AFOSR AWARD FA9550-18-1-0392
High-Pressure LPRE Combustion Dynamics: Low-Cost Computation and Stochastic Analysis

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Goals to Improve the Science and the Methodology

Better understanding of LPRE combustion instability and turbulent combustion dynamics.

Identify methods for improved performance and stable operation.

Use deliberate triggering to change the resonant mode to a less energetic and less consequential mode.

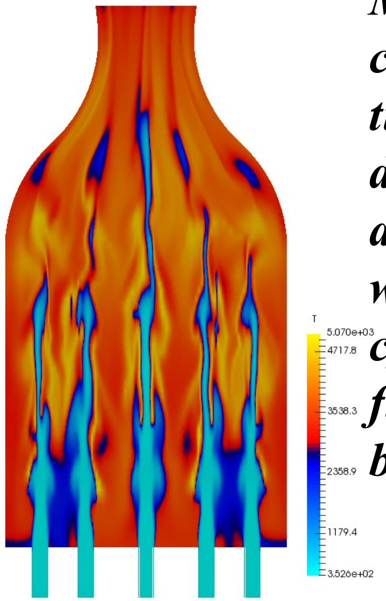
Better closure models for sub-grid physics and lower computational costs (e.g., flamelet model) for large-eddy simulations (LES).

Examine combustor flow using real fluid equations of state

Increase ability to analyze multi-injector engines.

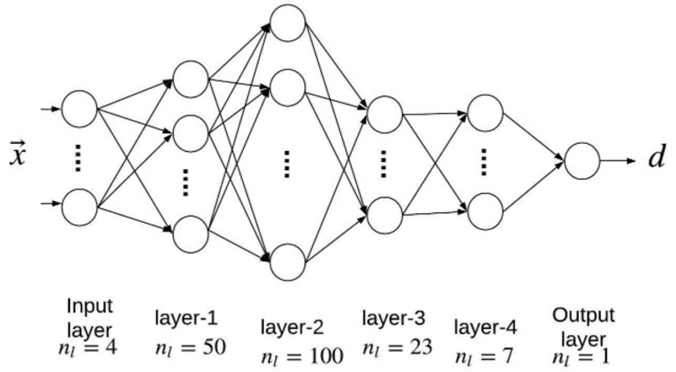
Greater accuracy and lower computational cost at various levels of fidelity.

Optimize design of deep learning neural networks (DLNN) to bypass look-up tables for the flamelet sub-grid model in LES.



Multi-injector rocket combustors– turbulent combustion dynamics, nonlinear acoustic oscillations with unstable limit cycles, unsteady flamelets, chaotic behavior.

Multi-output DLNN – more layers, more efficient.



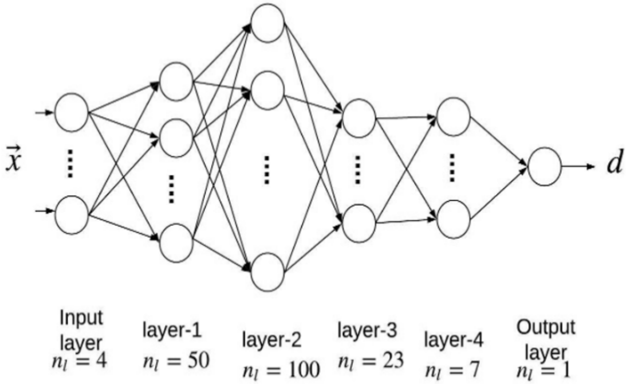
High-Pressure Combustion Dynamics
Configurations for Study

Single-coaxial-injector rocket engine
Purdue University CVRC experiment

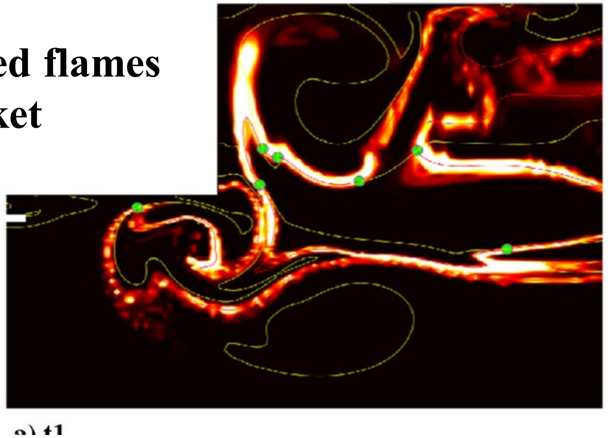
Various lengths, mixture ratios, wall Temperatures. LES/ RANS hybrid, use of flamelet theory for sub-grid. Triggering and spontaneous longitudinal mode.

DLNN Optimization

Numbers of deep layers, neurons, variables /NN



Multi-branched flames appear in rocket combustor computation. New flamelet theory is needed.

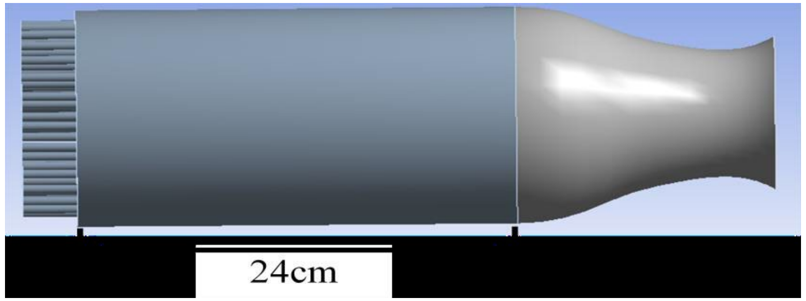


Ten- and Nineteen-Coaxial-Injectors LPRE

Various diameters, longitudinal and tangential modes, triggering and spontaneous instability, triggering for mode change, scaling laws, effect of helicity. Add and compare flamelet model.

Thirty-Injector LPRE mimicking Rocketdyne Jensen et al. 82-injector LPRE experiment

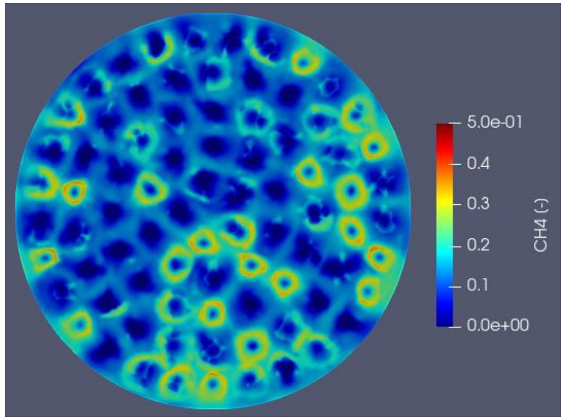
Various lengths, longitudinal and tangential modes, chaotic combustion dynamics, triggering and spontaneous instability, triggering for mode change, triggering for control, premixed flames vs. nonpremixed flames.



82-Coaxial-Injector LPRE

This mimics the Rocketdyne Jensen et al. experiment. We examine longitudinal and tangential modes. We show how a change in burning rate affects the preferred instability mode.

Snapshot: Methane mass fraction 2 cm downstream of injector plate.



Flamelet Theory and LES Sub-grid Modelling

Our strategy is to use the best available flamelet theory to represent well the detailed chemistry and molecular mixing but avoid the short time scales forcing excessive computational costs. First, we used a look-up table approach. Now, we have moved to the use of deep learning neural networks (NN). Simutaneously, we seek to improve the flamelet model.

