Modeling of Heterogeneous Solid Propellant Flames

T.L. Jackson* & J. Buckmaster**

****Senior Research Scientist, Center for Simulation of Advanced Rockets***
Adjunct Professor, Department of Theoretical & Applied Mechanics
***** Professor, Department of Aeronautical and Astronautical Engineering***
University of Illinois at Urbana-Champaign

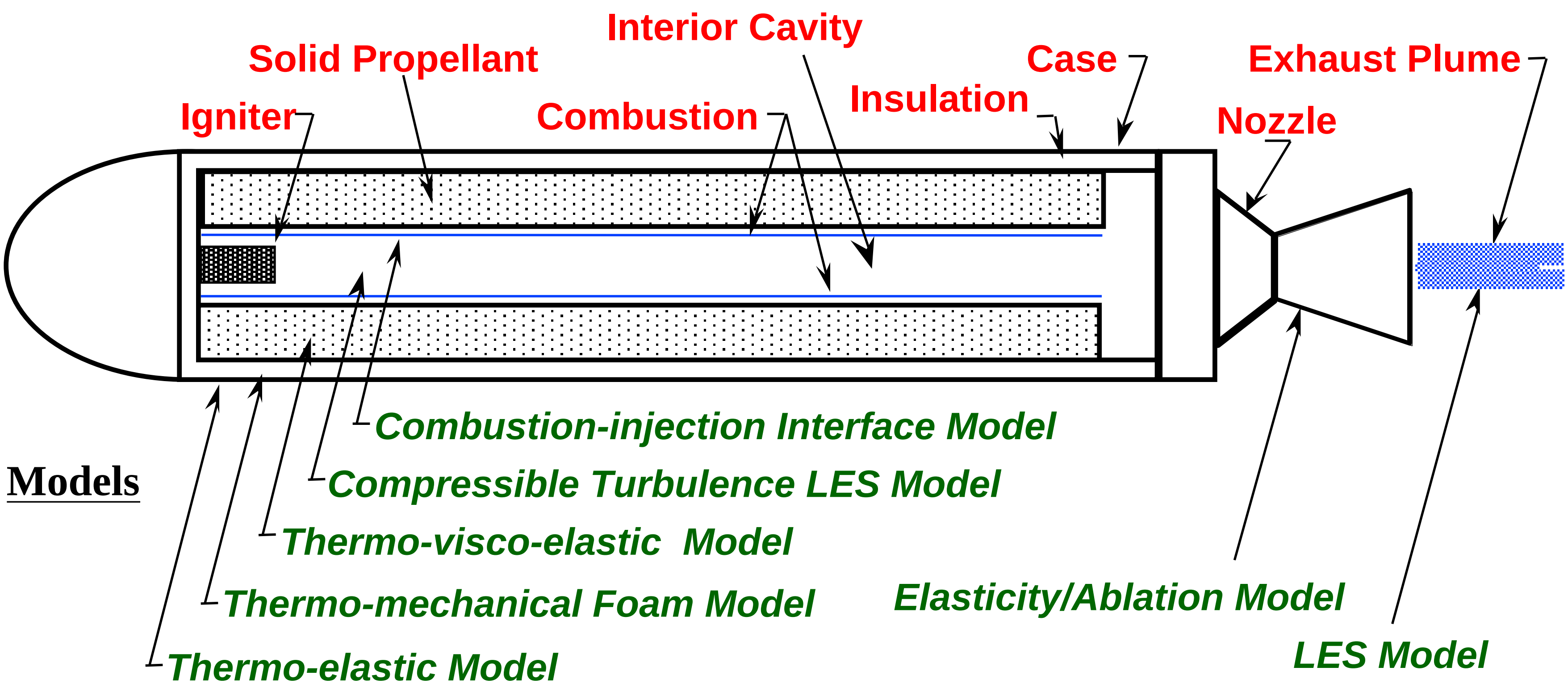
Center for Simulation of Advanced Rockets (CSAR)

- One of five ASCI (Accelerated Strategic Computing Initiative) centers funded by DOE (beginning October 1997)
- Goal of the center is the detailed, whole-system simulation of solid propellant rockets under both normal and abnormal operating conditions
  - develop appropriate software for the simulation of complex, large scale multi-component systems
  - subscale simulations of materials/accident scenarios
  - accurate models of physical components
  - interface code to enable component interactions
  - computational infrastructure to support large scale simulations
  - research collaborations with the three DOE laboratories (Los Alamos, Sandia, Lawrence Livermore)
- Currently have about 42 faculty, 25 professional staff, and 45 students

Idealized Solid Rocket

Components

Models



Center for Simulation of Advanced Rockets

University of Illinois at Urbana-Champaign

Introduction

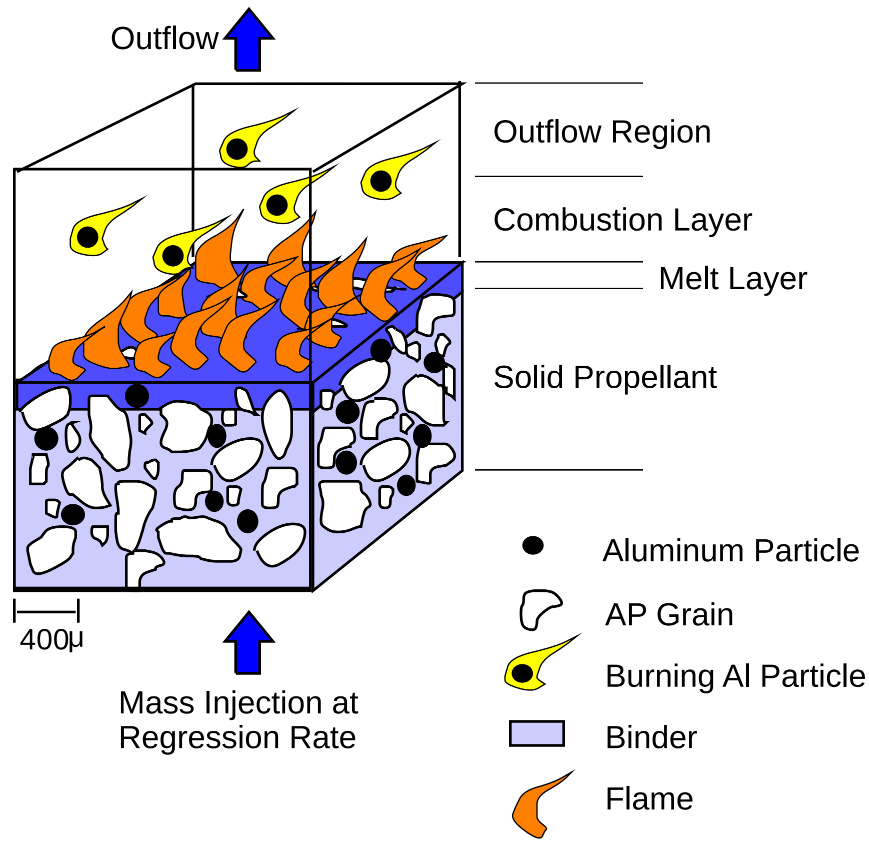
- Primary task is to develop appropriate software for the simulation of complex, large-scale multi-component systems
- Due to large disparity in scales, a DNS is not feasible
  - booster   30 meters in length
  - smallest scales   1-10 microns
- Sub-grid modeling of various physical components necessary for meaningful results
  - models must be relevant, with a view of how they are going to be incorporated into the system code
  - must consider time-line in building models
  - for combustion, proper sub-grid modeling is important as it provides the proper boundary conditions for the internal flow-field

CEM Group Research

- **Combustion interface code**
  - **Physical jump conditions across solid/gas interface**
  - **Algorithm to move the interface; mesh association and data transfer between solid/gas meshes**
  - **Need constitutive relations for burning rate, temperature jump, etc.**
    - **Assume a phenomenological law (e.g.,** $r_b = aP^n, \quad T = T_f$ **; other response functions)**
    - **Assume propellant is homogeneous and flat (1D analysis coupled to the solid; possible 'separate' 1D combustion code)**
    - **Sub-grid modeling (require numerical/modeling strategies)**
    - **Well defined experiments for validation/insight**

Sub-grid Combustion Model

- The sub-grid model will be developed at the 1 to 10 m resolution to describe the detailed physics
- Model will include energetic grains, oxidizers, binder, melt layers, flames, burnt gases, etc.
- Important questions
  - flame structure
  - generation of vorticity
  - turbulence generation
  - interaction with pressure and velocity fluctuations generated in the hot core flow
- Collaborative effort among the various disciplines within the center
- ASCI level research problem



