CFD Modeling of NOx Formation in a Rotating Detonation Engine

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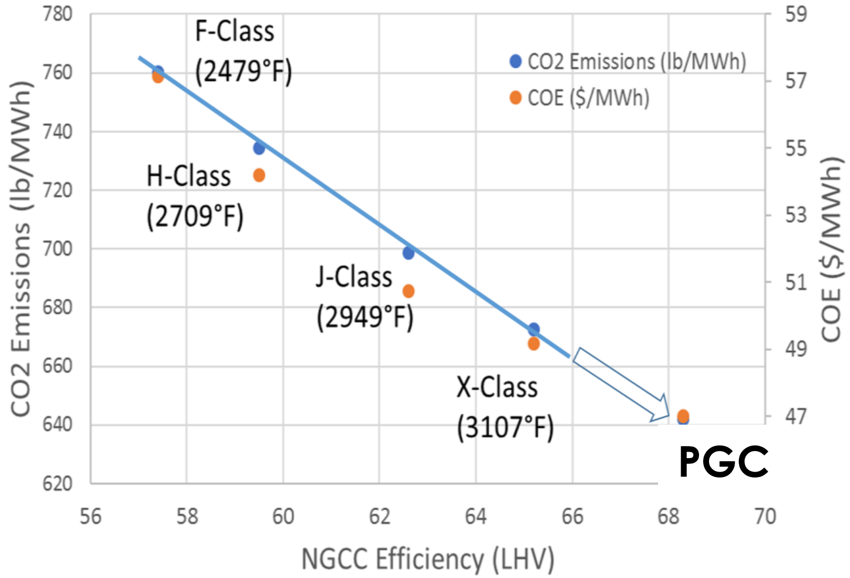
Background - Pressure Gain Combustion

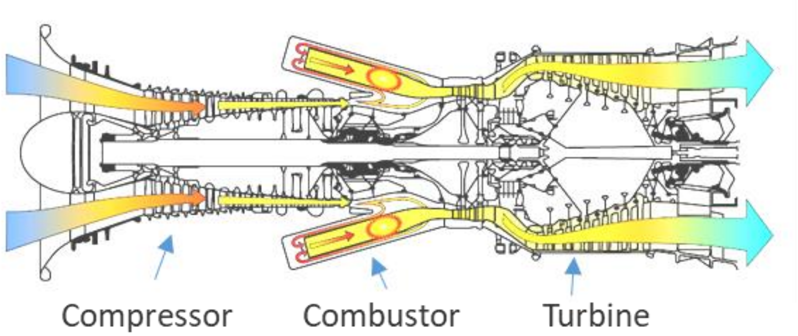
Rotating Detonation Engines

Motivation

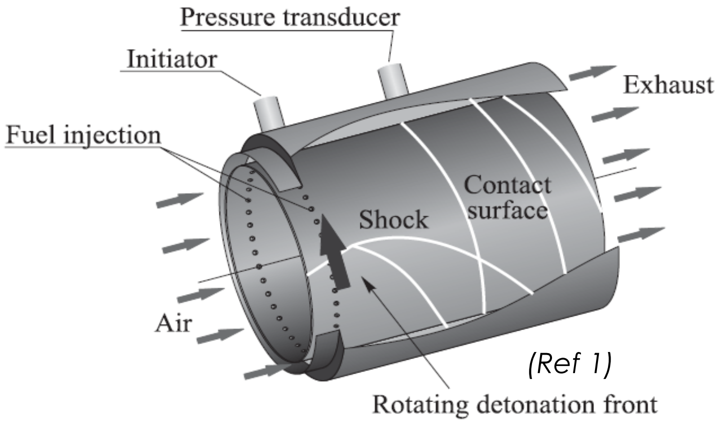
- **RDEs offer significant efficiency and COE benefit: Internal systems models suggest 4.9% increase in GT Efficiency (LHV) and 1.8% increase in Net Plant Efficiency (NGCC with H-Class RDE-GT Hybrid).**
- **Alternate and additive pathway to efficiency improvement.**
- **Creates a new class of machine reducing COE.**



Gas Turbine



RDE Combustor



(Ref 1)

- **Bulk axial flow with circumferential detonation wave**
- **Detonation wave, once initiated, is self-sustained.**
- **No moving parts – No complex valving required at the inlet compared to PDE's**
- **Potential for low NOx**