Added equations for LES

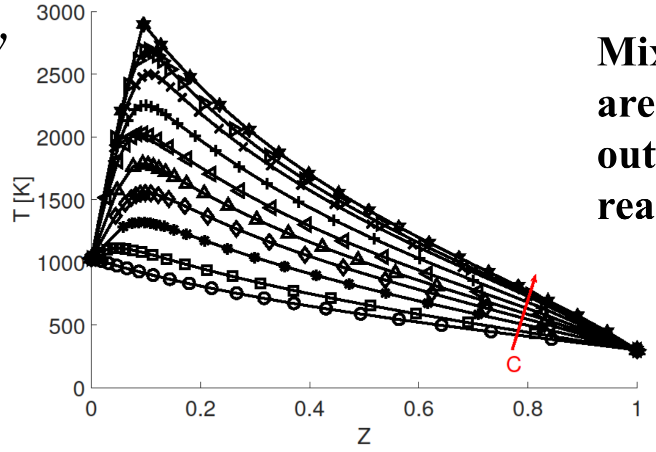
$$\frac{\partial \bar{\rho}\tilde{Z}}{\partial t} + \frac{\partial \bar{\rho}\tilde{v}_j\tilde{Z}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\frac{\lambda}{c_p} + \frac{\mu_t}{Sc_t}\right)\frac{\partial \tilde{Z}}{\partial x_j}\right]$$

$$\frac{\partial \bar{\rho}\widetilde{Z^2}}{\partial t} + \frac{\partial \bar{\rho}\tilde{v}_j\widetilde{Z^2}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\frac{\lambda}{c_p} + \frac{\mu_t}{Sc_t}\right)\frac{\partial \widetilde{Z^2}}{\partial x_j}\right] - \bar{\rho}C_x\omega(\widetilde{Z^2} - \tilde{Z}^2)$$

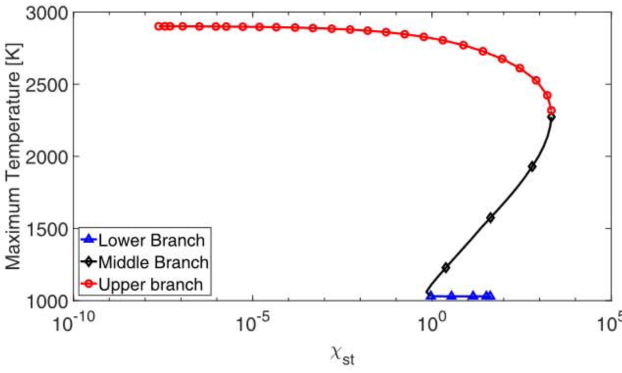
$$\frac{\partial \bar{\rho}\tilde{C}}{\partial t} + \frac{\partial \bar{\rho}\tilde{v}_j\tilde{C}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\frac{\lambda}{c_p} + \frac{\mu_t}{Sc_t}\right)\frac{\partial \tilde{C}}{\partial x_j}\right] + \tilde{\dot{\omega}}_C$$

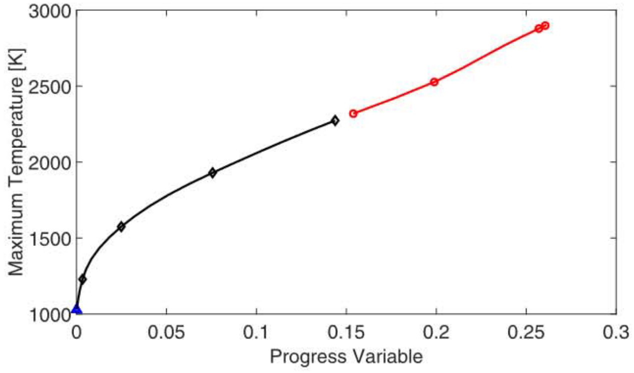
Flamelet Progress Variable Theory

The FPV approach is built around a single diffusion flame in a strained counterflow. Scalar dissipation rate increases with strain rate and residence time shortens compared to chemical time. Peak temperature drops. The progress variable C is a convenient but contrived quantity.



Mixture fraction Z (mean and variance), progress variable C are inputs to flamelet model together with pressure. Seven outputs, including flame temperature and $\dot{\omega}_C$, the sum of reaction rates for selected species, i.e., FPV reaction rate.





Advantages of FPV Approach

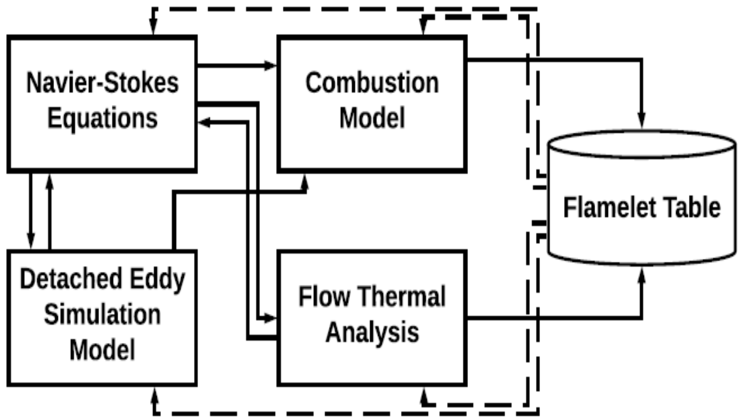
Reduces number of dependent scalars.
Eliminates short chemical-kinetic time scales and high computational cost.
Adds sub-grid mixing physics.

Disadvantages of FPV Approach

Does not account for multiple flames.
Ignores imposed shear strain or vorticity.
Does not address 3D flamelets.
No scaling between resolved flow and sub-grid.
Constant-density scalar dissipation rate.

Neural Network Representation of Flamelet Model for Rocket Engine Combustion

(a) Schematic of CVRC configuration [23]



(b) Top level architecture of CFD code

Focus has been on single-injector CVRC Engine with axisymmetric LES and unsteadiness due to both combustion instability and turbulence: it emulates well experimental evidence.

Original Approach: two sets of NNs learning off-line from table data.

New approach: one NN for each FPV output. Six learn from table data used by transient-case CFD. FPV reaction rate learns also from dynamic equilibrium data.

NN replaces look-up table for the Progress-variable Flamelet (PVF) Theory requiring less memory.

Training of the NN can require as little as 15% of the table data. Learning from the data most used by the CFD and data derived from physical constraints, i.e., "physics awareness"

The NN is used successfully for the triggered instability case without special training.

	# of neurons in each layer	FLOP	training error (%)	test on table (%)
$\tilde{T}_f$	4-15-10-15-1	375	0.59	4.83
$\tilde{e}_f$	5-15-10-15-1	390	0.0566	0.57
$\tilde{R}$	5-15-10-15-1	390	0.0526	0.65
$\tilde{\lambda}$	5-15-10-15-1	390	0.21	3.57
$\tilde{\gamma}$	5-15-10-15-1	390	0.0371	0.48
$\tilde{\alpha}_\gamma$	5-15-10-15-1	390	0.22	1.41
$\tilde{\dot{\omega}}_C$	4-15-20-25-35-25-20-15-5-1	3490	1.49	32.86

GUIDING CONCEPTS IN NEURAL NETWORK DESIGN

NN structure design is aimed at increasing accuracy while decreasing the data retrieval computational cost. A NN with the lowest number of neurons and layers that results in sufficiently small error is desired for each variable.

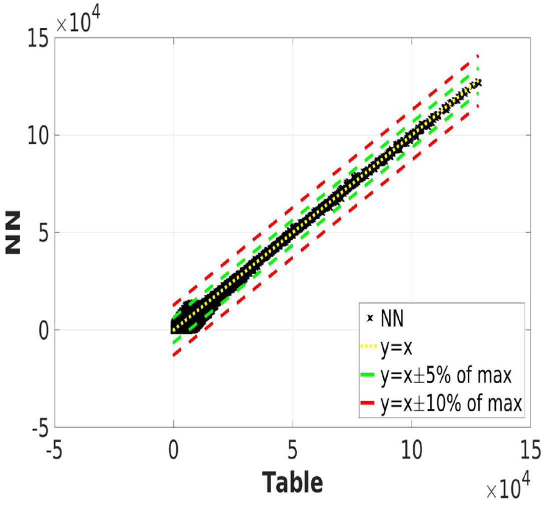
Physics-informed enhancements **of the training set improve results.**
1) the use of flame temperature as an extra input for all variables except PVRR;
2) the addition of specific boundary points to the training set ; and
3) the addition of points with C=0 based on empirical considerations.

NN weights are randomly initialized with the Xavier algorithm and are updated via the ADAM algorithm within the back-propagation procedure. Mini-batch training, as it is helpful to avoid local-minima in the training process, and regularization to avoid overfitting and improve NN performance on the test sets have been also used.

