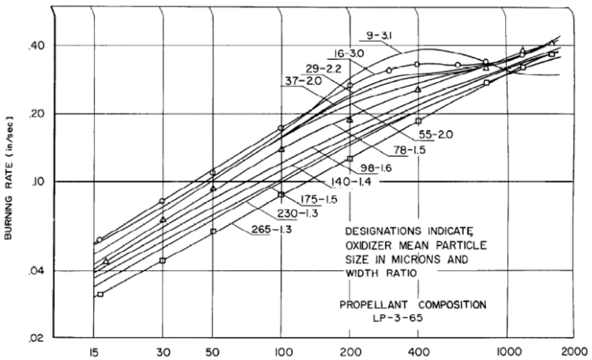


FIGURE 4 BURNING RATE VS PRESSURE
POLYSULFIDE PROPELLANTS, NARROW UNIMODAL
PARTICLE SIZE DISTRIBUTIONS

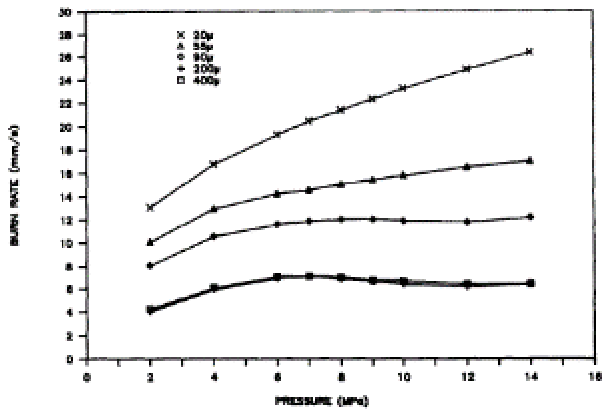
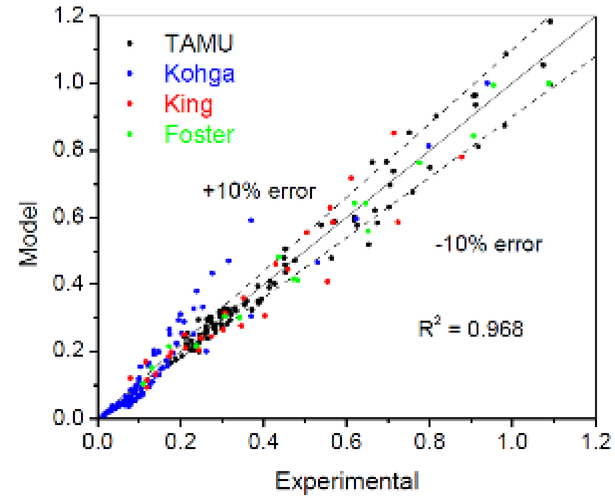


Fig. 6. Burning rates at 20°C for pentamodal AP pseudopropellant.



