Modeling and Simulation of Combustion of Solid Propellant Ingredients Using Advanced Capabilities

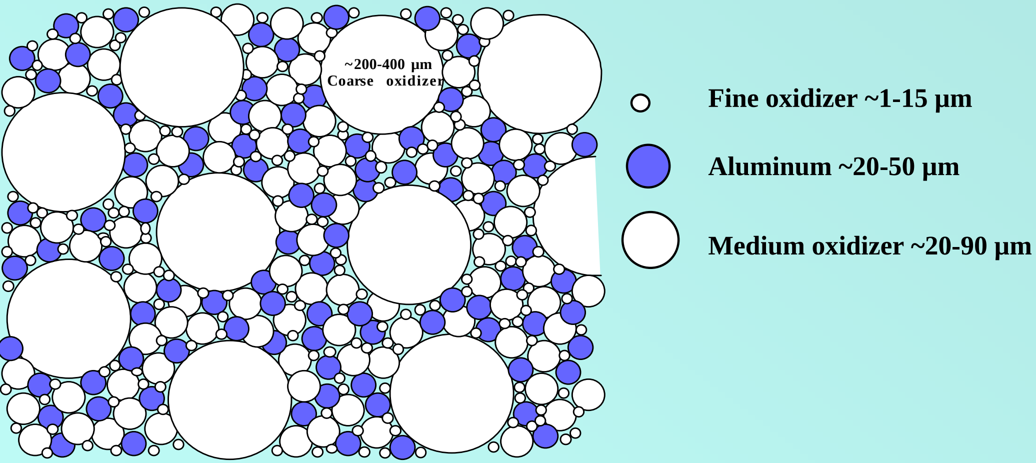
by

M. W. Beckstead and K. V. Puduppakkam

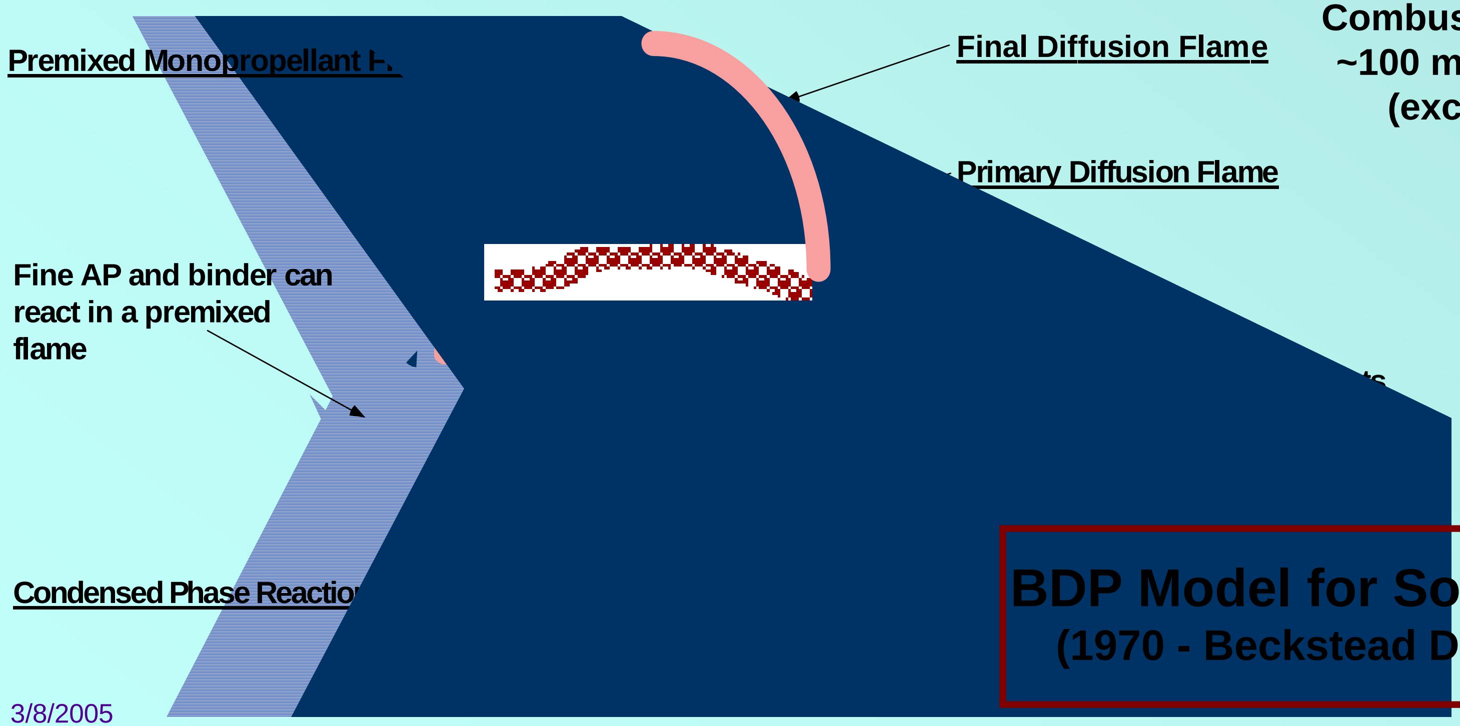
Brigham Young University

This work was sponsored partly by BYU, and partly by ONR Contract N00014-02-C-0292, Program Manager Dr. Judah Goldwasser, (subcontracted through SEA, Carson City, NV)

Typical Solid Propellant Mixture & Combustion
(looking at it under a microscope)



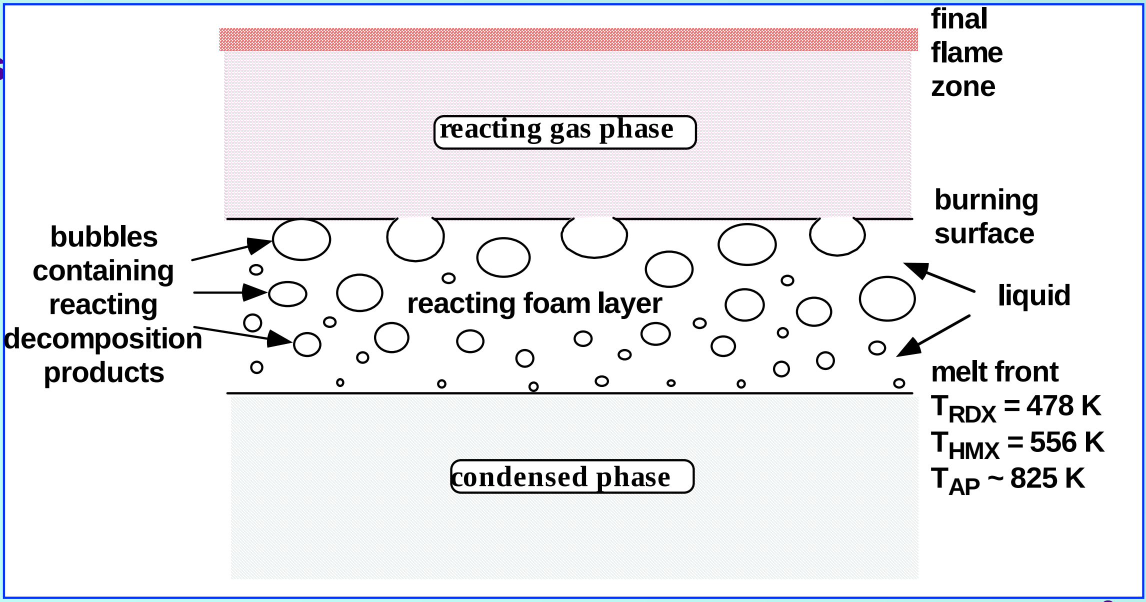
Combustion occurs within ~100 microns of surface (except Aluminum)



BDP Model for Solid Propellants
(1970 - Beckstead Derr Price Model)

Objective

- Assess progress in detailed kinetic modeling from 1995 til now
- Solid propellant ingredients - RDX, HMX, GAP, AP, . . .
  - 1-D & homogeneous
- Using available mechanisms
- Focus on chemical families
  - Nitramines
  - Azides
  - Nitrate esters
- Model pseudo-propellants (mix 2 or more ingredients)
  - Use same mechanisms
  - Average physical properties