Center for Simulation of Advanced Rockets

University of Illinois at Urbana-Champaign

Key Ingredients

- 3D
- propellant is heterogeneous (particle packing important)
- non-planar regression surface
- heat conduction within the solid
- account for AP decomposition and AP/binder flames
- fluid-mechanics effects
- effects of external flow field (acoustic waves, non-linear acoustic induced shear, turbulence) and interaction

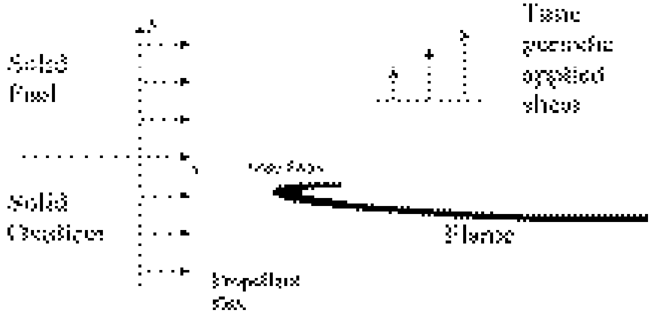
Major Obstacles to Overcome

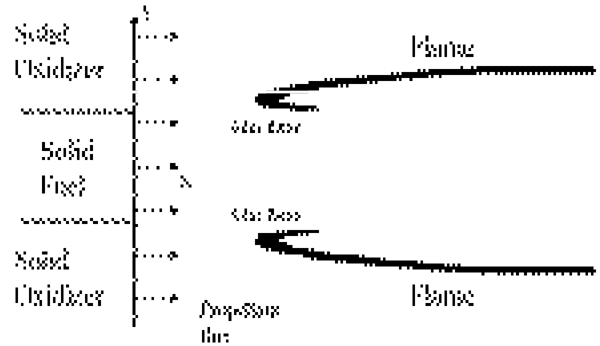
- Previous theories all one-dimensional
- Little is known about flame structure of heterogeneous propellants

Roadmap to Developing Sub-grid Model

- **Analyze simple flame geometries where the surface is 1D**
  - **flame is 2D; constant mass flux; no AP flame; 1-step kinetics; flat surface**
  - **provide an understanding of the complex combustion field that is generated by burning a heterogeneous solid propellant of the kind used in high-performance rockets**
  - **only a few previously calculated 2D flame structure**
- **Analyze simple flame geometries where the surface is 2D**
  - **flame is 3D; constant mass flux; no AP flame; 1-step kinetics; flat surface**
  - **AP particles represented by a level set function**
  - **no previously calculated 3D flame structure**
- **Incorporate more complicated physics**
  - **low Mach number equations**
  - **coupling to solid phase**
  - **advanced kinetic models**
  - **non-planar propellant surface**
- **Sub-grid code (RocFire)**
  - **verification - recover simple models**
  - **validation - comparisons with experiments**

Elementary Flame Configurations for Heterogeneous Propellants

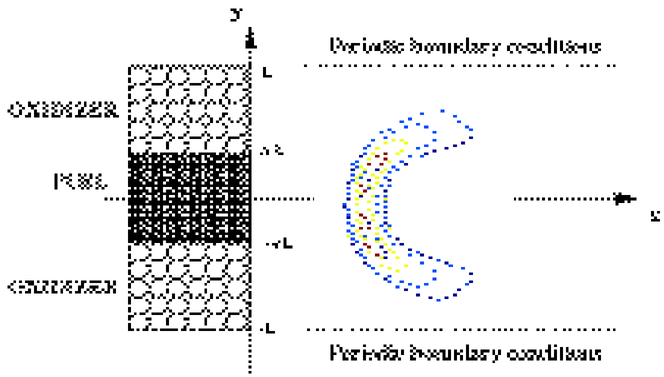


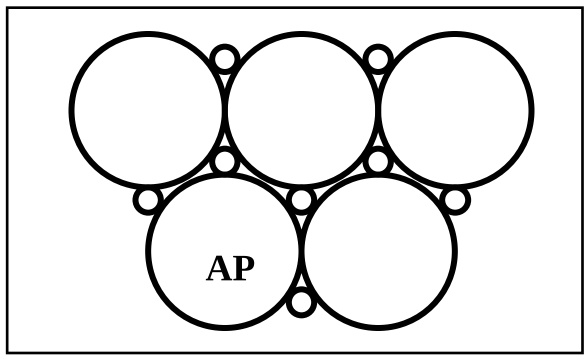


1/4 plane (with or without shear)

sandwich (e.g. Price, Brewster)

(Buckmaster, Jackson & Yao, C&F, 1999; Buckmaster & Jackson, C&F, 1999; Buckmaster & Jackson, AIAA 99-0323)





1D periodic (2D flame)

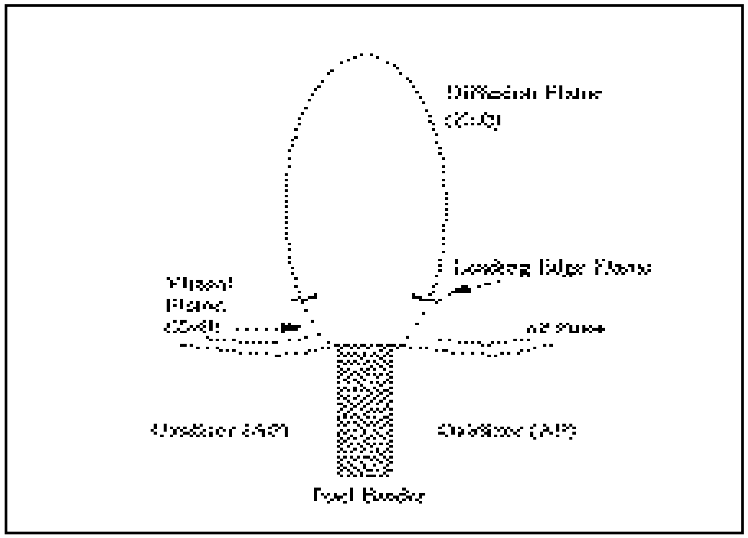
(Jackson & Buckmaster, JPP, 1999a, 1999b)

2D periodic (3D flame)

(Jackson, Buckmaster, Hoeflinger, in prep.)

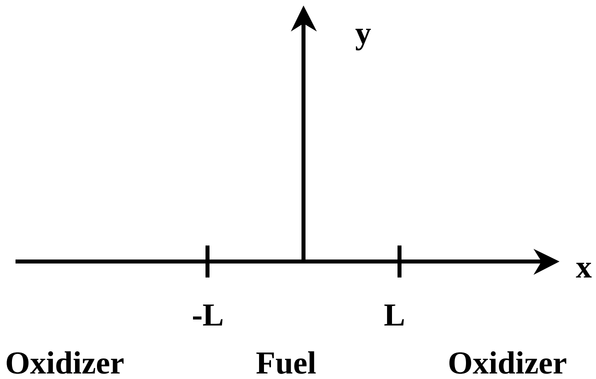
1. Sandwich Propellant Geometry

- Consider the following model propellant of Price
  - fuel-binder of thickness 0.1mm or so, layered between sheets of AP (ammonium perchlorate)
  - sketch of propellant flame for O/F/O sandwich



  - Price argues that the edge structures play an important role in the transfer of heat to the propellant, heat that is responsible for surface regression (the burning rate)

- **Configuration of sandwich problem**



- **Assume surface is flat, have constant mass flux**
- **Equations (X - oxidizer, Y - fuel)**

$$MX_y = \rho D \nabla^2 X - \alpha_x \Omega, \quad MY_y = \rho D \nabla^2 Y - \alpha_y \Omega$$

- **Flux boundary conditions**
  - **oxidizer** $\quad MX - \rho D X_y = k_x M, \quad MY - \rho D Y_y = 0$
  - **fuel** $\quad MX - \rho D X_y = 0, \quad MY - \rho D Y_y = k_y M$

- **Burke-Schumann analysis**

$$Z = \frac{X}{\alpha_x} - \frac{Y}{\alpha_y}$$

$$MZ_y = \rho D \;{}^2 Z$$

$$MZ - \rho D Z_y = M \begin{matrix} k_x / \alpha_x & \quad \mathit{Oxidizer} \\ k_y / \alpha_y & \quad \mathit{Fuel} \end{matrix}$$

- **Z=0 is the virtual flame, also called the stoichiometric level surface**

- **Convenient to first non-dimensional the system**

L	Reference length (fuel thickness 2L)
$Pe = \dfrac{ML}{\rho D}$	Peclet number
$\beta = \dfrac{\alpha_x / k_x}{\alpha_y / k_y}$	Stoichiometric coefficient
$Z = \dfrac{k_x}{\alpha_x} \quad S$	

$$S_y = (Pe)^{-1} \quad {}^2 S$$

$$S - (Pe)^{-1} S_y = \begin{cases} 1 & \textit{Oxidizer} \\ -\beta & \textit{Fuel} \end{cases}$$