1. *Wolanski, P., Proc. Comb. Institute, 2013*

Background – NOx Emissions

RDE NOx Emissions

Problem

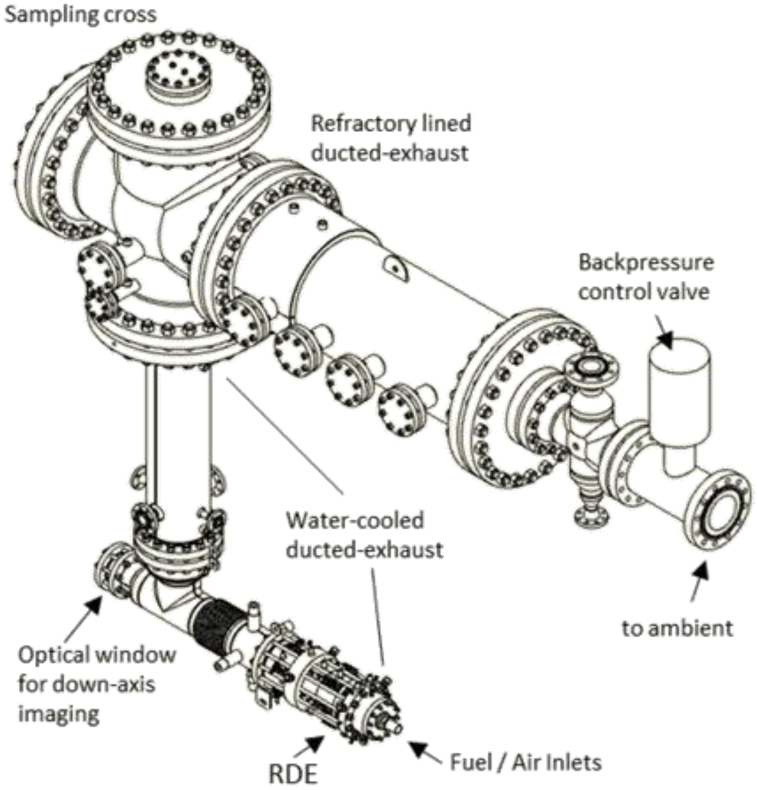
- NOx emissions from RDEs is not well understood and very little data is available.
- Most RDE CFD modeling approaches ignore turbulence-chemistry interactions, and many ignore viscous effects. Deflagrative burning not predicted well.