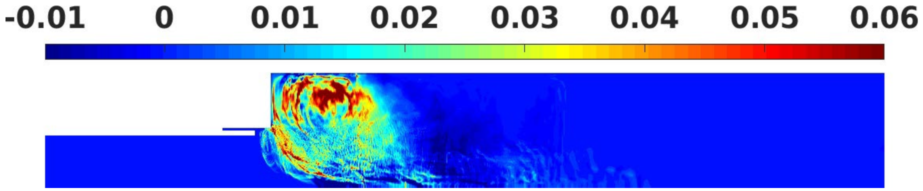
Accordingly, we significantly improved the accuracy of the output variables

Comparison of Results: CFD with Lookup Table vs. CFD with NN

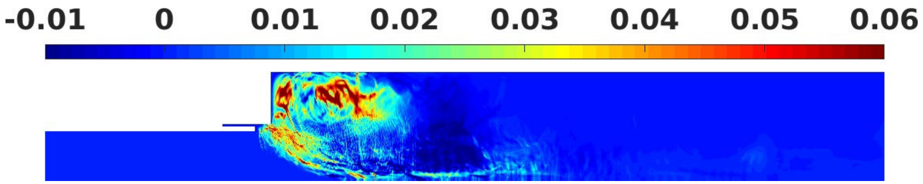
Training of Progress-variable reaction rate is greatest challenge



Lookup Table-Rayleigh Index

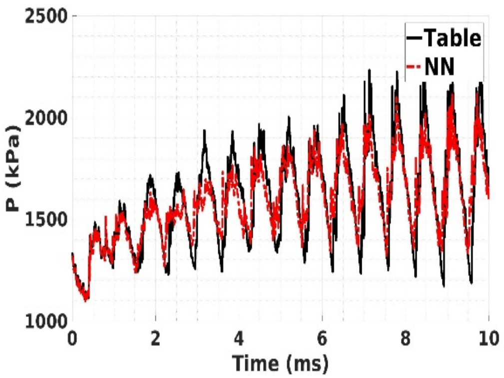


NN-Rayleigh Index

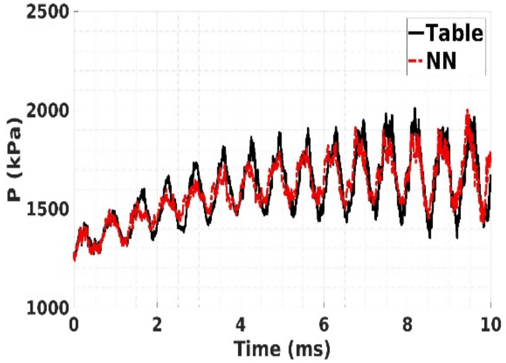


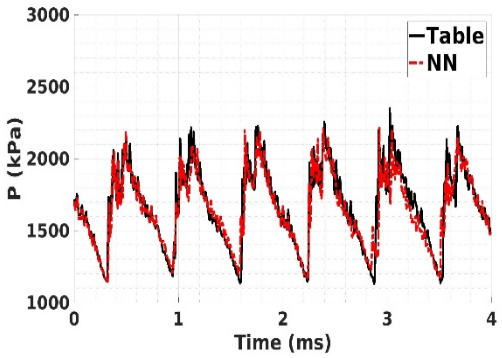
Pressure in oxidizer post r=0.5 cm, x = -10 cm