Summerfield et al. 1961

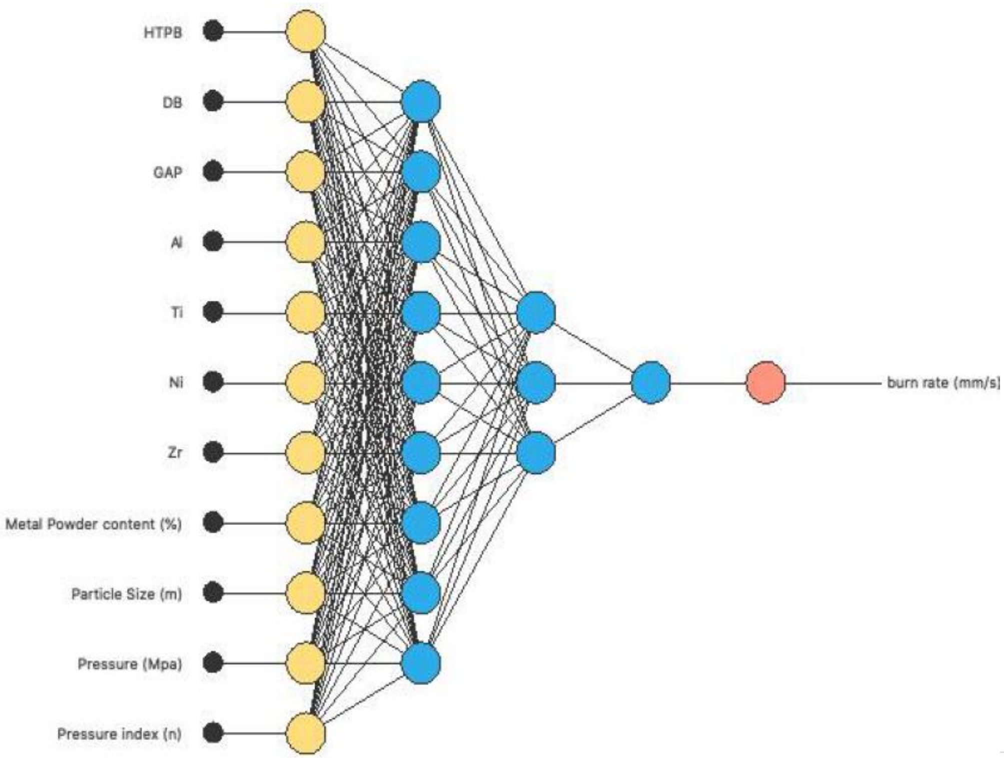
Fong and Smith 1987

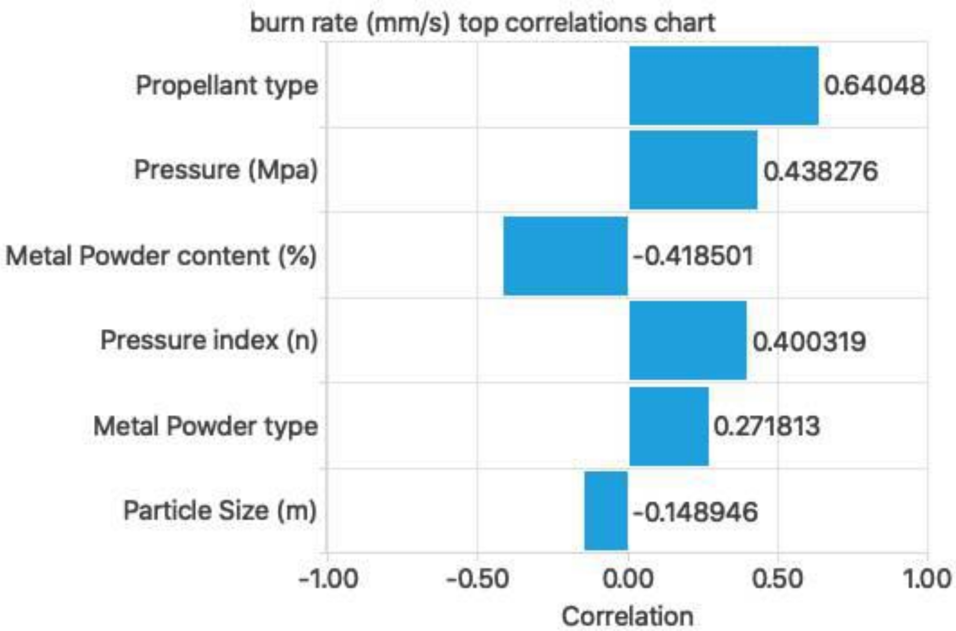
Marrow thesis-TAMU 2018

- Others such as Miller et al. 1982, Atwood et al. 1999, Price et al. 2003 evaluated AP particle size dependence on propellants
- None have been used as a predictive tool in propellant formulization development burning rates or ballistics
- Models do not generalize and materials change
  - Particle size distributions often not reported or with limited information
- ML collaboration by Abrukov et al. 2020 and Mariappan et al 2020 (AIAA propulsion and energy)

Machine Learning Effort

- **Abrukov et al. AIAA P&E meeting 2020**
- Russia/India Collaboration on ML
  - Network with 3 layer: Scaling, Perception (neuron) and Unscaling
  - Neurons- mathematical function the takes inputs and multiplies them by weighting function and adds the output
  - 11 inputs with 9 neurons at first layer
  - 9 input and 9 neurons at the second layer
  - 9 inputs and 1 neuron at third layer



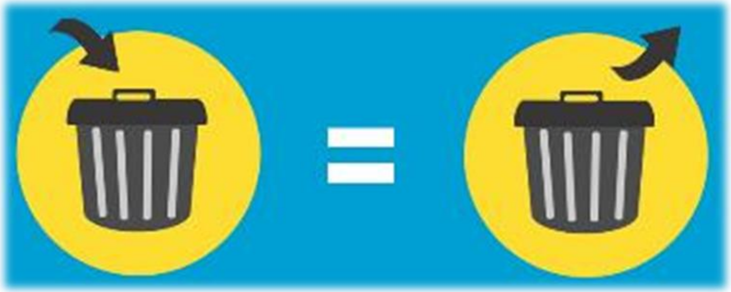


- **Correlation important propellant properties**
  - Results on 20 propellants, 5 pressures (145 to 1250 psi), single AP size, and multiple metals (Al, Ni, Zr)
  - AP Size not correlated with burning rate
  - Materials now well characterized

DATA-DRIVEN EFFORT

Work is "data-driven":

AI & ML models are trained on data.