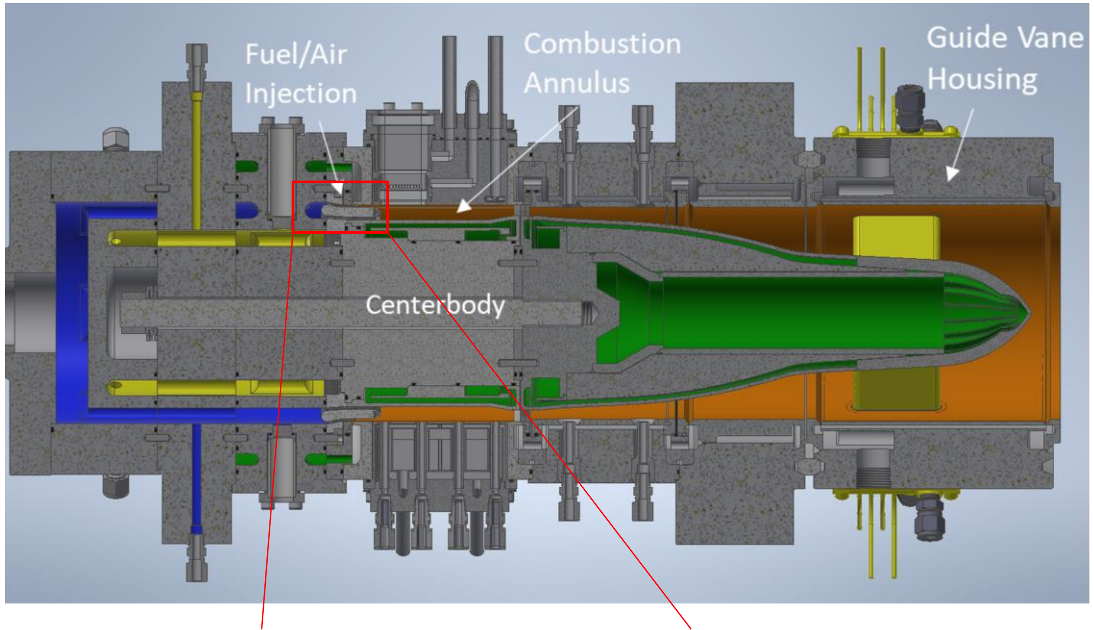
Approach

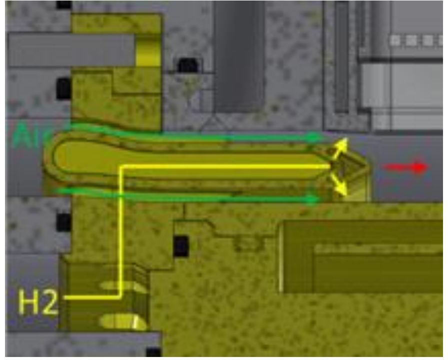
- Experimentally characterize NOx emissions from a water-cooled RDE over a range of equivalence ratios and back-pressures.
- Assess the ability of a zero-dimensional Partially Stirred Reactor (PaSR) model with detailed chemical kinetics to capture the physics of a Rotating Detonation Engine.
- Validate the PaSR model using new experimental data.

NETL Water-Cooled RDE

Hydrogen-Air







ID = 128.5 mm
OD = 148.8 mm
Pintle Style Injector (120 x 0.75mm holes)

Typical Operating Envelope

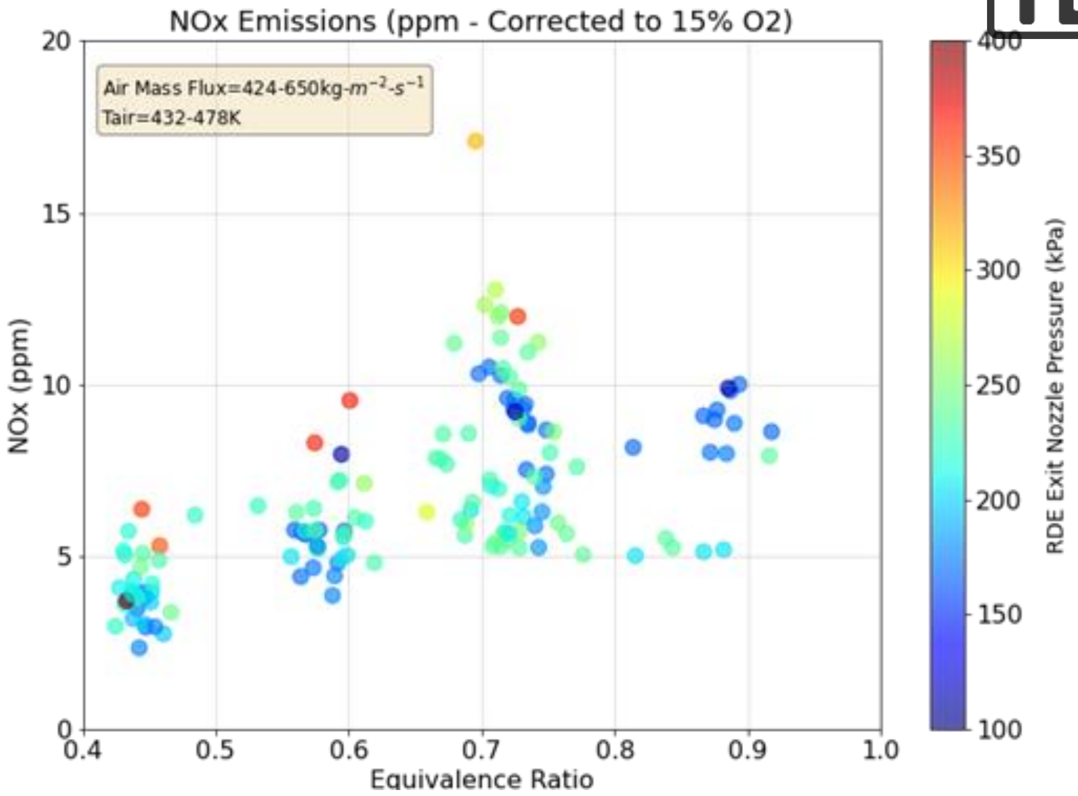
Air Mass Flux [kg m^{-2} s^{-1}]	phi	T_{air} [K]	P_{back} [kPa]
450	0.45, 0.6 0.75, 0.9	400, 475	101.3, 135 170, 240
500	0.45, 0.6 0.75, 0.9	400, 475	101.3, 135 170, 240
625	0.45, 0.6 0.75, 0.9	400, 475	101.3, 135 170, 240
650	0.45, 0.6 0.75, 0.9	400, 475	101.3, 135 170, 240