Pressure in chamber shear layer=1.13 cm, x = 8 cm

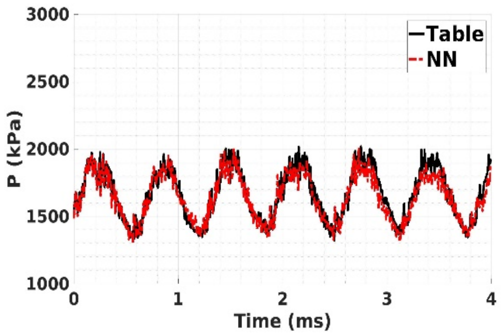


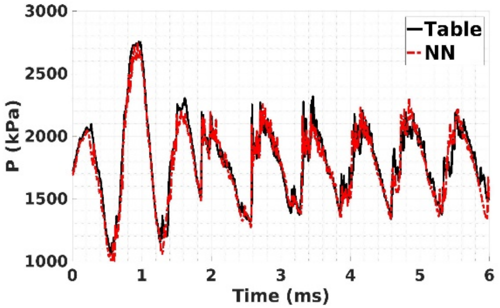
Transient for spontaneous instability



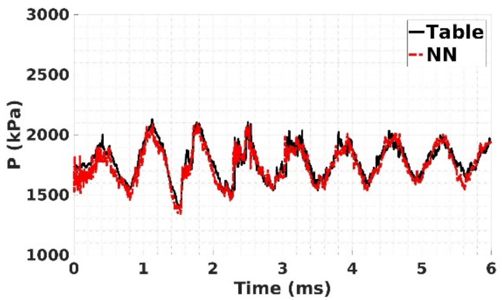


Dynamic equilibrium for spontaneous instability



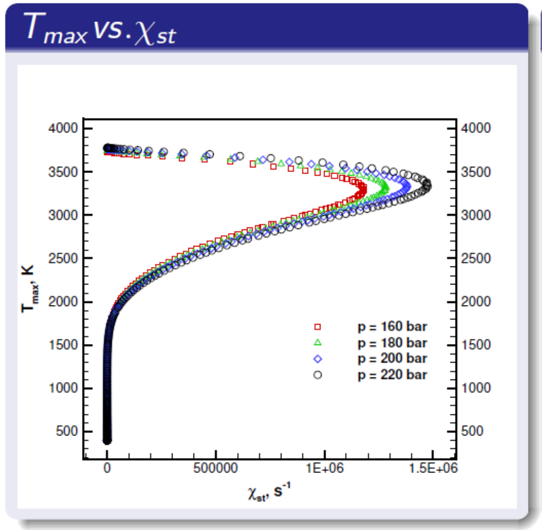


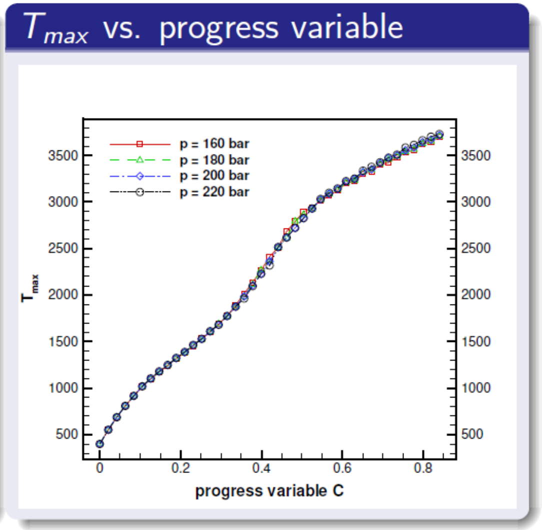
Triggered instability



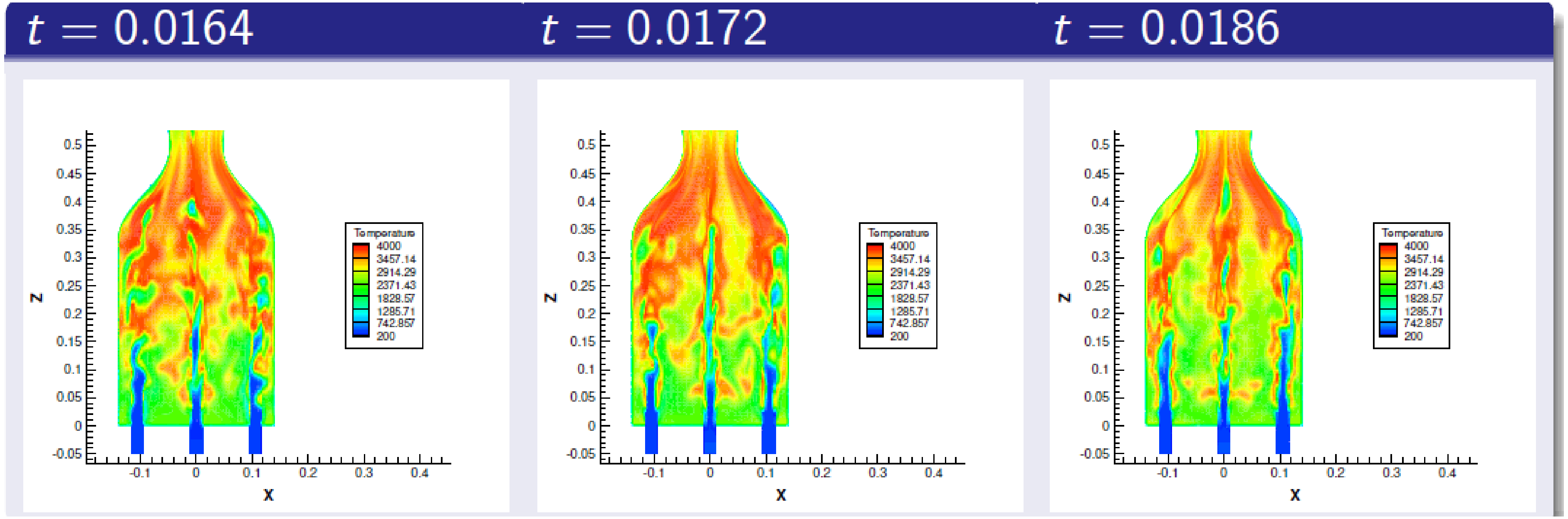
A new flamelet table is created for multi-injector methane-O2, high pressure engines

Prof. Hai Wang, Stanford CHO system
12 SPECIES: H2 H O2 O OH HO2
H2O CH3 CH4 CO CO2 CH2O
39 REACTIONS
Pressure range: 160 -220 bar
Lower flame temperatures and lower burning rates compared to one-step kinetics applied to resolved scale.

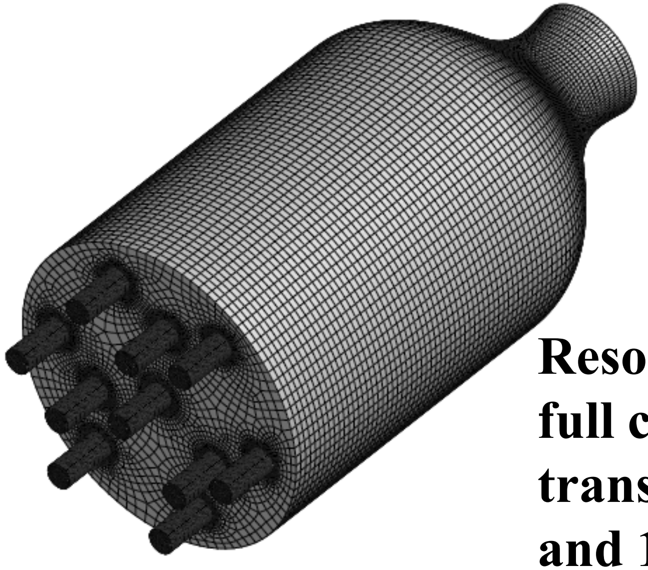




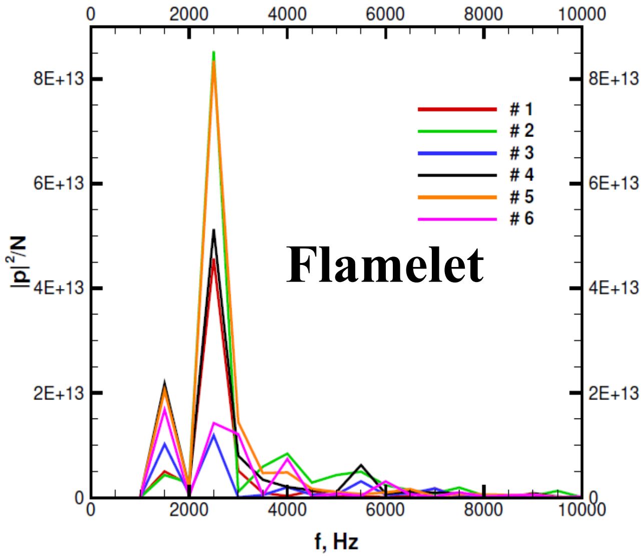
Results for 10-injector engine with flamelet progress variable.



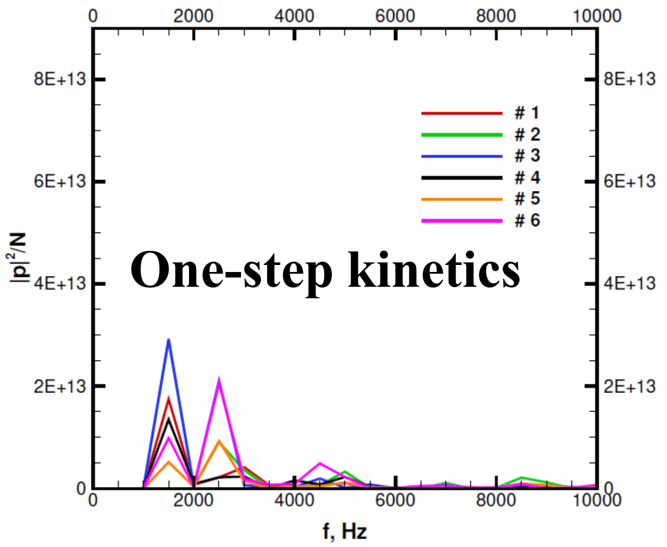
3D LES for 10-coaxial-injector methane-O_2 Engine: One-step kinetics vs. Flamelet



Resolution of full chamber, transonic nozzle, and 10 injector ports

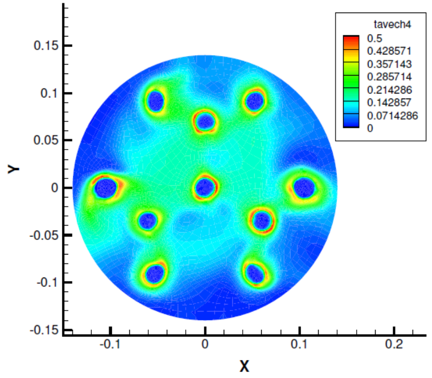


(a) At $z = 0.01$ for FPV

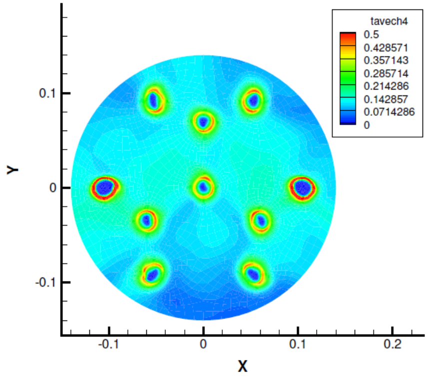


(b) At $z = 0.01$ for one step kinetics

progress variable approach



one-step kinetics



Flamelet has lower burning rate at same pressure levels as shown by magnitudes of reactant mass fractions. The flamelet model accounts for sub-grid molecular mixing.

The slower burning flamelet favors the 2500 cps tangential mode over the 1500 cps longitudinal mode; vice-versa for the faster burning one-step kinetics model.

The flamelet model moves much of the combustion away from the pressure antinode of the longitudinal mode, thereby making the tangential mode relatively stronger.