Garbage in, Garbage out

Stories of three approaches to formulation data:

New DoD experiments

Historical DoD data mining

Analysis of open data

Experimental Objectives

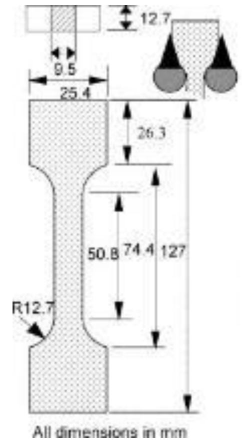
- Focus on reduced smoke compositions for formulation and testing
- Systematically study the chemical effects of binder molecular weight, curative, oxidizer particle size, concentration, and coarse to fine ratio on propellant burning rates
  - Well characterized particle sizes
  - Identify pressure dependency and temperature sensitivity for propellants
    - Test pressures up to 8000 psi to capture slope break
  - Testing at NAWCWD-CL and NSWC-IHEODTD to eliminate manufacturing variability
  - Develop relationship with burning rate and Pressure, Temperature, and Particle size/concentration as described by equations:

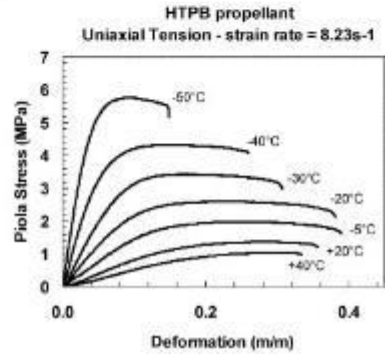
$$\mathbf{r_b} = aP^n e^{\sigma_p (T_i - T_{ref})}$$

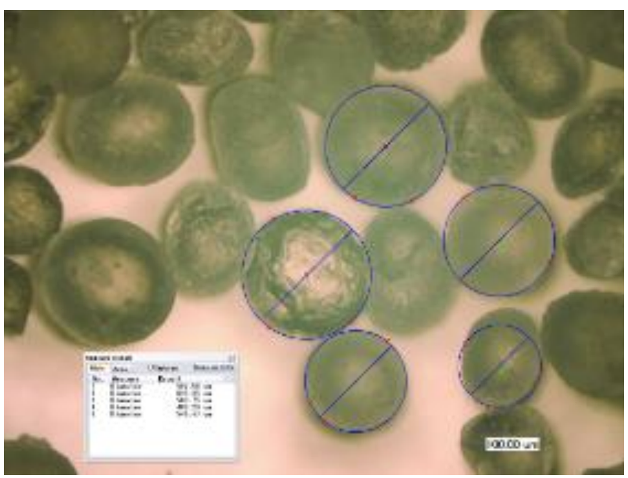
$$\sigma_p = \left(\frac{\partial \ln r}{\partial T_i} \right) \Bigg|_p$$

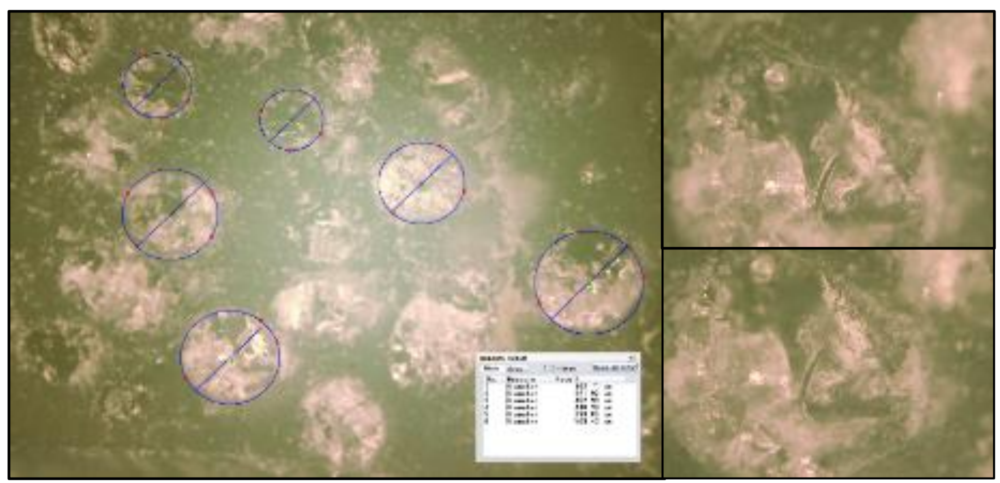
Propellant Characterization

- Characterize large data set of materials for basic AP/HTPB composite propellants
  - Identify potential AP grinding
    - Increases in ballistic data
  - Link Mechanical properties to ballistics
    - Strength testing for stress and strain
    - Viscosity of mixture
  - Compare facility testing from different locations