Center for Simulation of Advanced Rockets

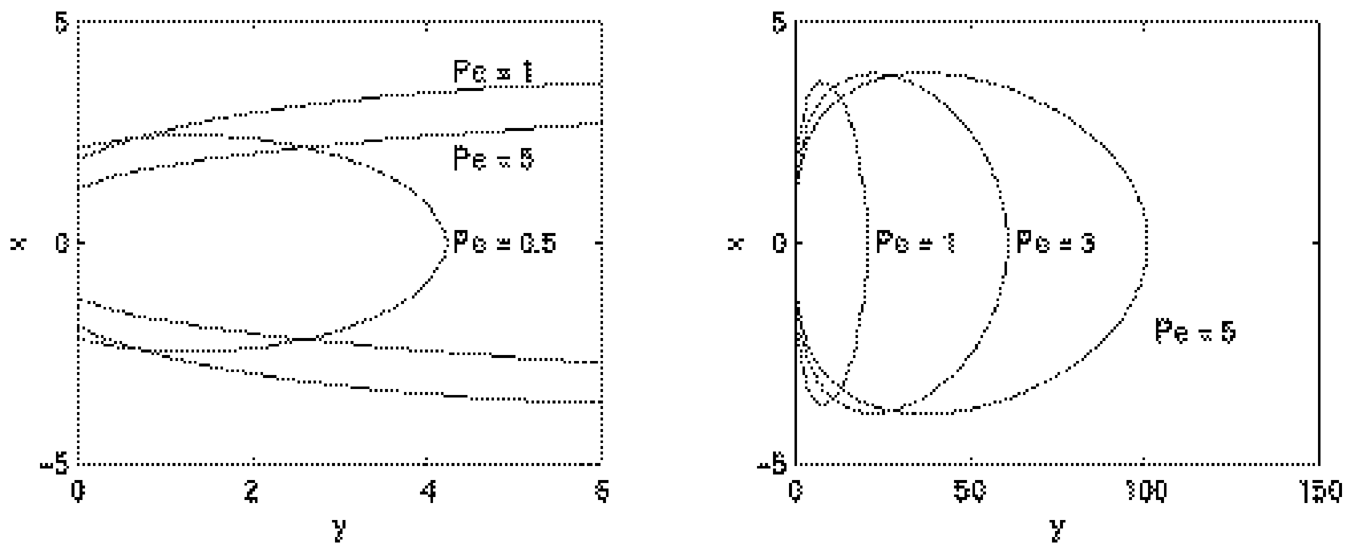
University of Illinois at Urbana-Champaign

- **Solution**

$$Z = \frac{k_x}{\alpha_x} - \left(\frac{k_x}{\alpha_x} + \frac{k_y}{\alpha_y}\right) \phi(x,y)$$

$$\phi = \frac{4}{\pi}\int_0^{\infty} \frac{\sin\omega}{\omega} \cos(\omega x) \frac{e^{yPe\left(1-\sqrt{1+4\omega^2/Pe^2}\right)/2}}{1+\sqrt{1+4\omega^2/Pe^2}}\, d\omega$$

- **Stoichiometric level surface (Z=0) for =7**



Center for Simulation of Advanced Rockets
University of Illinois at Urbana-Champaign

- **Finite rate chemistry effects**
  - **add temperature equation** $Mc_pT_y = \lambda \quad {}^2T + Q\Omega$
  - **bc** $T = T_w$
  - **reaction rate** $\Omega = BXYe^{-E/RT}$

- **Non-dimensional system**

$$L(X,Y,T) = (-1,-1,1)\delta XYe^{-\theta/T}$$

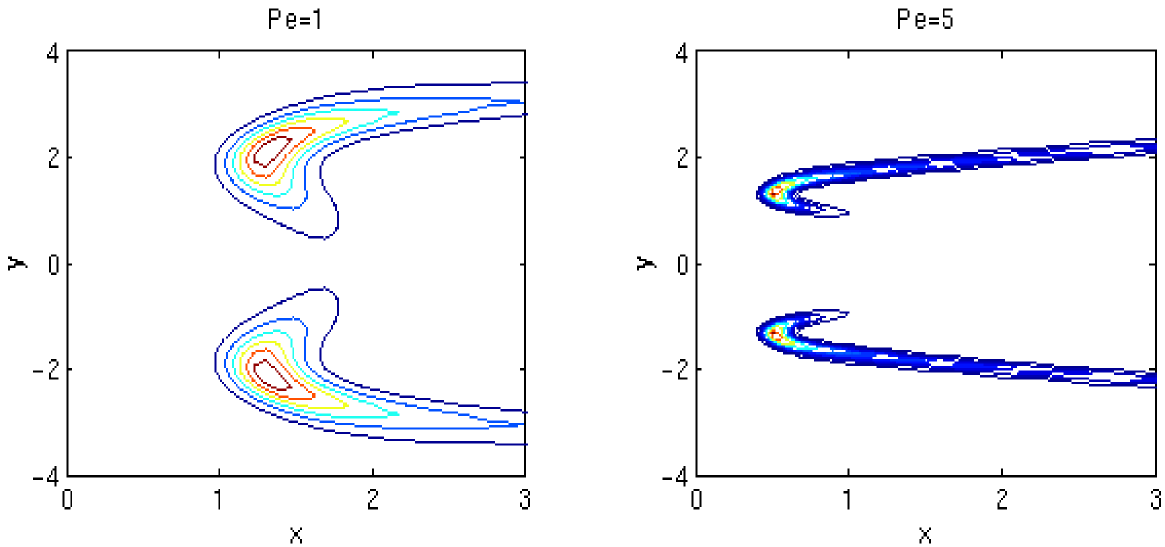
$$L \quad \frac{f}{fy} - Pe^{-1} \quad {}^2$$

  - **plus mass flux b.c. for X,Y; Dirichlet b.c. for T**
  - **- Damkohler number**

Center for Simulation of Advanced Rockets

University of Illinois at Urbana-Champaign

■ Reaction rate contours for =7, =4.8d7, =6



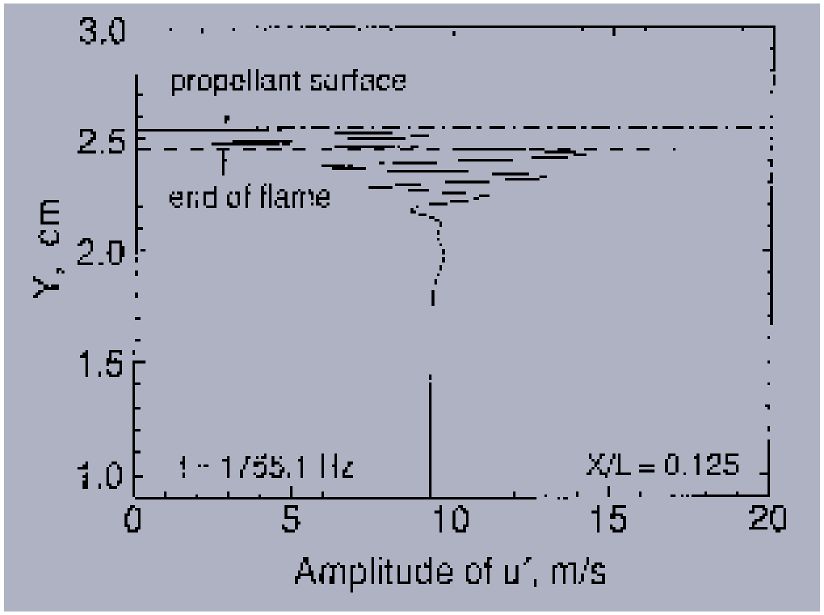
- edge flame, followed by trailing diffusion flame
- as Pe increases, trailing diffusion flame displaces according to the dictates of the SLS
- edge flames play an important role in regression rate
- Price observed enhanced regression for those portions of the propellant close to the edge flame
- Other propellant configurations can be studied (1/4 plane; F/O/F sandwich, axisymmetric, etc.) within this framework

Center for Simulation of Advanced Rockets

University of Illinois at Urbana-Champaign

2. Effects of Time-Periodic Shear

- **Interaction between axial acoustic waves and the rotational mean flow in the rocket chamber (Taylor, 1956; Culick, 1966) can generate large time-dependent shear flows at the propellant surface (Flandro, 1995)**
- **Numerical studies by Yang, et al (1995a, 1998) support this**