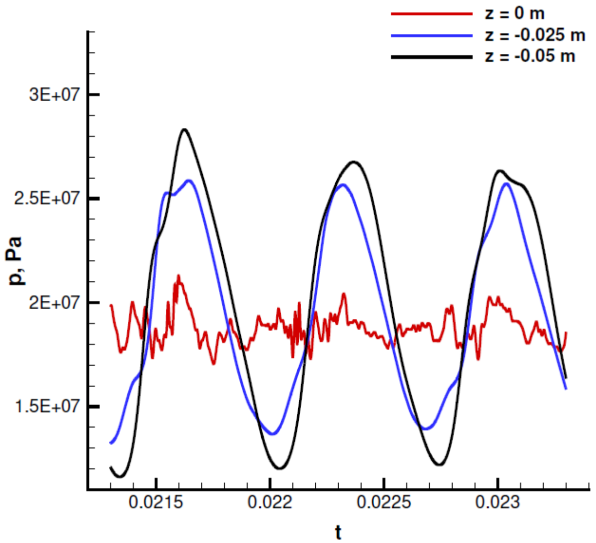
Injector Ports – Quarterwave Oscillations

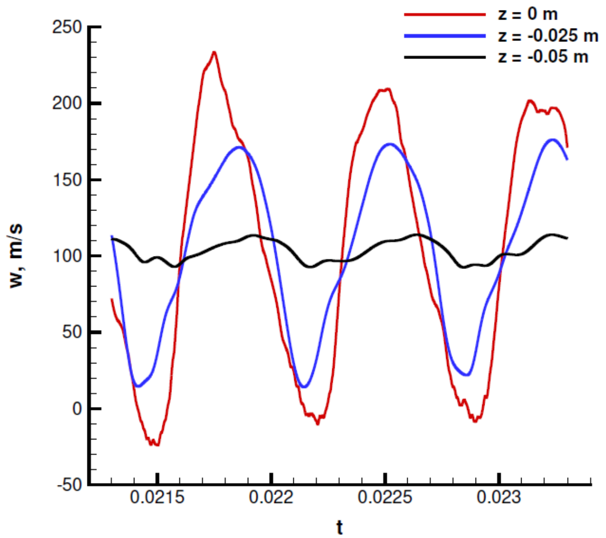
For 10-injector engine, better resolution for injector ports compared to 19-, 30-, and 82-injector analysis.

z **= 0 at injector-plate face (injector exit, open end); z = - 0.05 m is injector-port inlet (closed end).**

Oscillatory behavior in the central port using the progress-variable flamelet model.
Similar oscillatory behavior occurs with the one-step kinetics model. Similar resonance in each injectors.
However, the oscillation magnitude reaches a maximum value in the central injector .

Quarterwave character: Pressure antinode (velocity node) at port entrance; a pressure node (velocity antinode) occurs at port exit. Phase angle difference between pressure and the axial velocity is about 90 degrees.



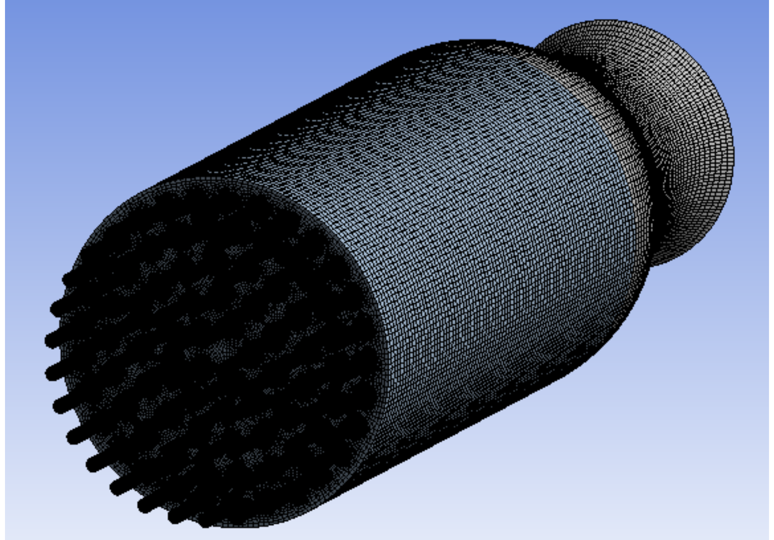


The theoretical frequency of this quarter-wave-length resonance is 1895 Hz.

The actual resonance frequency is 1500 Hz.

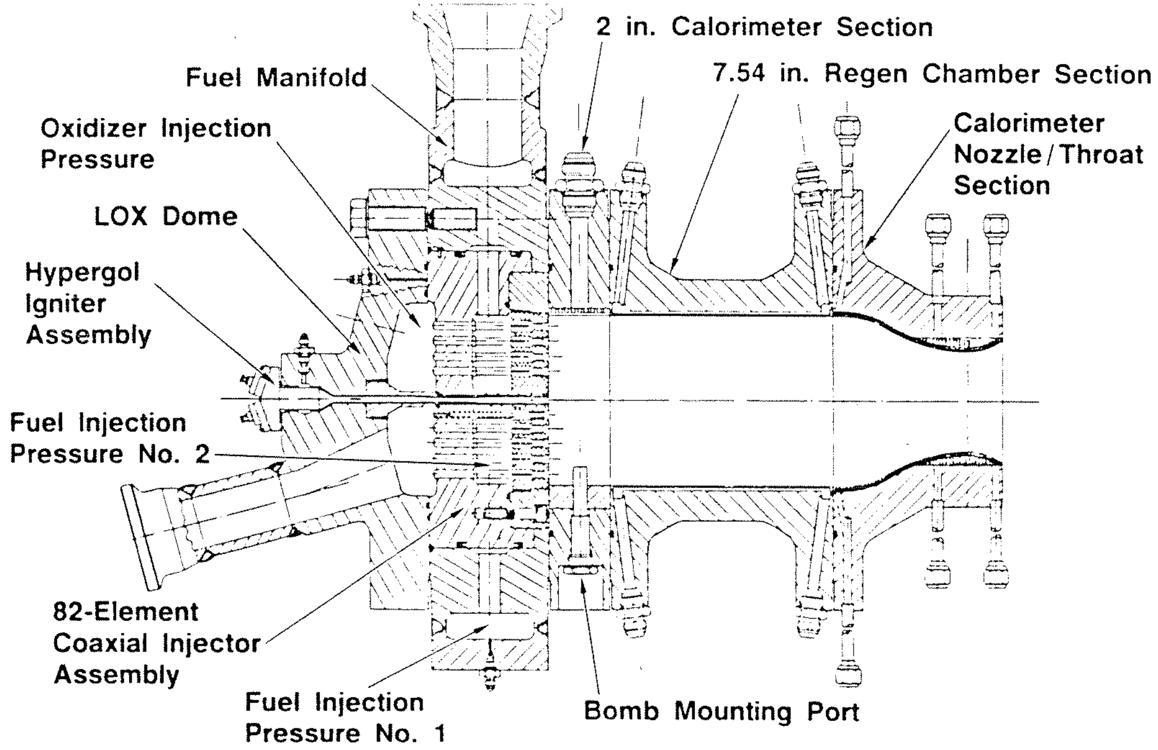
The 1500 cps is expected since it is driven by the longitudinal-mode oscillation in the combustion chamber.

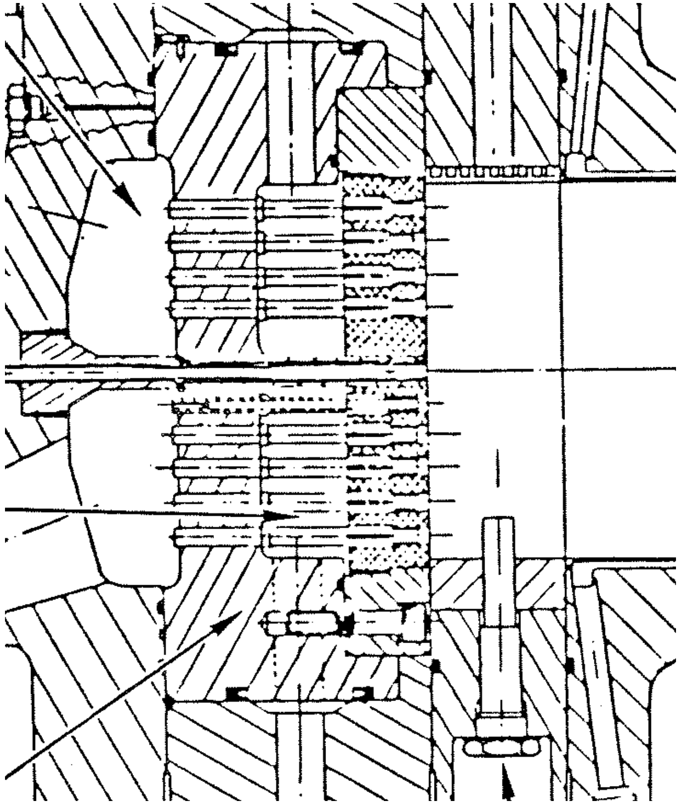
Comparison of Jensen *et al.* Rocketdyne Experimental Engine to our CFD Simulation