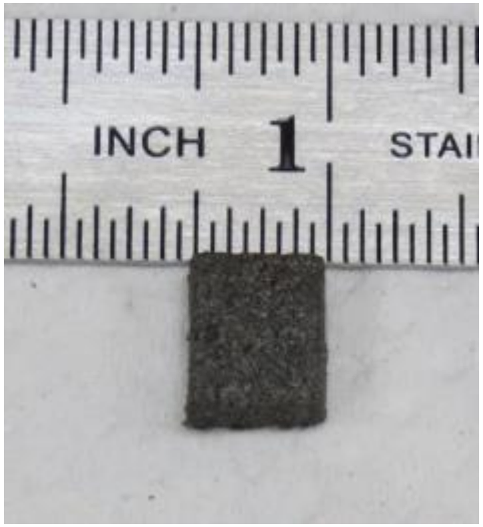


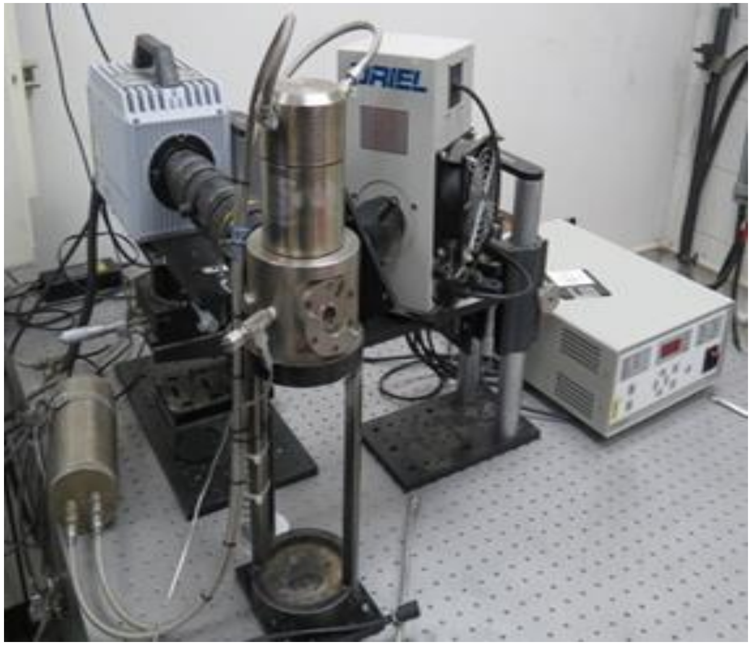




Experimental Facility: NAWCWD-CL

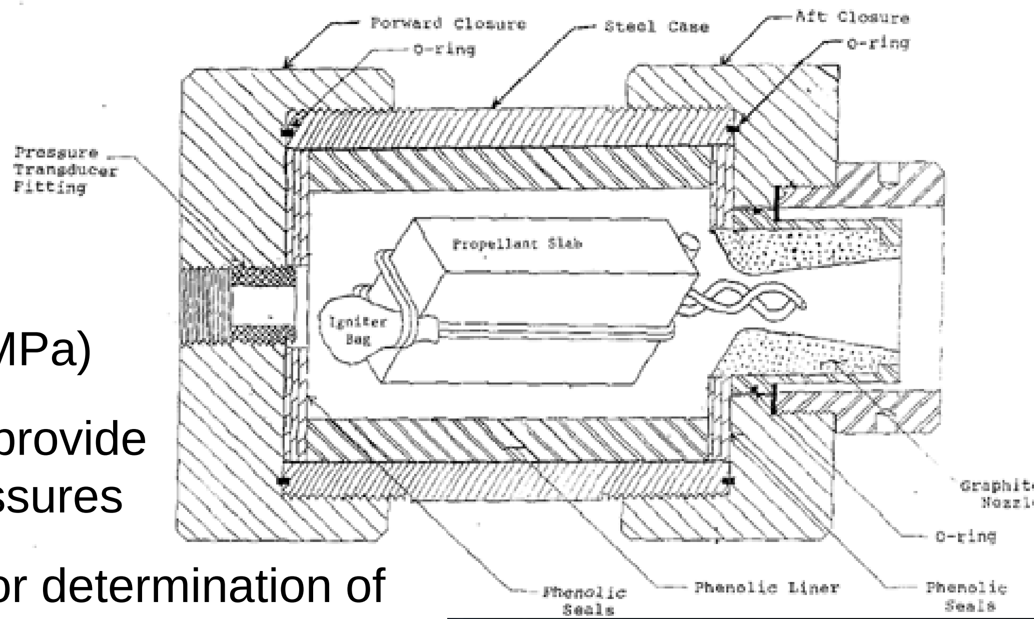
- Burned at 1.7 to 10.3 MPa (250 to 1500 psi) (LPWB)
- Burned at 10.3 to 55 MPa (1500 to 8000 psi) (HPWB)
  - Nitrogen used as pressurizing gas
  - Visual burning rate measurement
- Photron Fastcam SA1.1
  - 700 frames per second
  - K2 lens system with CF2 objective
- Nichrome wire Ignition .3 mm (.012 in.)