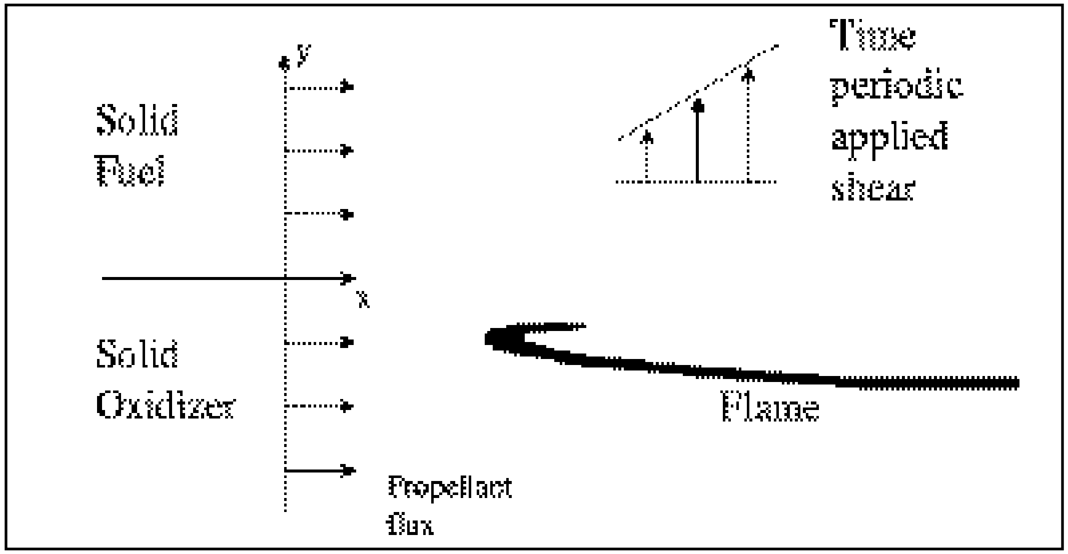
$$\frac{du'}{dy} = 2.67x10^{5} \quad \sec^{-1}$$

$$freq = 10^{-5}\sec$$

Center for Simulation of Advanced Rockets

University of Illinois at Urbana-Champaign

- **Model 1/4 plane of fuel and oxidizer - single edge flame**



- **Non-dimensional equations**

$$L(X,Y,T) = (-1,-1,1)\delta XYe^{-\theta/T} \qquad L \quad \frac{f}{ft} + \underset{\sim}{v} \quad \underset{\sim}{} - \quad ^{2}$$

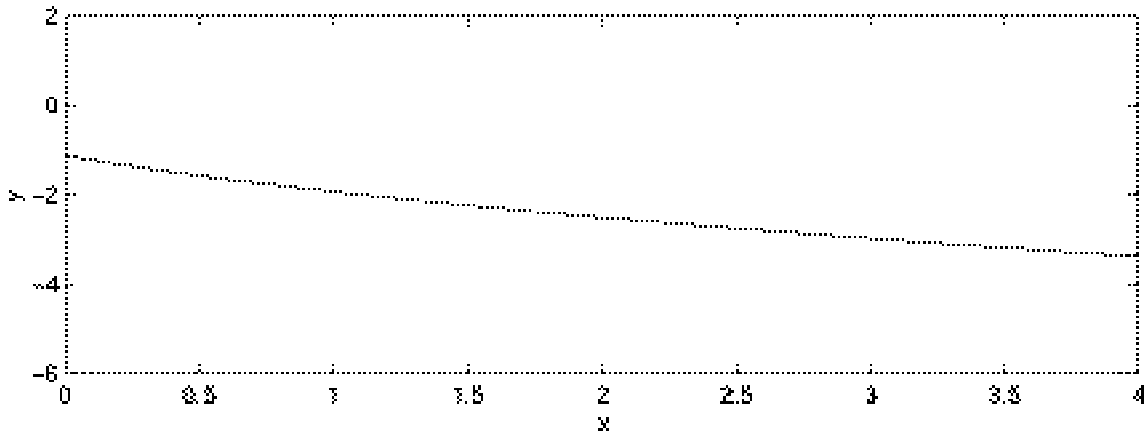
- **shear** $\underset{\sim}{v} = (1, v) \qquad v = ax\sin(\omega t)$
- **mass flux b.c. for X,Y; Dirichlet b.c. for T**

Center for Simulation of Advanced Rockets

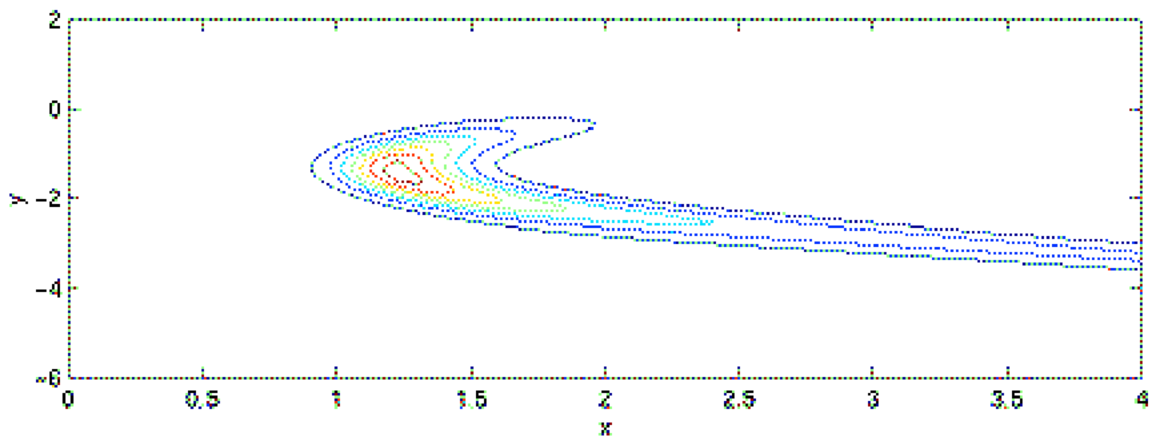
University of Illinois at Urbana-Champaign