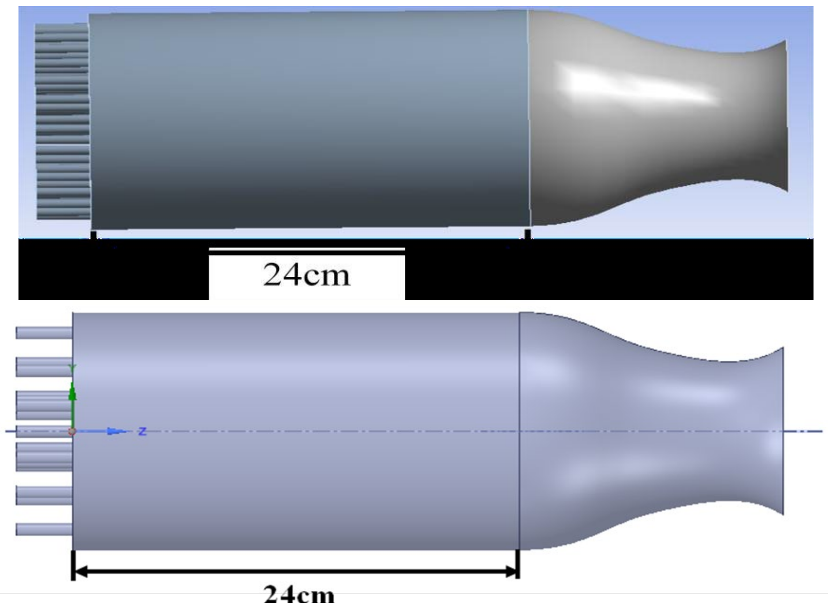
Even with 16.5 million nodal points in the mesh, the internal details of the injector port are not well resolved

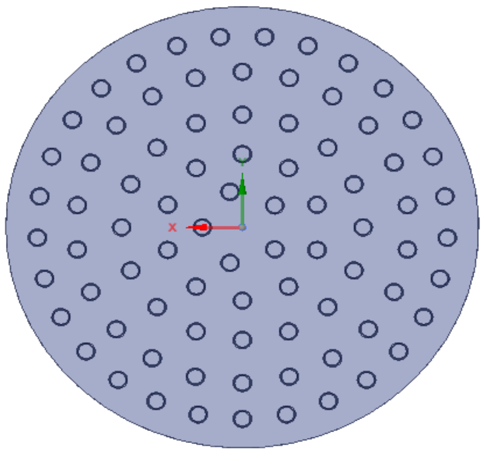
Design sketches for the experimental engine



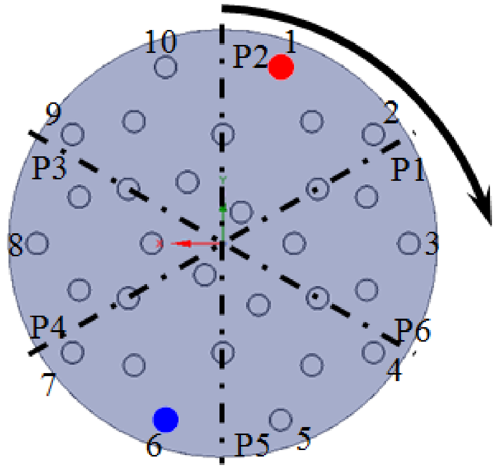


Simulation of 82-injector Rocketdyne LPRE

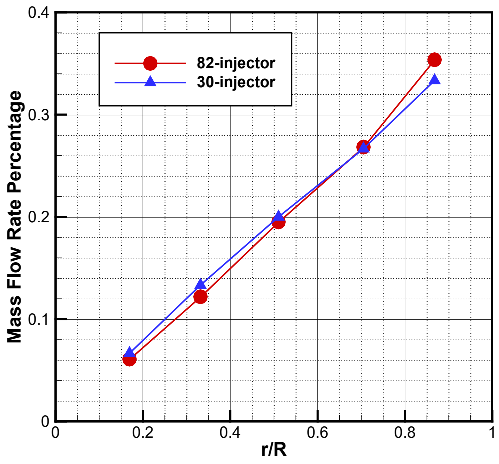




82-injector plate



30-injector plate



The 82-injector engine follows the design of the Rocketdyne experimental engine, except for details internal to the injector ports.

The 30-injector case matches the 82-injector case in chamber and nozzle sizes; mixture ratio; injector exit velocities; total mass flux; mean chamber pressure; total port exit area.

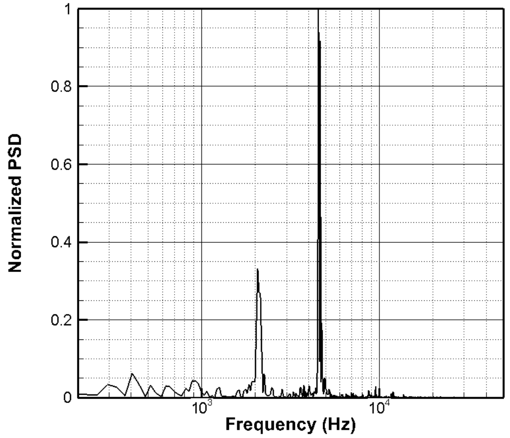
The radial and azimuthal distributions of injected mass flux are matched carefully.

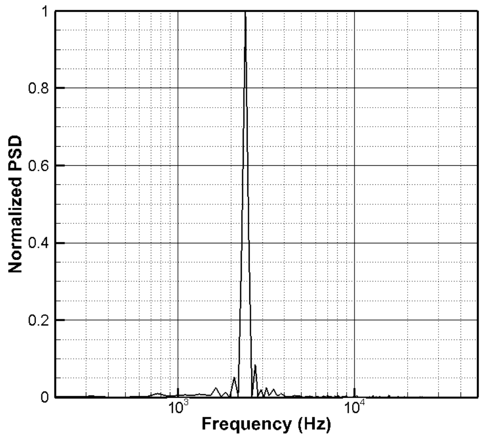
Some details of the internal injector port design is not perfectly mimicked.

Stability Behavior of 30-injector LPRE vs. 82-injector LPRE

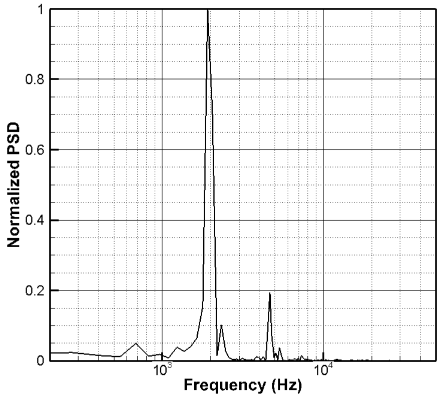
A decrease in mixing rate or chemical rate favors tangential mode by moving combustion away from longitudinal pressure antinode