INDIAN HEAD EXPERIMENTAL EFFORT – Mini Slab

- Standard Slab: 1” x 2.6” x 6”
  - ~1 lbs, up to 10kpsi (69 MPa)
- Mini Slab: 0.75” x 1.75” x 2.5”
  - ~100 grams, up to 5kpsi (34 MPa)
- Unlike strands, a single firing can provide burning rate data over a range of pressures
- Temperature conditioning allows for determination of temperature sensitivity
- Data collected: chamber pressure, thrust
  - Data deduced: burning rate, specific impulse, c*, temperature sensitivity
- Slab motor has been used regularly for ~30 years on all types of propellants → lots of data to mine



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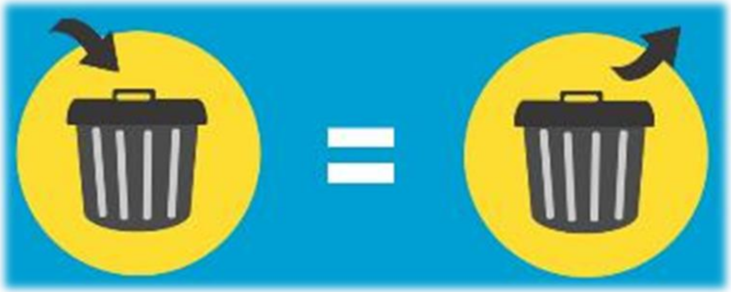

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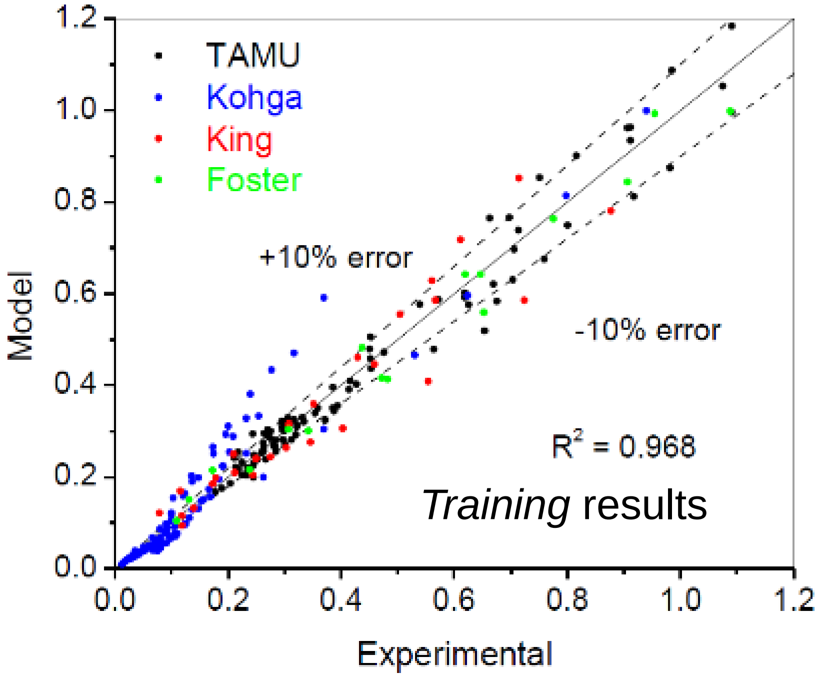
MODERN EMPIRICAL CORRELATION

Start with Vielle's Law: $BR = aP^n$

Make prefactor and exponent dependent on particle diameter ***D*** and solids concentration ***C***

$$a = 0.438\boldsymbol{D}^{-0.942+1.034\boldsymbol{C}}\boldsymbol{C}^{14.702-0.045\boldsymbol{D}}$$

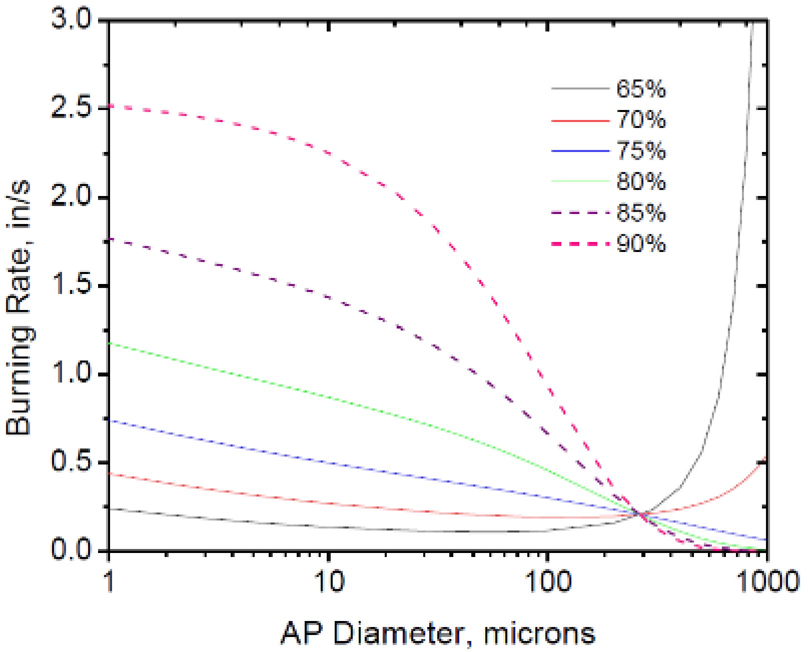
$$n = 1.736 - 0.002\boldsymbol{D} - 1.397\boldsymbol{C}$$