- Maximum back-pressure of 20 atm.
- Typical test time of 20-30 sec.
- Thermal equilibrium reached within 10 sec.
- High-speed pressure, OH*, Ions, Imaging, Calorimetry and steady-state gas sampling (O2, NOx).

Experimental Results

NOx Emissions

Gas Sampling Cart

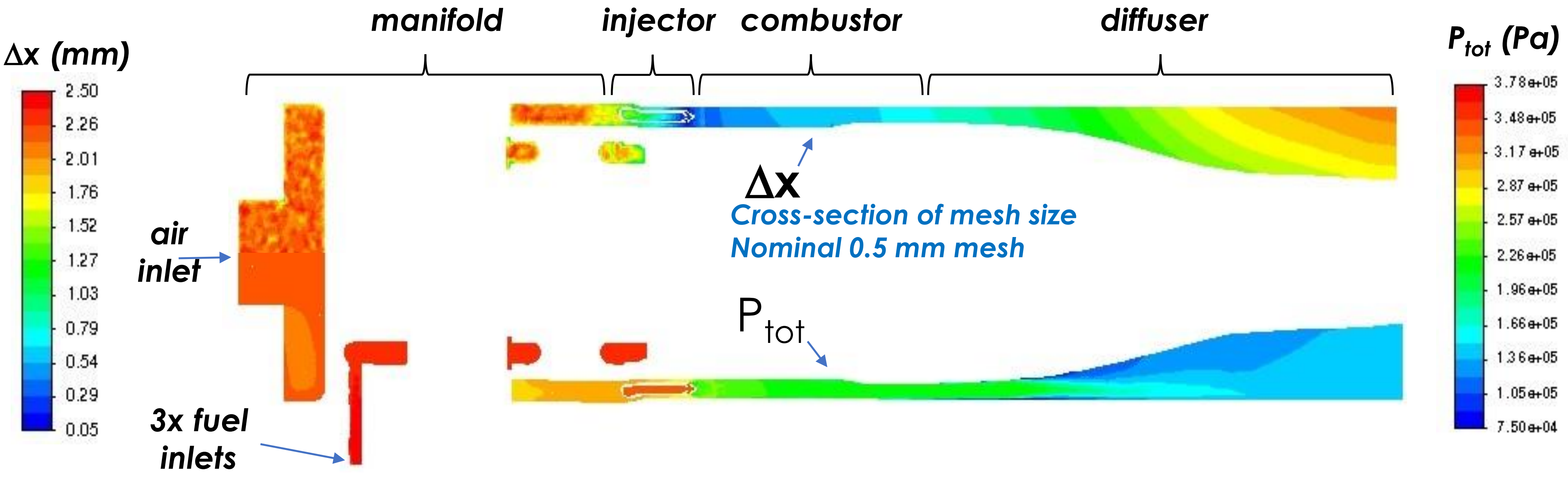


- NOx emissions increase with increasing equivalence ratio.
- NOx also increases with pressure, consistent with constant pressure combustion.
- Single digit NOx observed over range of operating conditions.

Modeling Approach

ANSYS Fluent

- Hybrid mesh with polyhedral cells in manifolding and injectors and hex cells in annulus.
- ANSYS Fluent pressure-based solver. Mass flow inlets, pressure outlet and 300K walls.
- LES with BCD for momentum, 2nd upwinding for scalars and 1st Euler in time. Derived from 1D detonation simulations.
- Sandiego H_2/Air mechanism with nitrogen chemistry.