- **Parameter** $\beta = \dfrac{\alpha_x / k_x}{\alpha_y / k_y}$

- **Stoichiometric level surface for = 7 (no shear)**

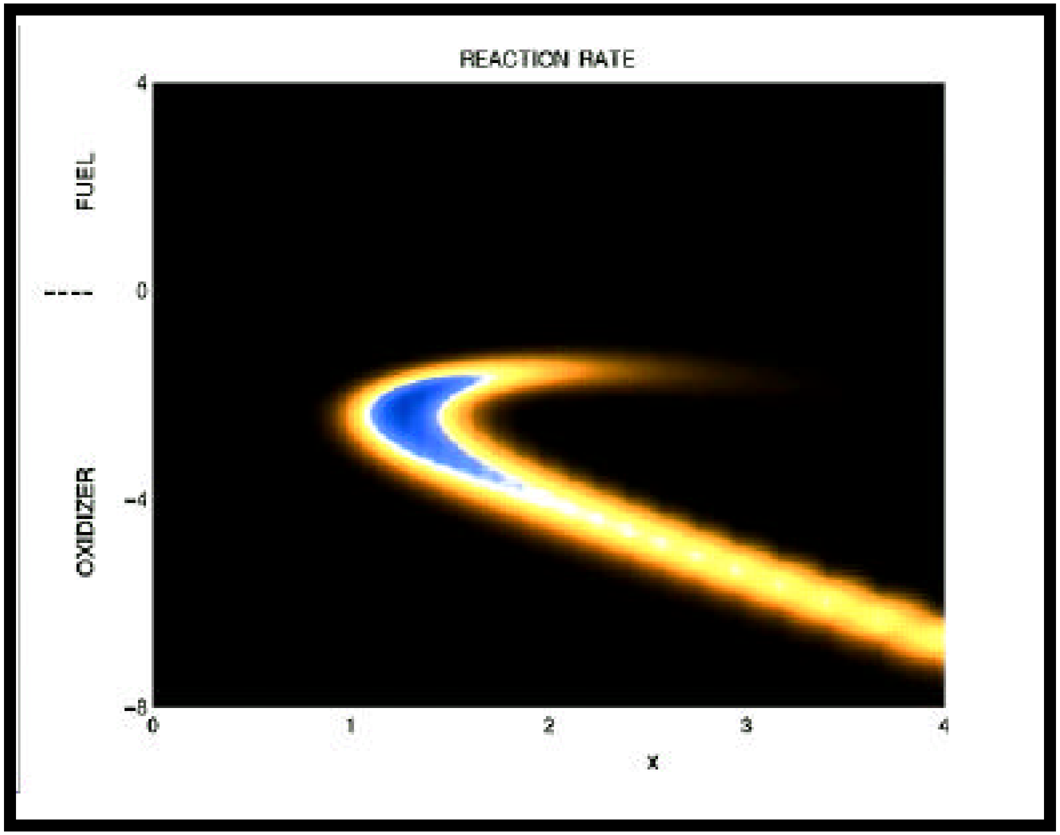


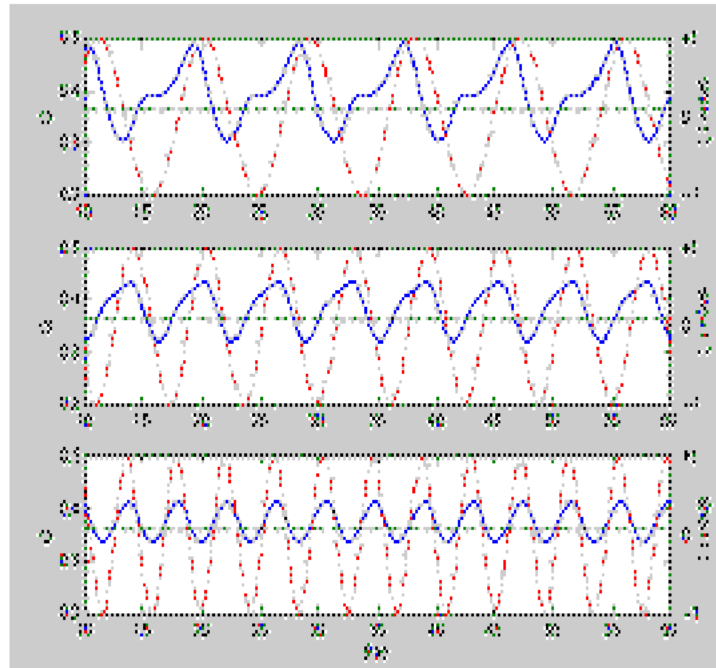
- **Plot of reaction rate contour with a = 0 (no shear)**



- **Inclusion of shear - plot of the reaction rate and the total integrated heat flux to the propellant surface**

$$Q(t) = \int_{-\infty}^{+\infty} \frac{\partial T}{\partial x}(0, y, t)\,dy$$





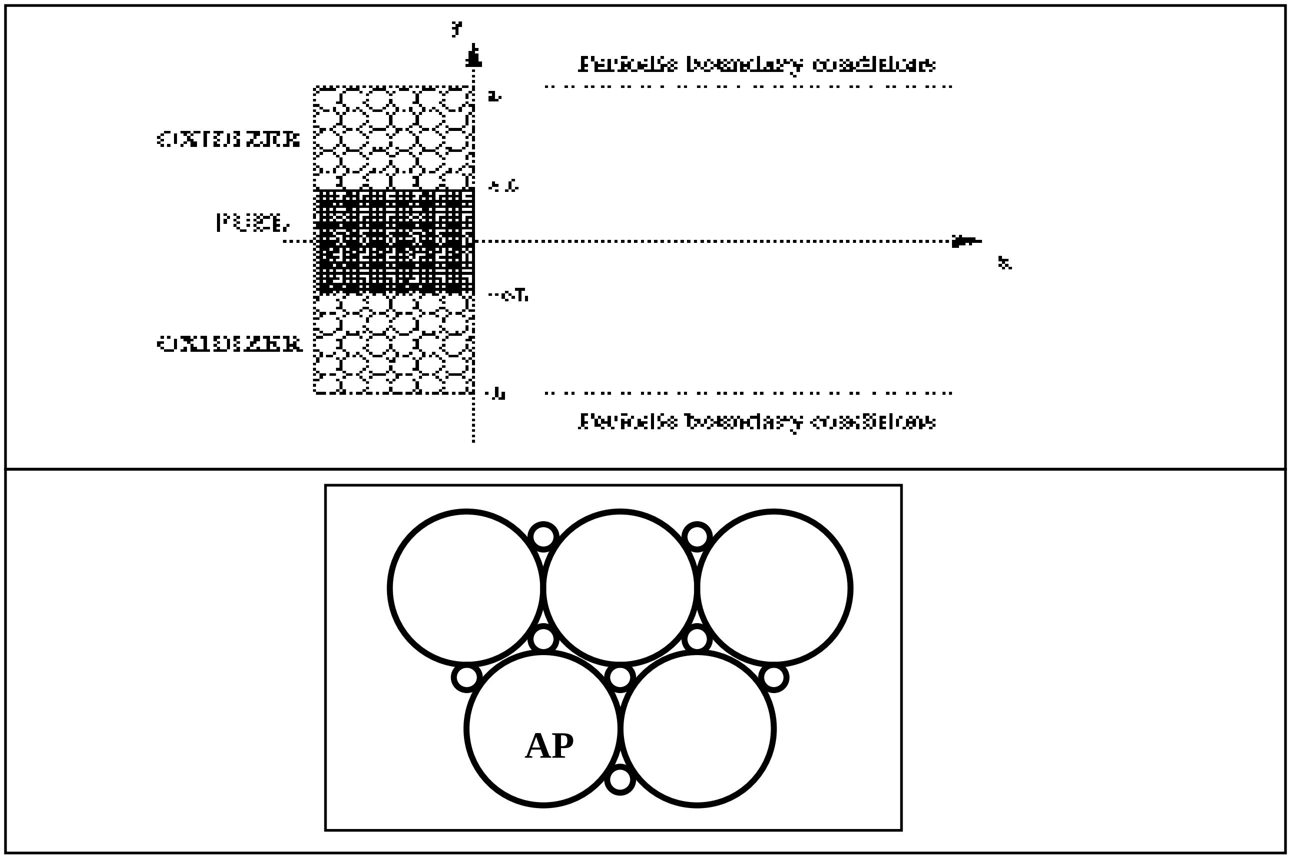
- **At the lower frequencies the response is significantly nonlinear**

Center for Simulation of Advanced Rockets

University of Illinois at Urbana-Champaign

3. Non-premixed Periodic Flames

- So far we have discussed isolated flames
- We now consider a propellant whose surface is periodic, either 1-d or 2-d (the combustion field will be 2-d or 3-d, respectively)



Center for Simulation of Advanced Rockets

University of Illinois at Urbana-Champaign

3a. Periodic Array
(1-d surface, 2-d combustion field)

- **Equations**

$$L_1(X,Y) = (-1,-1)\delta XYe^{-\theta/T} \qquad L_1 \quad \frac{f}{fx} - Pe^{-1} \quad {}^2$$

$$L_2(T) = \delta XYe^{-\theta/T} \qquad L_2 \quad \frac{f}{fx} - \frac{Le}{Pe} \quad {}^2$$

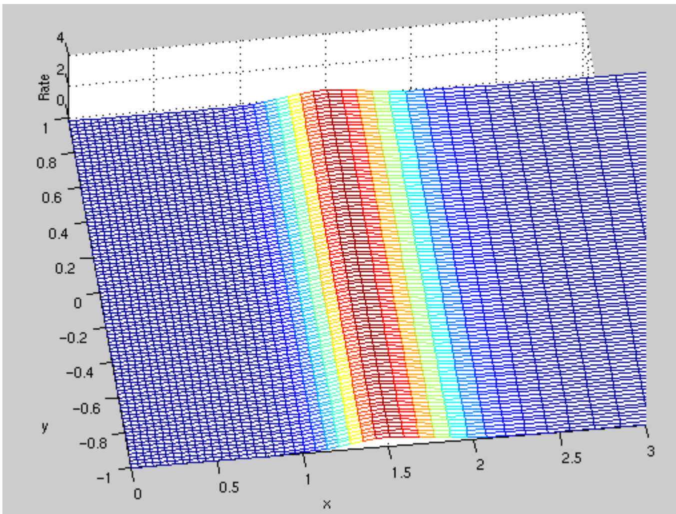
- **Mass flux b.c. for X,Y; Dirichlet B.C. for T**
- **Parameters , Pe, Le, (fuel thickness 2)**
  - **for stoichiometry, = (1 -)/**

Center for Simulation of Advanced Rockets

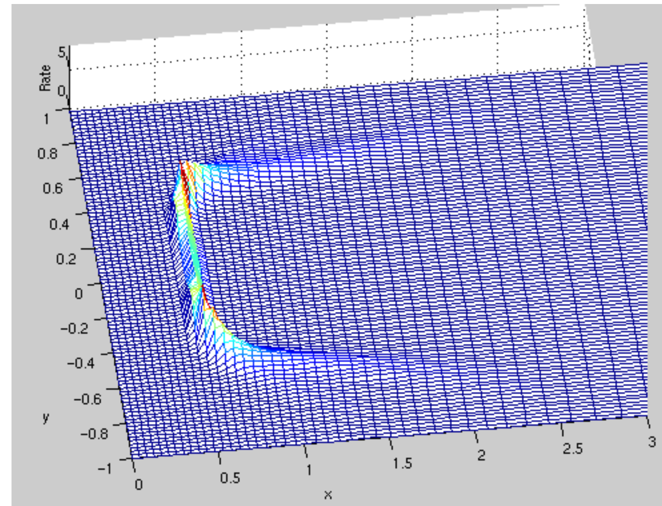
University of Illinois at Urbana-Champaign