Above: training results with R^2 0.968, RMSE 0.054 in/s
NOT SHOWN: test results with R^2 0.818, RMSE 0.477 in/s

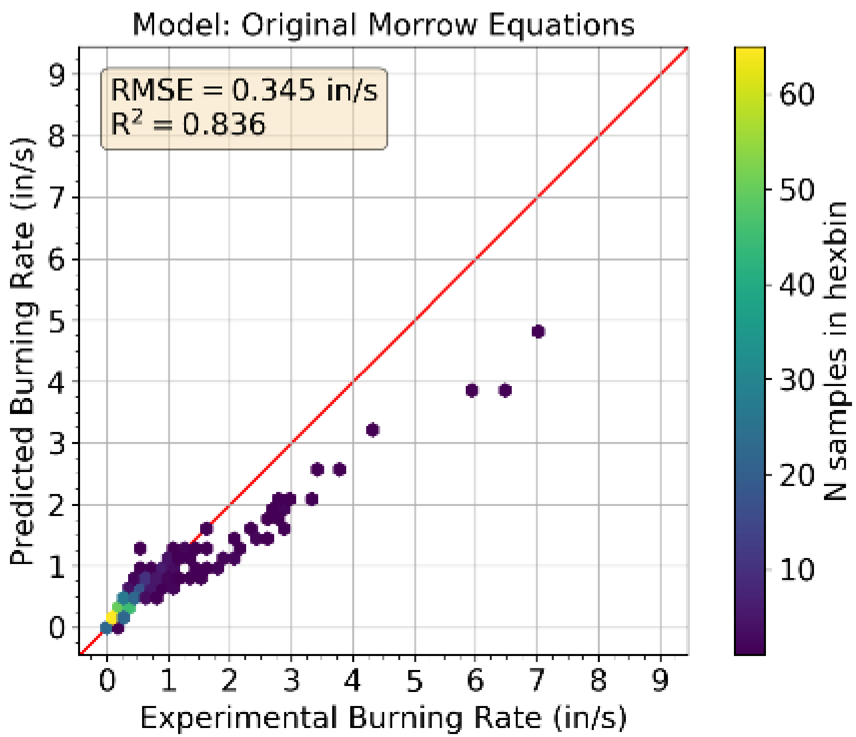
Correlating the Effects of AP Particle Size and Concentration on AP/HTPB Composite Propellant Burning Rates, Gordon R. Morrow, Master's Thesis, 2017. Prof. Eric L. Peterson, TAMU.

Empirical, physics-inspired model fits the training data, but fails outside of trained particle size data.

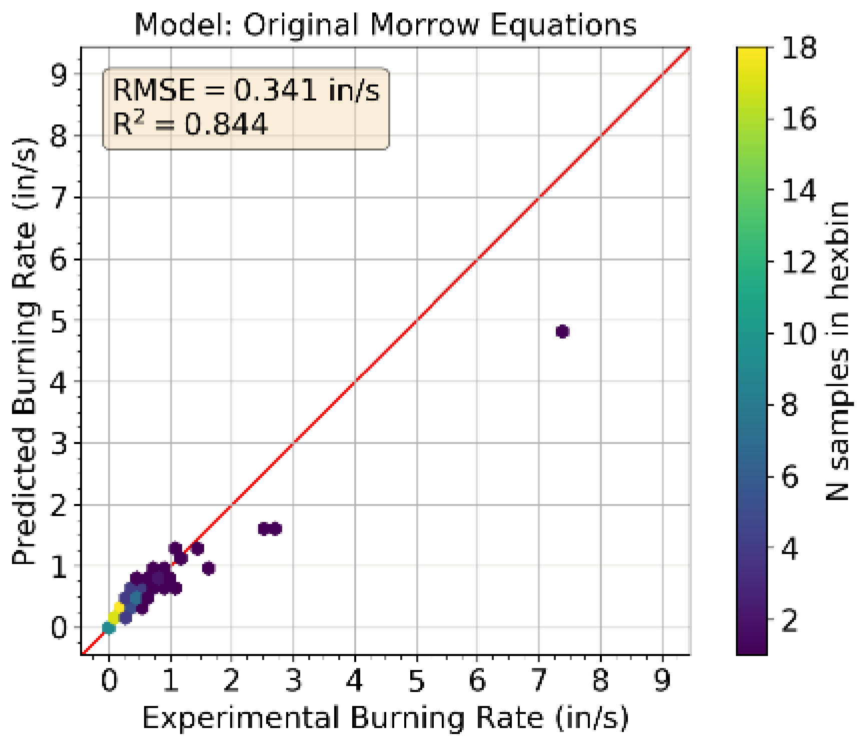


Let's try something else with the data…

Shuffle all 8 datasets together and partition to train/test. Morrow’s model performance is shown below. Note large number of samples near 0.1-0.3 in/s.