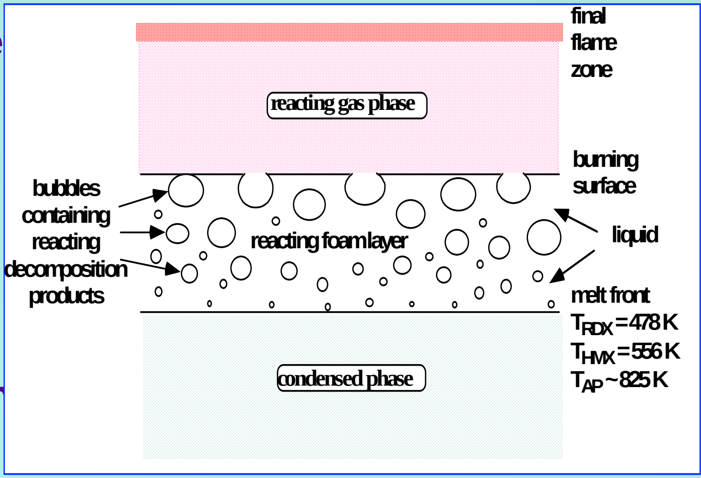
Monopropellants Modeled with Detailed Kinetics since 1995

- Work prior to 1995 summarized previously

Monopropellant	Chemical family	Researcher	Year
RDX	Nitramine	Liau et al.	1995
		Prasad et al.	1997
		Davidson et al.	1997
		Miller et al	2000
HMX	Nitramine	Davidson et al.	1996
		Prasad et al.	1998
		Kim	1999
GAP	Azide	Davidson et al.	1996
		Puduppakkam et al.	2003
NG	Nitrate ester	Miller et al.	2000
BTTN	Nitrate ester	Puduppakkam et al.	2003
AP		Jing et al.	1998
ADN		Liau, et al.	1998
		Liau, et al.	1999

Approach to Combustion Modeling

- One-Dimensional & Steady-state
  - Limited transient work done - more cpu intensive
  - Liau ignition model
  - Erikson oscillatory model
- Gas phase modeled by modified PREMIX code
  - Mass, energy and species conservation eq'ns
  - Detailed kinetic mechanisms
  - Yetter RDX mechanism provided solid foundation
- Solid region
  - Heat transfer only - no reactions in solid
- Condensed phase region - liquid/gas bubbles
  - Energy and Species Eq'ns
  - Evaporation usually considered
  - Semi-global condensed phase reaction(s)



<u>**Typical Dimensions**</u>
(decrease with pressure)

from surface to flame
~ 10 to 100 μm

liquid layer
~1-100 μm

- Burning rate determined by matching heat flux at boundary
- Different modelers use slightly different approaches/assumptions

Gas Phase Kinetic Mechanisms

Ingredient	Species	Reactions	Comments
RDX	45	232	Based on 1 mechanism
HMX	45	232	
AP	33	79	
ADN	33	180	
AP/HTPB	44	157	Based on 3 mechanisms
GAP	74	460	Based on 4 mechanisms
BTTN	75	462	
RDX/GAP	76	488	
RDX/GAP/BTTN	76	488	

- BYU combined mechanism: 76 species & 488 reactions
- Redundant reactions eliminated (Yetter reactions used)
- Chlorine containing reactions eliminated
- 4 reactions from GRI and AP mechanisms inconsistent with Yetter mechanism for RDX monopropellant combustion

Condensed Phase Kinetic Parameters

- **Consistent trends within chemical families**
- **Global or key step usually identified**
- **Measured Ts data can be used for global kinetic reaction**
    - **(Miller/Anderson approach)**

Calculated Burning Rate Curves

Mono-propellant	% data within	± error
RDX	85	15
BTTN	100	15
AP	83	7
GAP	80	10
NG	82	15

- **Burning rate predictions very reasonable over a wide range of pressures**

Calculated Pseudo-Propellant Burning Rates

- **Pseudo-propellants have lower burning rates than monopropellants**
- **RDX/GAP/BTTN has higher burning rate than RDX/GAP**
- **Pressure exponent similar for RDX, BTTN, pseudo-propellants, different for GAP.**
- **RDX/GAP/BTTN calculation was a blind prediction (<4% error)**

Calculated Temperature Profiles
(at 5 atm)

- **Huge variation in temperature profiles**
- **BTTN yields significant dark zone**
- **GAP/RDX and GAP/RDX /BTTN show slight inflection**
- **RDX - no dark zone and very high gradient (same as AP)**