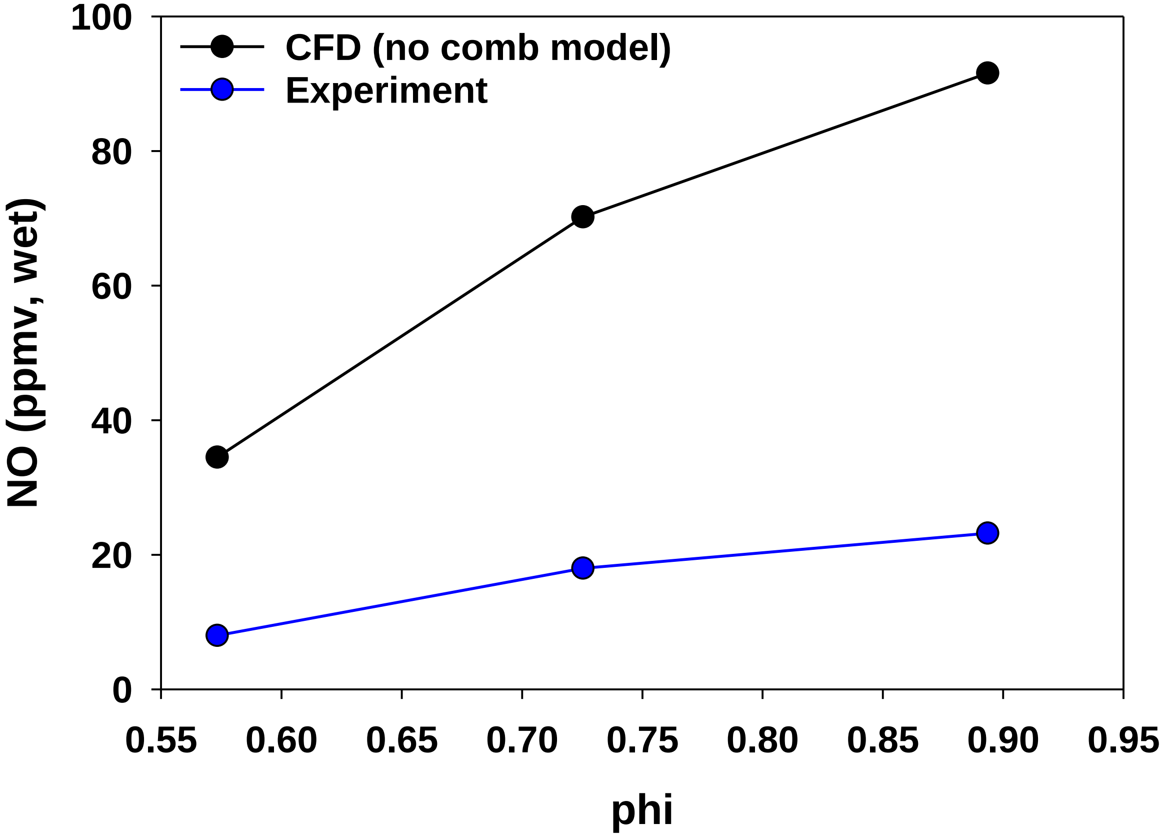


Early Modeling Results

LES with No Combustion Model

- FLUENT LES, 10M cells (0.5 mm)
- 1st ddt to prevent overshoot
- SanDiego mechanism
  - 19 species / 64 reactions (H2/Air)
  - Includes thermal, NNH, NH3, N2O and NO2 chemistry)

Case	ϕ	Fuel (kg/s)	Air (kg/s)	T_{fuel} (K)	T_{air} (K)	P_{back} (kPa)
Run 4	.573	.00973	.5807	333	432	130
Run 12	.725	.01191	.5621	331	431	133
Run 15	.894	.01362	.5218	330	432	131



- **Ignoring turbulence-chemistry interactions results in severe over prediction of NOx emissions, even with added dissipation to prevent numerical overshoot/oscillations at detonation wave.**

Partially Stirred Reactor Model

Developed by Magnussen, Chomiak and others…

- **The PaSR model assumes that each computational cell is comprised of both reacting and non-reacting zones where mass is exchanged between the two through turbulent mixing.**
- **Source term modification through ratio of turbulent mixing to chemical reaction time scales.**
- **Detailed chemistry with stiff ODE solver and LES approach.**