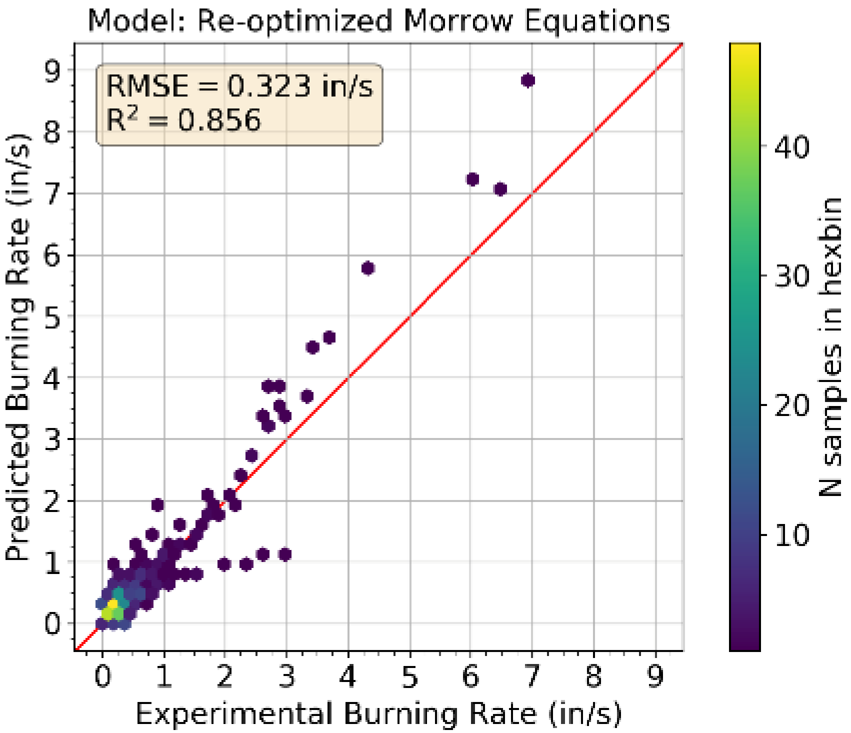
Training Results



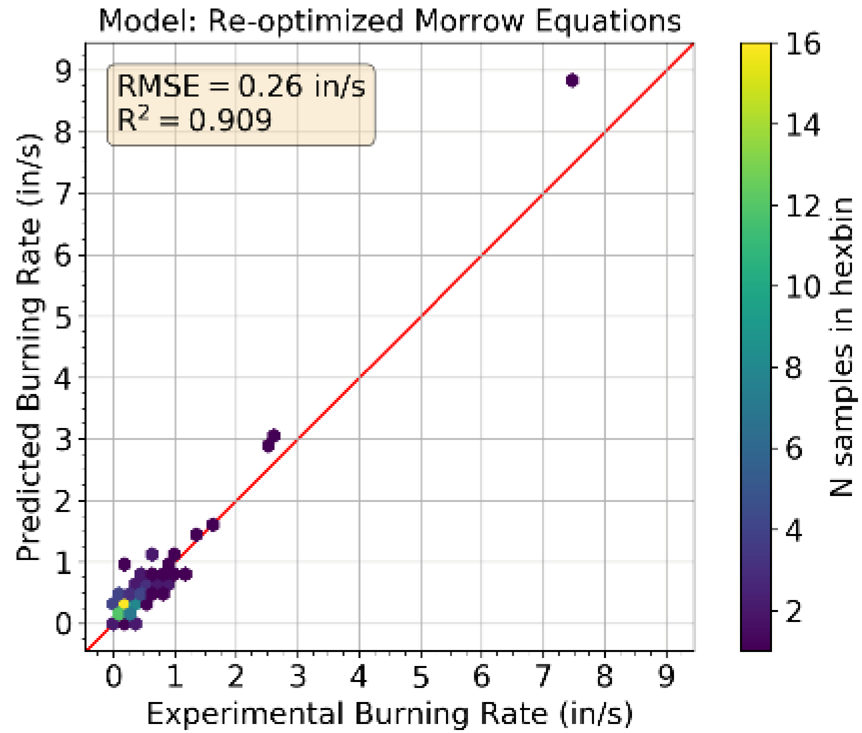
Test Results

Use non-linear least squares to re-optimize Morrow parameters.

Results improve, but model has significant errors.