Calculated Dark Zone Temperature Profiles

BTTN calculations

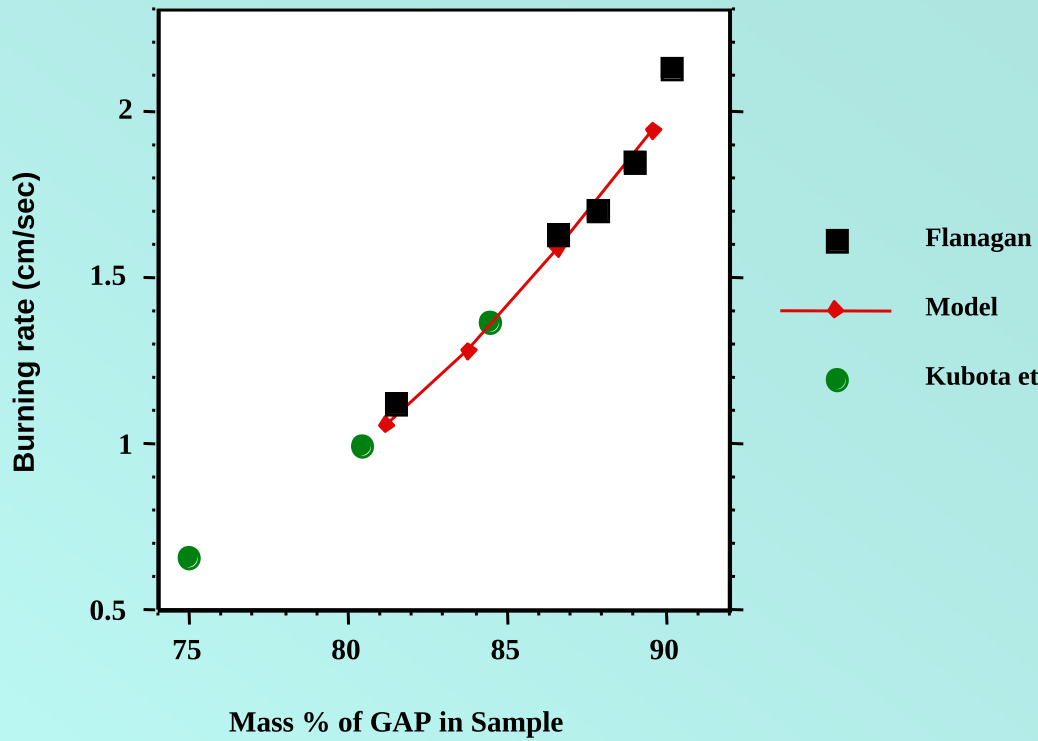
RDX calculations

- **Nitrate esters exhibit dark zones - calculation show the same**
- **RDX with laser augmentation exhibits a dark zone - calculations show the same**

Burning Rate Variations with Concentrations

GAP/RDX calculations

GAP/HMDI calculations



Rate decreases for RDX/GAP mixture - calculations show consistent trend

Large dependence of burning rate on azide content

Model calculations match well with experimental data

"Homogenized" AP/HTPB Binder Calculated Rate

Comparison with Literature Data

- Homogeneous AP/HTPB
  - Fine AP < 10 μm
  - No diffusion flame
- 1000 psi
- AP model plus some GRI reactions
- 44 species and 157 steps
- Experimental data (Foster)
  - 12 μm AP/HTPB