- Plot of reaction rate for = 7, = 1/(1 +) = 0.125, and Le = 1

Pe = 1



Pe = 5

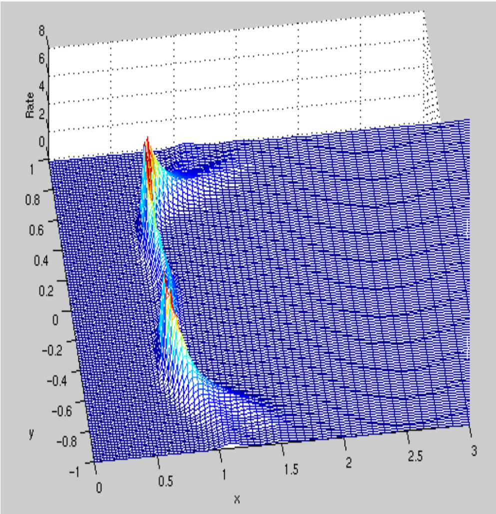


- **For small Pe, the mixing between the propellant surface and the flame is so through that essentially a 1-D deflagration is generated**
- **For increasing Pe, the combustion field is dominated by a strong premixed edge structure and a “hole” over the oxidizer**

Center for Simulation of Advanced Rockets

University of Illinois at Urbana-Champaign

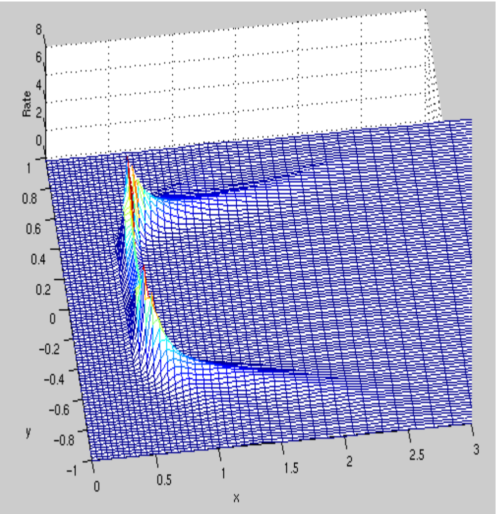
■ Surface plot of reaction rate for = 7, Pe = 10, Le = 1



= 0.2

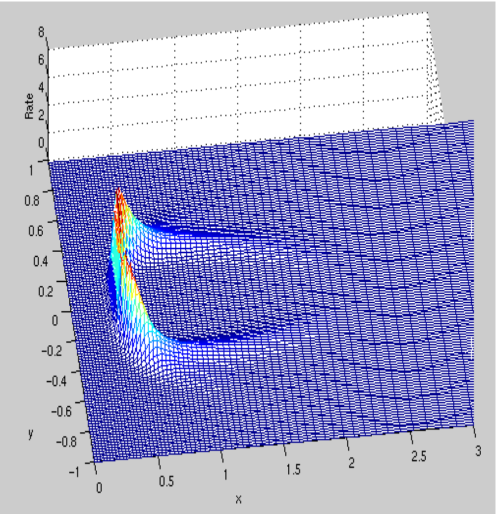
Fuel rich

(underventilated)



=1/(1+)=0.125

Stoichiometric



= 0.1

Fuel lean

(overventilated)

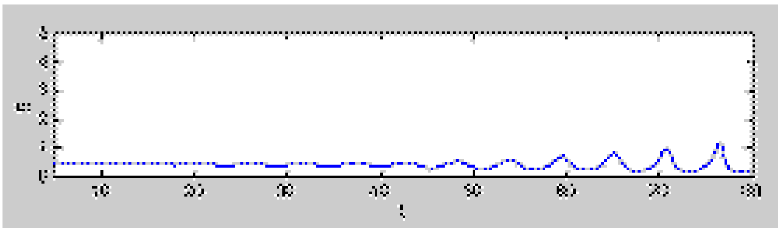
- **flame structure changes as the stoichiometry parameter varies**

Center for Simulation of Advanced Rockets

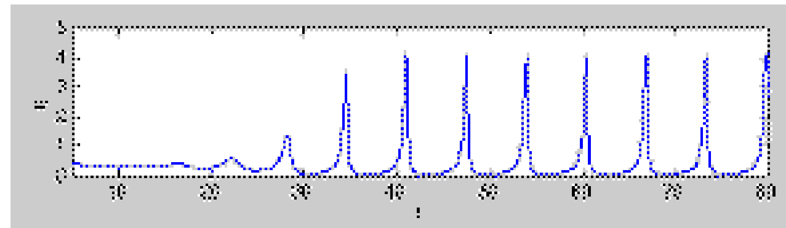
University of Illinois at Urbana-Champaign

- Maximum reaction rate as a function of time for = 7

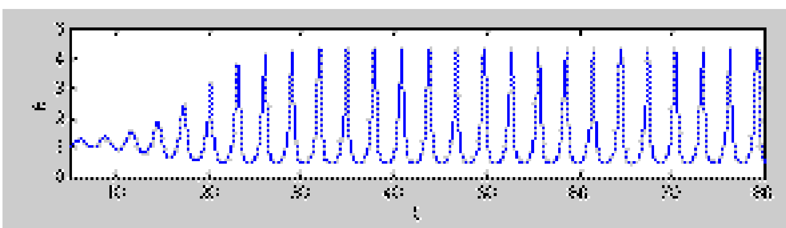
Le = 1.6, Pe = 1



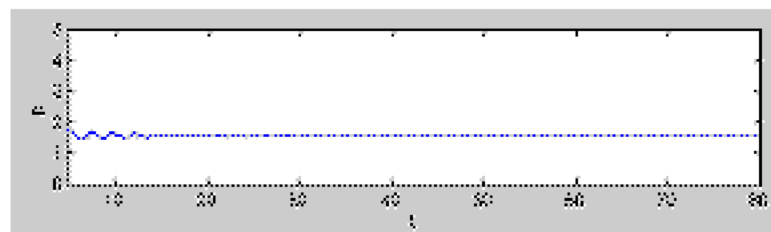
Le = 2.0, Pe = 1



Le = 2.0, Pe = 3



Le = 2.0, Pe = 4

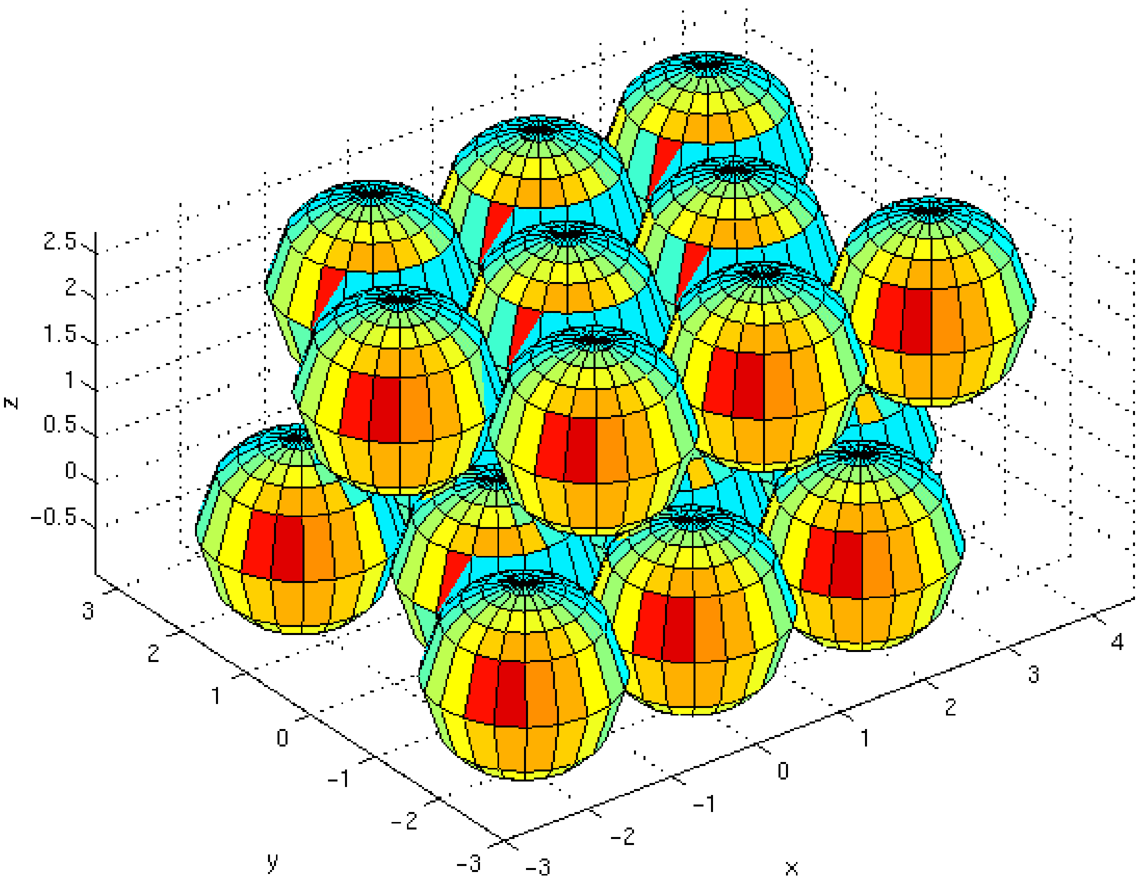


- Time periodic oscillating solutions are obtained for sufficiently large values of Le
- Oscillations can be damped by increasing Pe