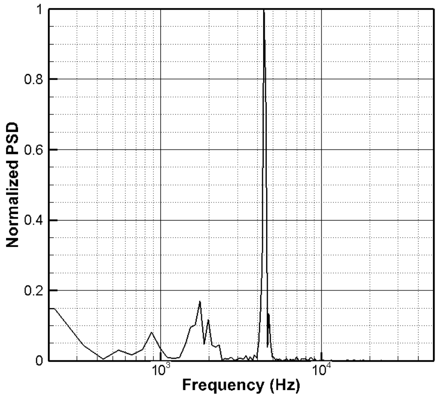
Spectral Analysis near Injector Plate

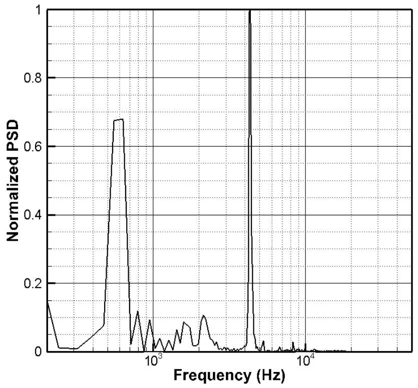




30-injector –full reaction rate   82-injector full rate

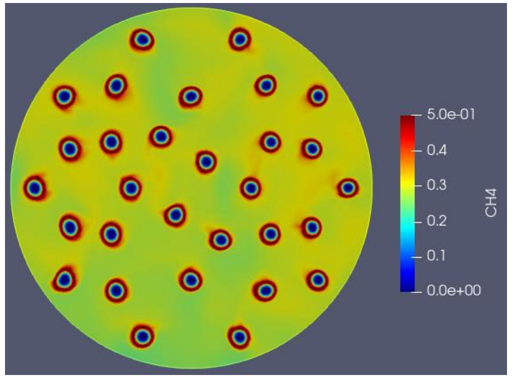


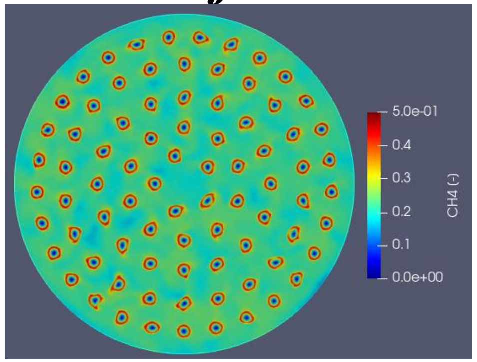




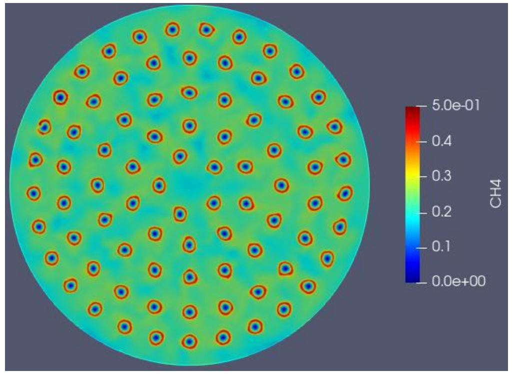
82-injector –half rate, 0.375 reaction rate, and 0.25 rate

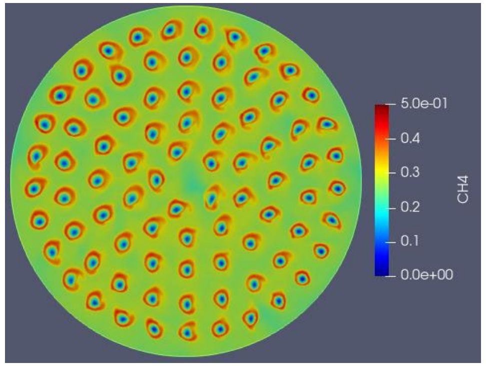
Methane Mass Fraction near Injector Plate





30-injector –full reaction rate   82-injector full rate





82-injector –half reaction rate   and quarter rate

Flamelet Theory and LES Sub-grid Modelling – *More Improvements*

Goals:

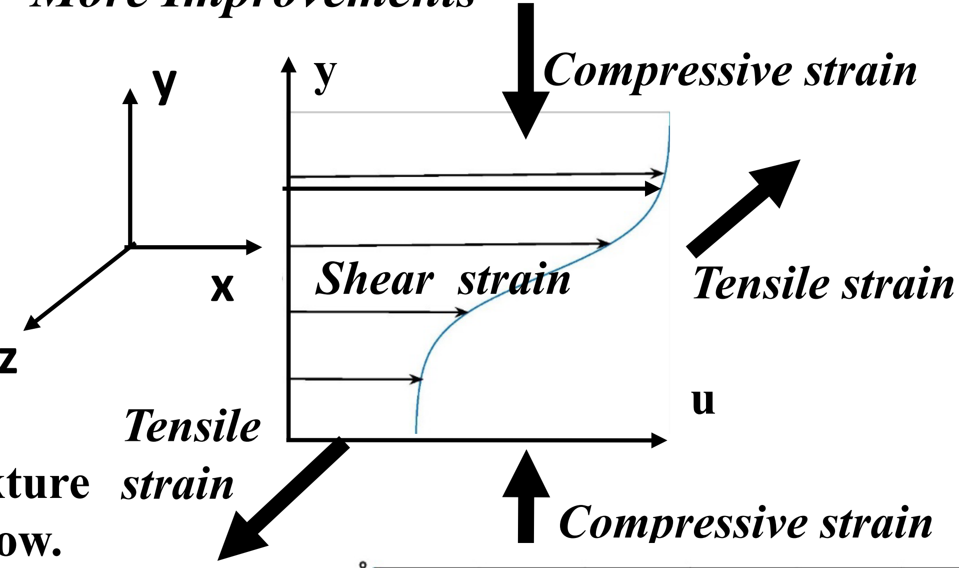
Account for multiple flames. ***Well handled.***

Variable-density formulation. ***Well handled.***

Consider imposed shear strain or vorticity. ***Done, more to come.***

Allow 3D flamelets. ***Done, more to come.***

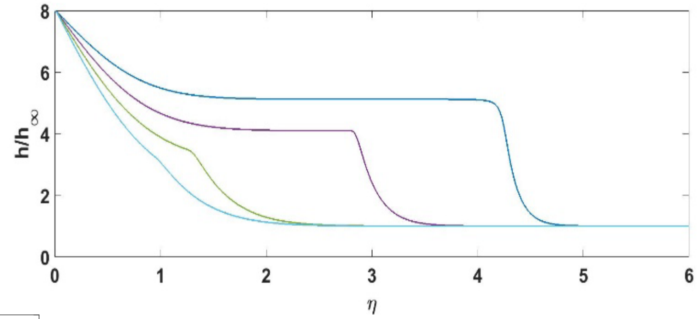
Properly scale between resolved flow and sub-grid. ***Underway.***

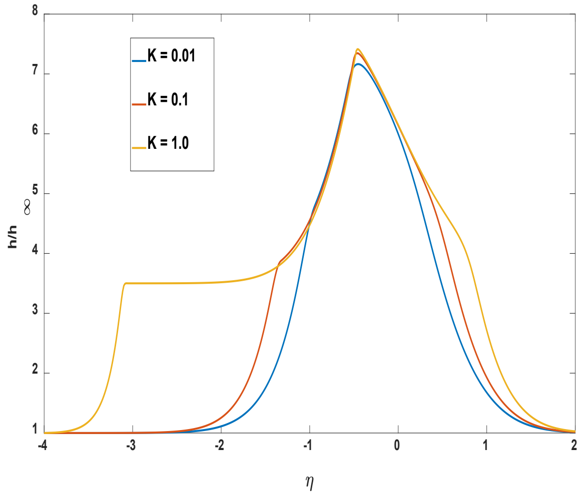


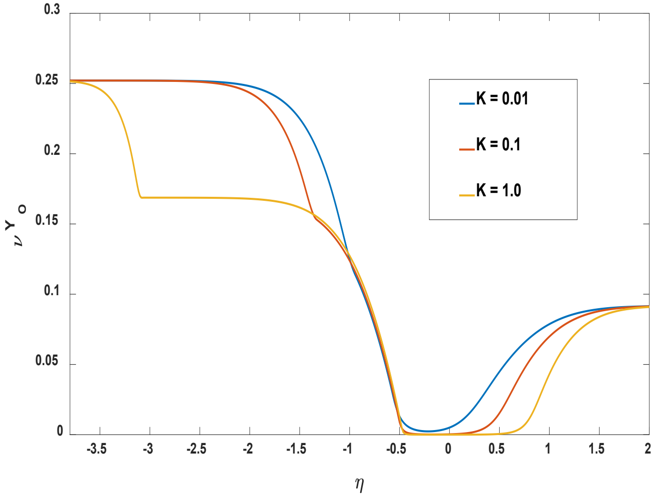
--- Consider a mixing layer with a fuel-rich mixture and a fuel-lean mixture flowing in parallel. A normal strain is imposed via transverse counterflow.