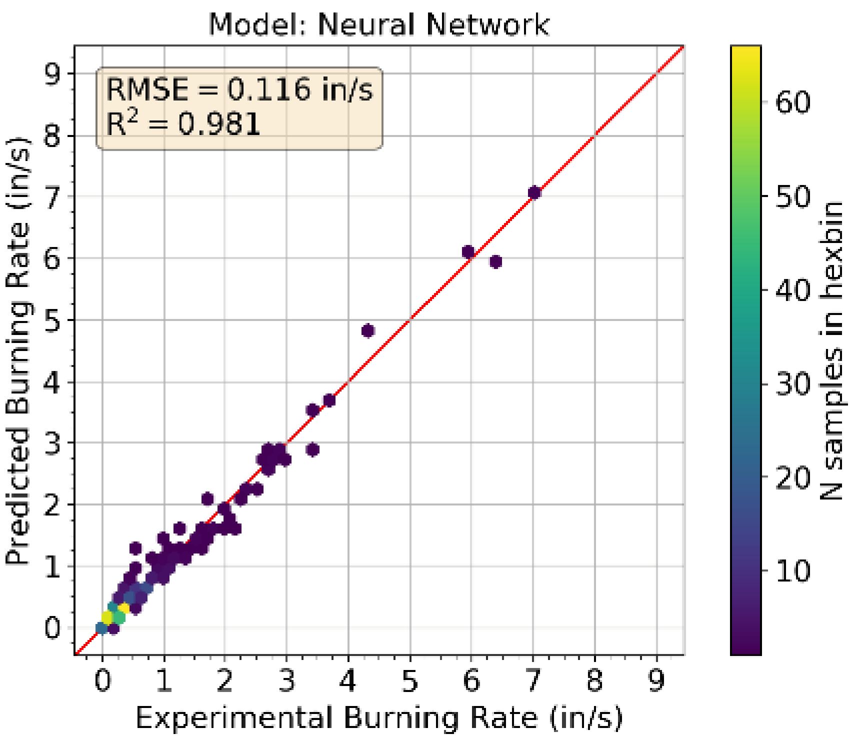
Training Results



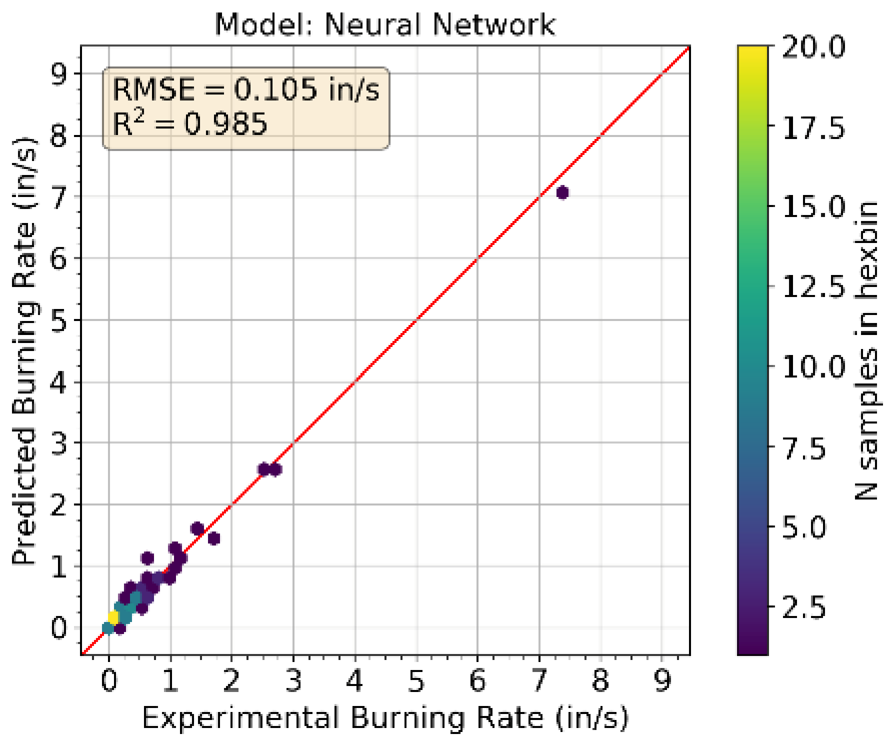
Test Results

A neural network beats Morrow's correlation by any metric.

Machine learning can improve formulation property predictions.



Training Results



Test Results

Summary

- Explored the literature to curate large data set
  - A lot of unknowns in open literature (polymer chain length, cure ratio, AP size distribution)
  - Need well characterized inputs for model
- Work to collect burning rate data over wide pressure range with a connection to mechanical properties in progress.
  - Searching all available data sources
  - Open to collect propellant data from those willing to share
    - Reach out to anyone on the team
- Each method has advantages and disadvantages
  - Determine what you want from your data

Questions?