3b. Three-dimensional Heterogeneous Flames (1-d surface, 2-d combustion field)

- **We are concerned exclusively with the gas phase, with solutions constructed subject to boundary conditions at the propellant surface**
- **Constant mass flux; propellant surface is flat**
- **We account for large and medium AP particle size**
  - **to account for smaller AP particles, necessary for stoichiometric purposes, the binder is modeled as a homogeneous mixture**
- **One-step kinetics; solutions are constructed using a numerical strategy**
- **Finite Peclet number effects are accounted for (results shown for Pe=5; Pe = ML/ D)**
- **Numerical code parallelized using OpenMP**

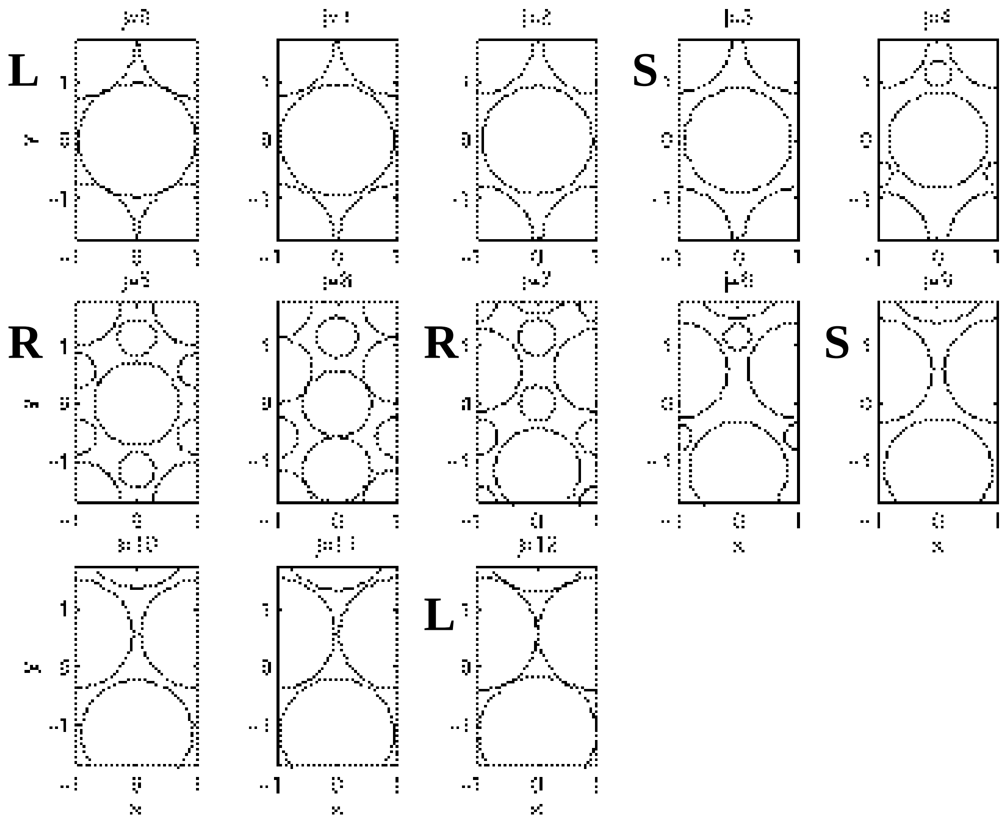
- **Example of particle packing showing only the largest AP particles (periodic packing)**

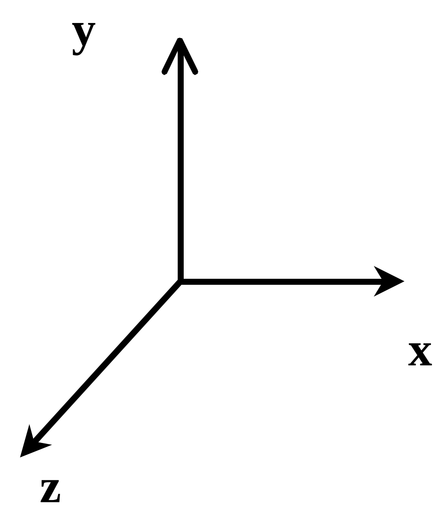


Center for Simulation of Advanced Rockets

University of Illinois at Urbana-Champaign

- Level set surface representation of AP particles
- Take 25 slices through the volume
- Only consider first 13 slices (last 12 found by reflection)
- Surface stoichiometry varies from slice to slice
  - L - leanest; R - richest; S - closest to stoichiometry

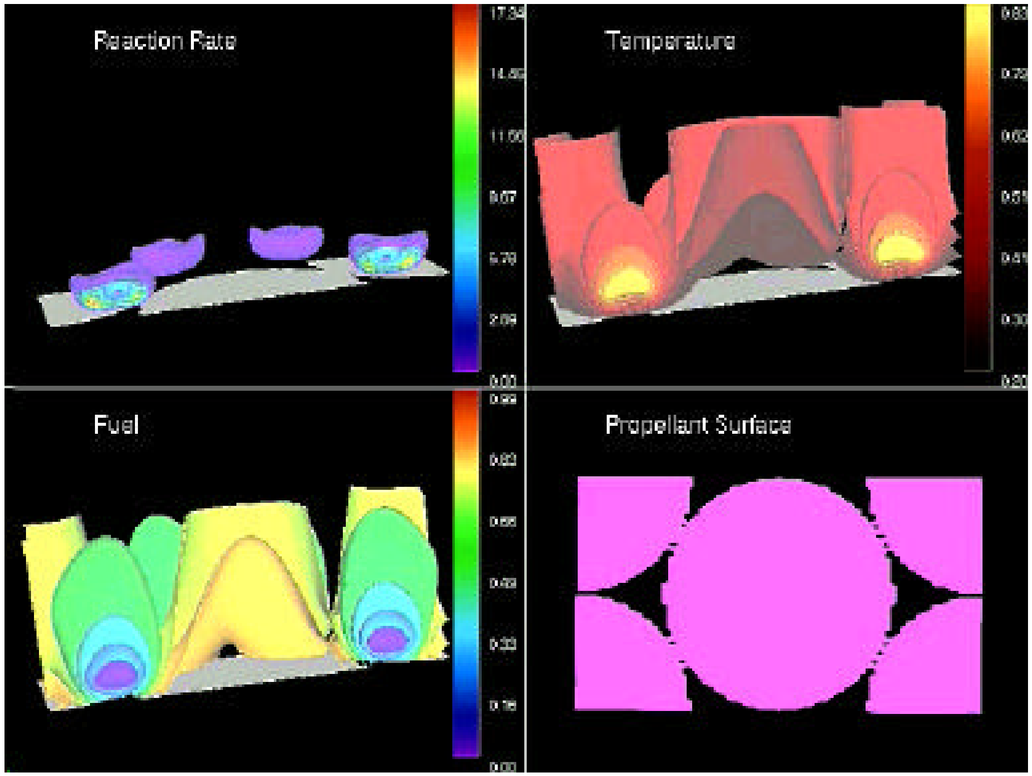




Center for Simulation of Advanced Rockets

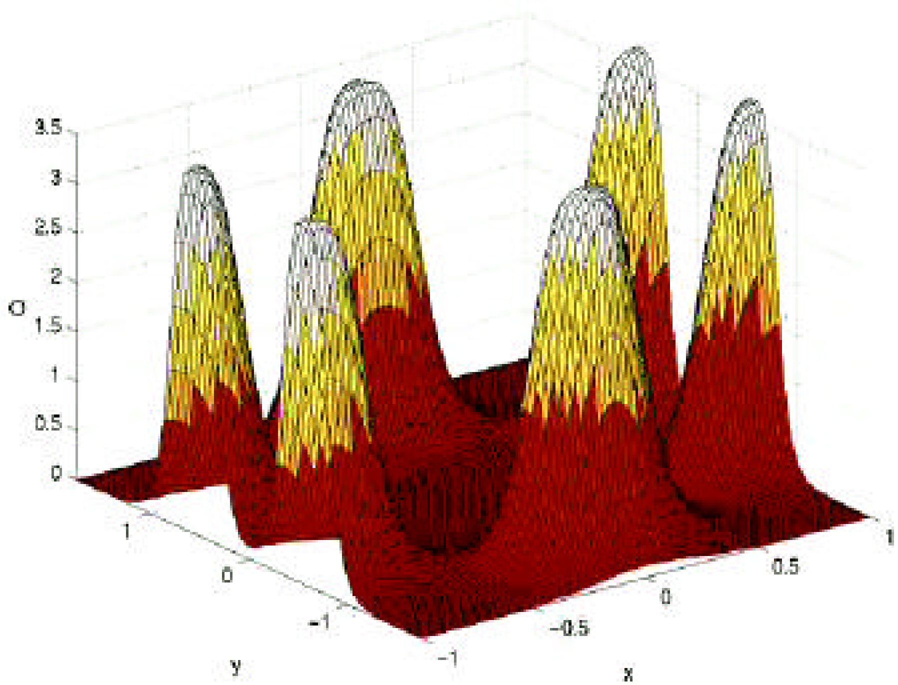
University of Illinois at Urbana-Champaign