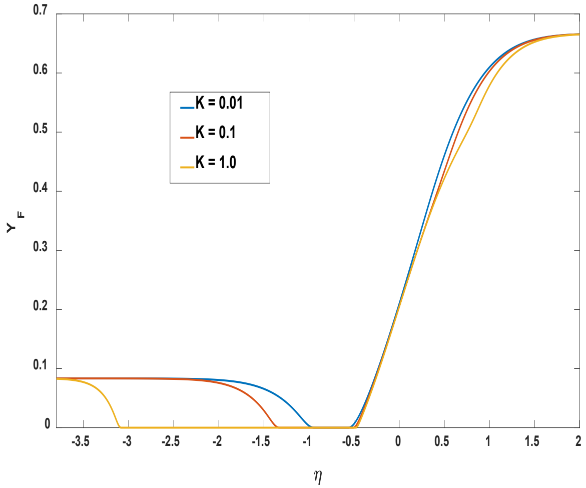
--- K is a normalized Damkohler number which increases with pressure and decreases with increasing imposed normal strain.

---Three flames result: a central non-premixed flame and two premixed flames. The premixed flames can be heat-diffusion controlled by the nonpremixed flame.









Heated wall, inflowing combustible premixture. Enthalpy vs. similarity variable. Two lower very-fuel-lean cases require wall heating while the top two modestly fuel-lean cases survive independently of wall heating

Sample Recent Publications ---- High-Pressure Combustion Dynamics: Low-Cost Computation and Stochastic Analysis

T. M. Nguyen and W. A. Sirignano, "Spontaneous and Triggered Longitudinal Combustion Instability in a Rocket Engine", *AIAA Journal*, online, 2019, https://doi.org/10.2514/1.J057743

J. Xiong, T. H. Morgan, J. Krieg, F. Liu, and W. A. Sirignano, "Nonlinear Combustion Instability in a Multi-Injector Rocket Engine", *AIAA Journal* 58 (1), pp. 219-35, 2020. https://doi.org/10.2514/1.J058036

J. Xiong, F. Liu, and W. A. Sirignano, "Combustion Dynamics Simulation of a 30-injector Rocket Engine", *Combustion Science & Technology,* in press, August 2020. Available online. https://www.tandfonline.com/doi/full/10.1080/00102202.2020.1847097

J. Xiong, F. Liu, and W. A. Sirignano, "Combustion Dynamics Simulation of an 82-injector Rocket Engine", paper in draft to be submitted to journal.

L. Zhan, J. Xiong, F. Liu, and W. A. Sirignano, "Inclusion of Flamelet Look-up Table in 3D Multi-injector Combustor Analysis" , paper in draft to be submitted to journal.

Z. Shadram, T. M. Nguyen, A. Sideris, and W. A. Sirignano, "Neural Network Flame Closure for a Turbulent Combustor with Unsteady Pressure", (with Z. Shadram, T. M. Nguyen, and A. Sideris), *AIAA Journal*, Vol. 59, No. 2, 2021, pp. 621–635. doi:10.2514/1.J059721, URL https://doi.org/ 10.2514/1.J059721.

Z. Shadram, T. M. Nguyen, A. Sideris, and W. A. Sirignano, "Physics-aware Neural Network Flame Closure for Combustion Instability Modeling in a Single-Injector Engine," paper in draft to be submitted to journal.

W. A. Sirignano, "Combustion with Multiple Flames Under High Strain Rates", *Combustion Science & Technology*, in press, online, 2019. https://doi.org/10.1080/00102202.2019.1685507

C. Lopez-Camara, A. Jorda Juanos, and W. A. Sirignano, "Strain Rate and Pressure Effects on Multi-branched Counterflow Flame", *Combustion & Flame*, *Combustion & Flame* 221, p.256-69, November 2020. http://arxiv.org/abs/2005.14516

W. A. Sirignano, "Mixing and Combustion in a Laminar Shear Layer with Imposed Counterflow", *Journal of Fluid Mechanics* 908 (10), A35, 2021. https://doi.org/10.1017/jfm.2020.936

W. A. Sirignano, "Diffusion-controlled Premixed Flames," *Combustion Theory and Modelling*, invited paper in press for special issue in honor of Professor Moshe Matalon, 2021. https://doi.org/10.1080/13647830.2020.1863474

High-Pressure Combustion Dynamics
Opportunities

- **Introduction of flamelet table for all multi-injector LPRE**
- **Pursue further triggering for control**
- **CFD with real-gas equations of state**
- **Further optimization of use and design of DLNN for multi-injector LPRE**
- **Better resolution of injector port oscillations for multi-injector LPRE**
- **Continued examination of chaotic combustion dynamics**
- **Further examination of consequence of premixed vs. nonpremixed combustion**
- **Further improvements of flamelet model**

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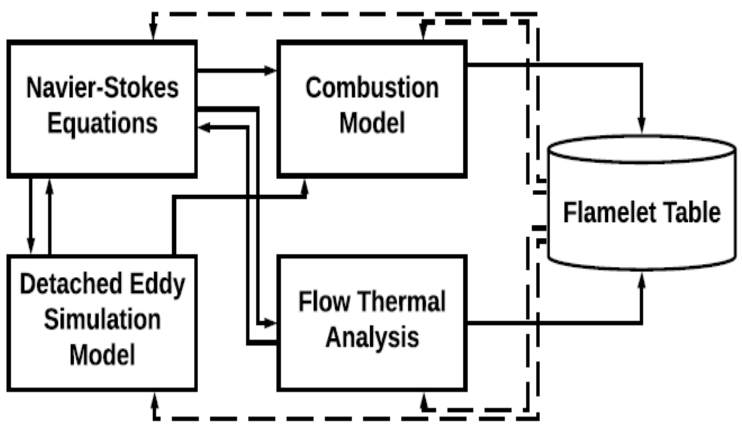
Graduate Student Researchers Z. Shadram and C. Lopez-Camara

Neural Network Representation of Flamelet Model for Rocket Engine Combustion

(a) Schematic of CVRC configuration [23]



(b) Top level architecture of CFD code

Focus has been on single-injector CVRC Engine with axisymmetric LES and unsteadiness due to both combustion instability and turbulence: it emulates well experimental evidence.

Original Approach: two sets of NNs learning off-line from table data.

14-cm oxidizer-post cases	Model	Relative Error (%)		Correlation (%)		RMS Ratio (%)	
		mean	std	mean	std	mean	std
Dynamic equilibrium	NNa	7.18	2.47	78.50	12.69	93.71	4.58
	NNb	6.23	2.34	82.10	13.71	93.91	2.85
Transient	NNa	5.02	1.32	18.74	18.74	75.84	2.35
	NNb	5.02	1.40	79.61	14.89	103.63	2.89

NN replaces look-up table for the Progress-variable Flamelet (PVF) Theory requiring less memory.

Training of the NN can require as little as 15% of the table data. Learning from the data most used by the CFD and data derived from physical constraints, i.e., “physics awareness”

The NN is used successfully for the triggered instability case without special training.

New approach: one NN for each FPV output. Six learn from table data used by transient-case CFD. FPV reaction rate learns also from dynamic equilibrium data.

	# of neurons in each layer	FLOP	training error (%)	test on table (%)
$\tilde{T}_f$	4-15-10-15-1	375	0.59	4.83
$\tilde{e}_f$	5-15-10-15-1	390	0.0566	0.57
$\tilde{R}$	5-15-10-15-1	390	0.0526	0.65
$\tilde{\lambda}$	5-15-10-15-1	390	0.21	3.57
$\tilde{\gamma}$	5-15-10-15-1	390	0.0371	0.48
$\tilde{\alpha}_\gamma$	5-15-10-15-1	390	0.22	1.41
$\tilde{\dot{\omega}}_C$	4-15-20-25-35-25-20-15-5-1	3490	1.49	32.86