Model matches experimental data well, especially at high pressures

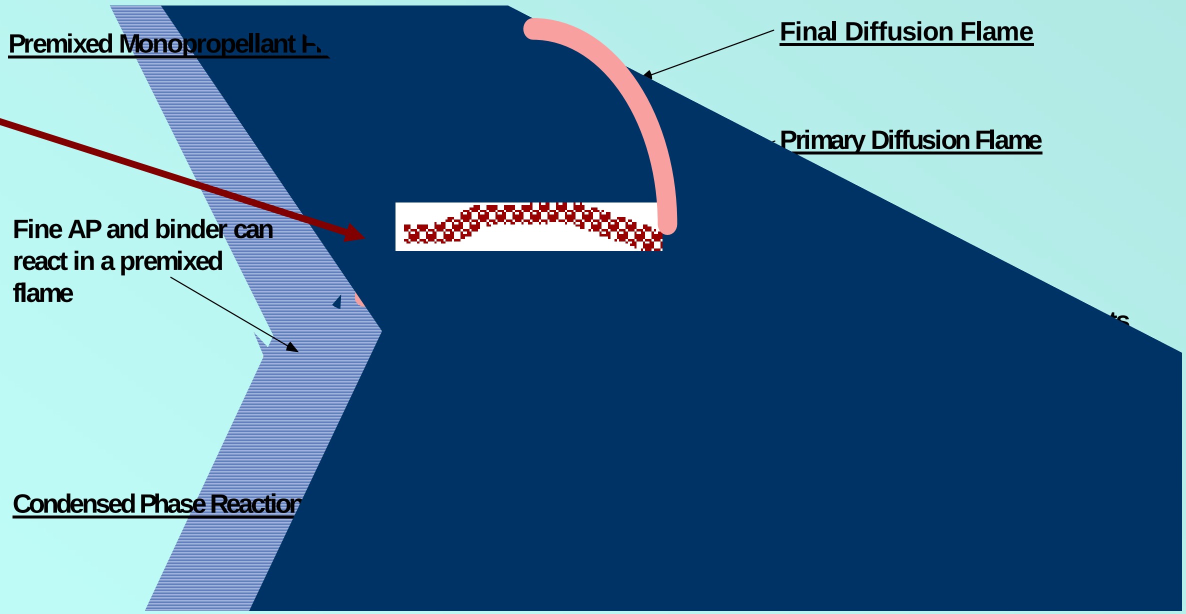
Low Pressure exponent ~ 0.4

FUTURE WORK

Extend Current Approach to Typical AP/HTPB Propellants

Will require modeling the primary diffusion flames

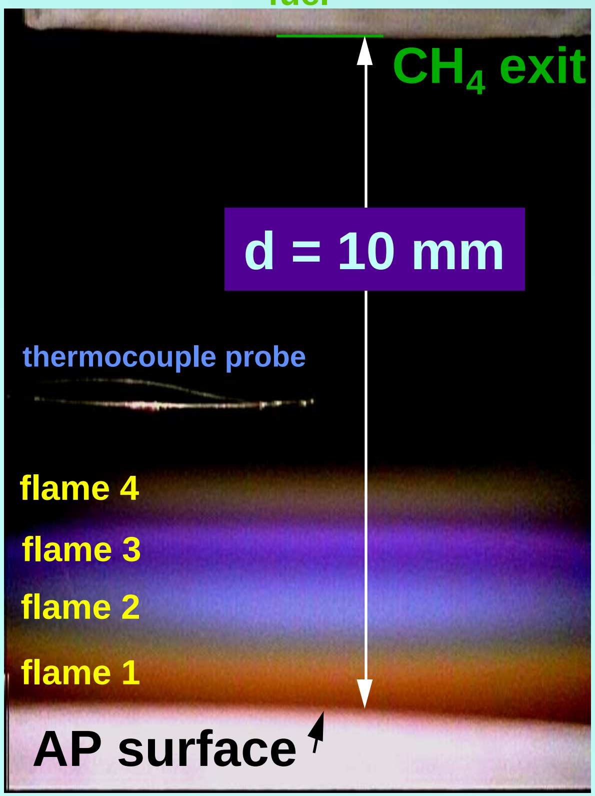
AP/HTPB Propellant Flames



Diffusion Flames Dominate AP Propellant Combustion

NAWC 1D AP/CH_4
Counter-Flow Diffusion Flame

v_{fuel} = 26 cm/s



v_{apgas} = 49 cm/s

BYU Calculated Diffusion Flame
For AP/HTPB Propellant

Final diffusion flame

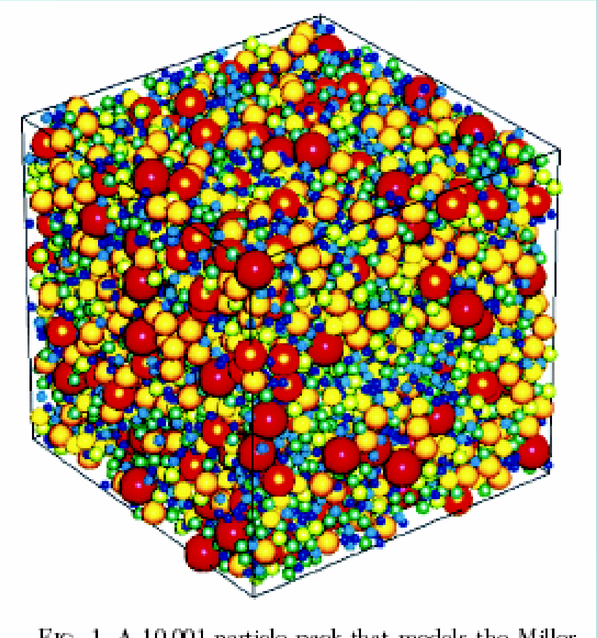
AP monopropellant flame

Primary diffusion flame

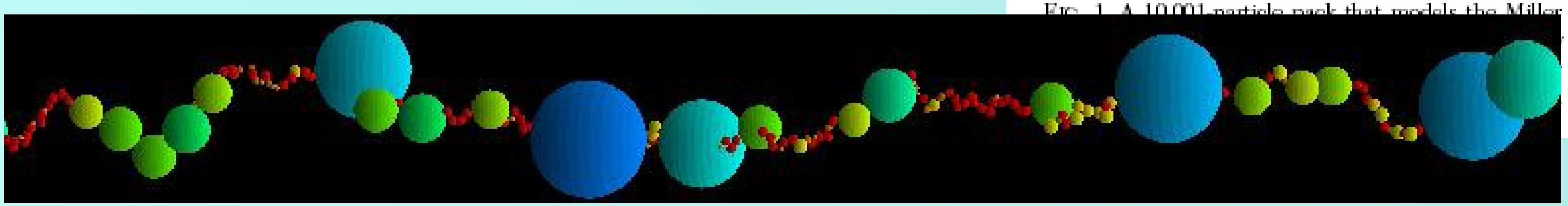
Premixed binder flame

D_{AP} = 400 μm
Binder: 77.5% AP
δ_{binder} = 89 μm
P = 20 atm

Finding an Average Rate for Complex Geometries



- Defining complex particle packing is possible
  - ATK/Thiokol - Lee Davis' ParPack
  - UIUC - Jackson/Buckmaster RocPack
  - GIT - Menon DNS calculations
- Find a burning path through particle pack
  - DNS calculations time consuming and miss details
  - How to define a representative path?
  - Assumptions to make in calculating overall rate?
  - How to incorporate the diffusion flames?
  - How many particles to include?