■ Movie showing burning heterogeneous propellant



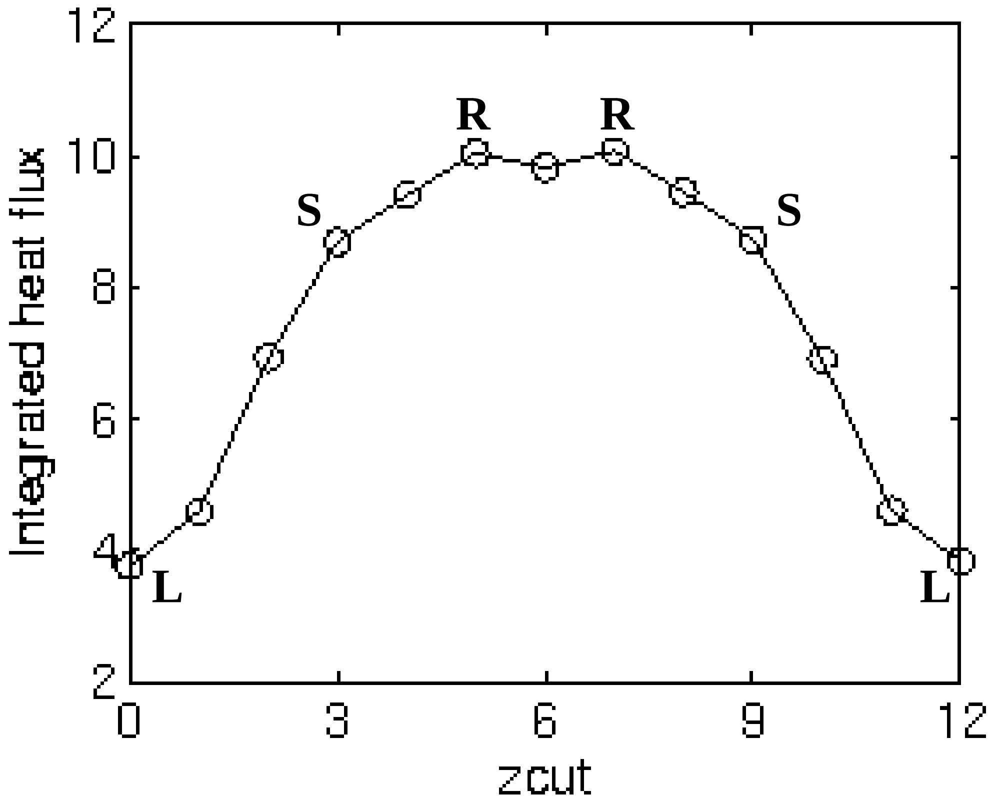
- flame structure changes as the propellant burns

■ Movie showing heat flux to the propellant surface



- heat flux has a 3d structure
- may not be as dramatic when the AP mono-propellant flame is accounted for

- **Integrated heat flux as a function of the 13 cuts**



Center for Simulation of Advanced Rockets
University of Illinois at Urbana-Champaign

4. Incorporation of Fluid Mechanics Effects

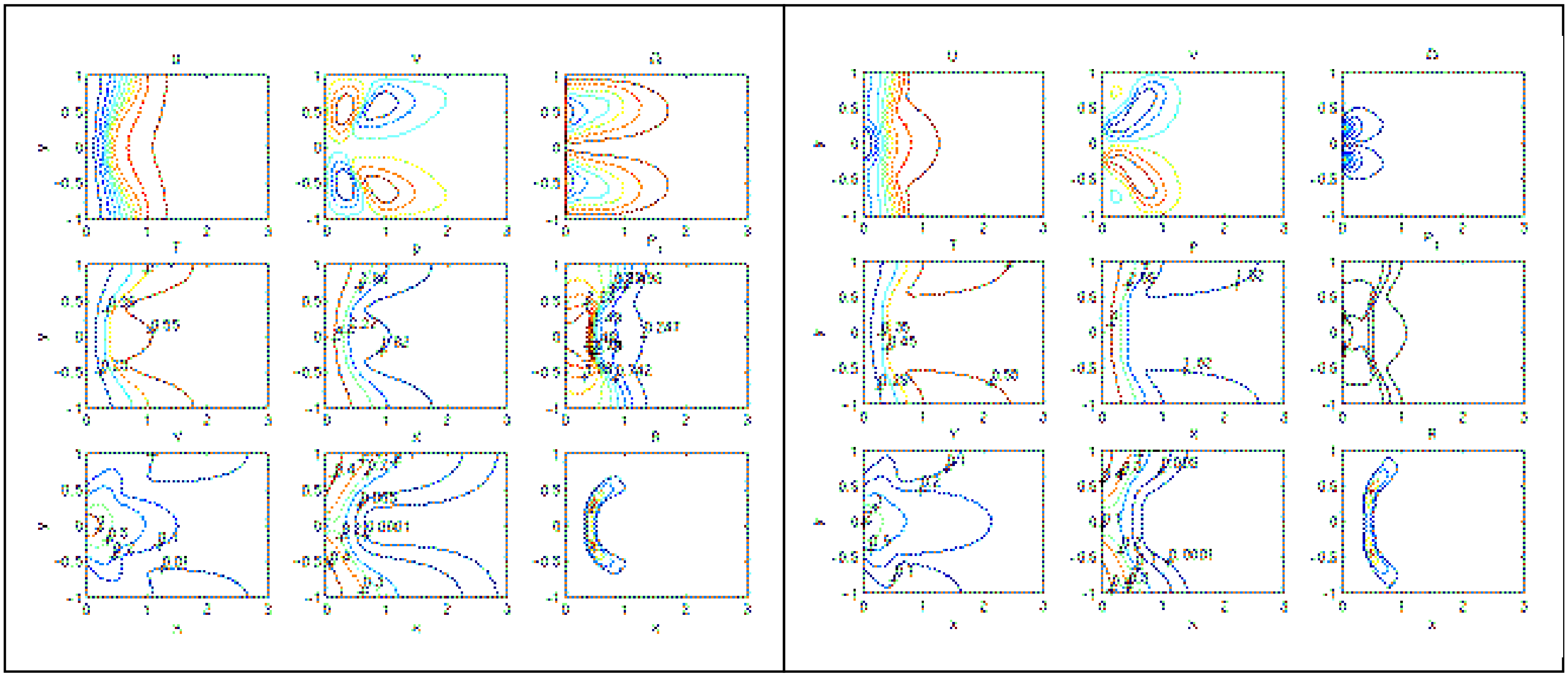
- **Full conservation equations for a chemically reacting system**
- **Combustion field: M 0.01 - 0.001**
- **Numerical solution of low Mach number equations require careful consideration due to time scales**
- **Numerical stiffness due to finite-rate kinetics**
- **Various strategies under investigation**

- **Example to follow: periodic array of heterogeneous propellant**

Results for Pe = 5, M = 0.01

1) Constant surface density; constant regression rate & mass flux
2) Variable surface density (AP - 1.95; Binder - 1.01); constant regression rate; variable mass flux

1) Constant Mass Flux | **2) Variable Mass Flux**



Center for Simulation of Advanced Rockets

University of Illinois at Urbana-Champaign

Future Work

- Complete coupled solid/gas problem ("eigenvalue problem")
  - Fluid mechanics essential for multi-dimensional problems
  - Account for regression boundary
  - Account for solid
  - Account for AP mono-propellant flame
- Incorporate into 3D propellant geometry
- Investigate flame structure for stochastic representation of propellant surface (more realistic particle packing)
- Investigate interaction with core region (unsteady process)
- Investigate ignition/flame spread problem
- Begin full-scale coupled problem (RocFire)