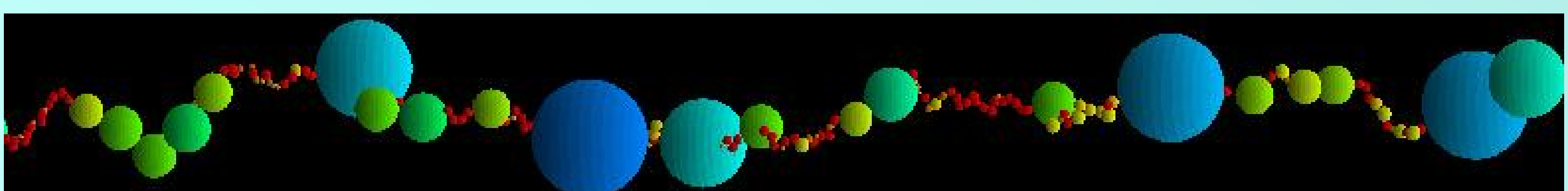


- Preliminary algorithm – Slower burning binder
  - Start with the highest particle
  - Shortest path to next particle
- Faster burning binder
  - Will need a different approach?

Particle Size Effect for Advanced Ingredients (non-AP)

- Inverse particle size effect in some advanced propellants (ADN)
- A reduced effect anticipated with energetic binders (depending on r_{binder} vs r_{solid})
- Smaller particles burn with a premixed flame
- Large particles approach monopropellant rate

Complex burn rate path?



Summary and Conclusions

- Tremendous progress in modeling solid propellant ingredients
- Detailed kinetic data improving in quantity and quality
- Models developed for several key ingredients
- Predicted combustion trends consistent with experimental data
- Pseudo-propellant trends consistent with experimental data
- Biggest challenges
  - Condensed phase description
  - Particle size effects
  - Describing diffusion flames (AP propellants)
  - Defining overall rate for propellant surface
- Future potential - very promising
  - Potential for a standard comprehensive mechanism
  - Combining with packing model
  - A priori propellant predictions??