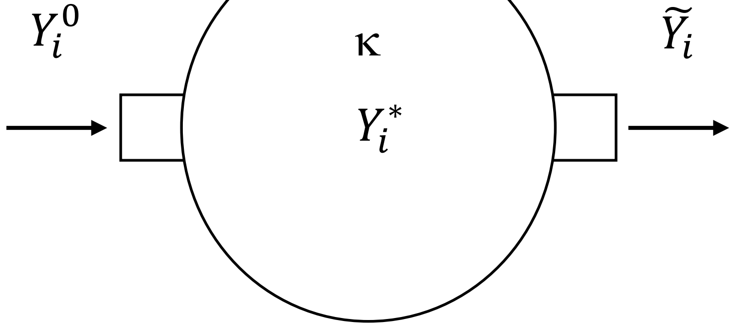
Source terms

$$\overline{\dot{\omega}_i} = \kappa \frac{\tilde{\rho}(Y_i^* - Y_i^0)}{\tau^*}$$

Mixing Constant

$$\kappa = \frac{\tau_c}{\tau_c + \tau_{mix}}$$

Partially Stirred Reactor



LES Turbulent mixing time

$$\tau_{mix} = C_{mix} \frac{k}{\varepsilon} \qquad \varepsilon = C_\varepsilon \frac{k^{1.5}}{\Delta}$$

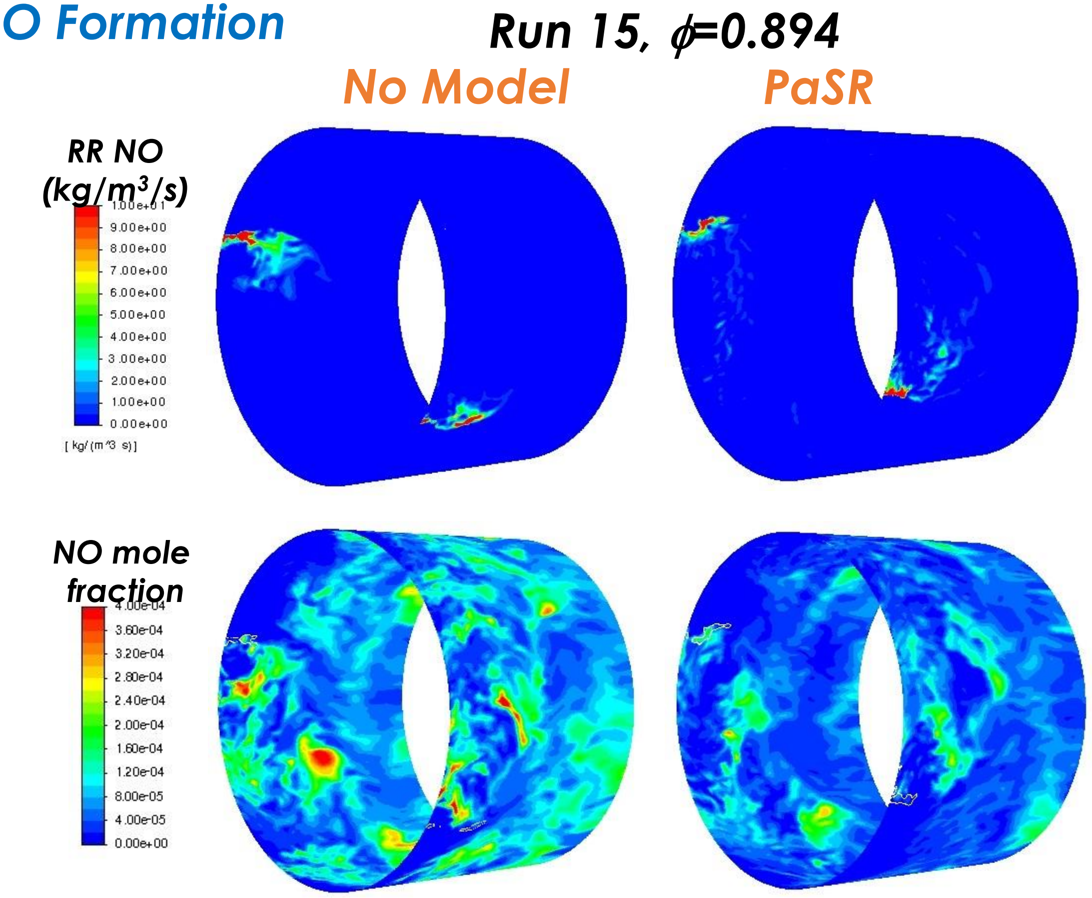
C_{mix} assumed to be 0.25

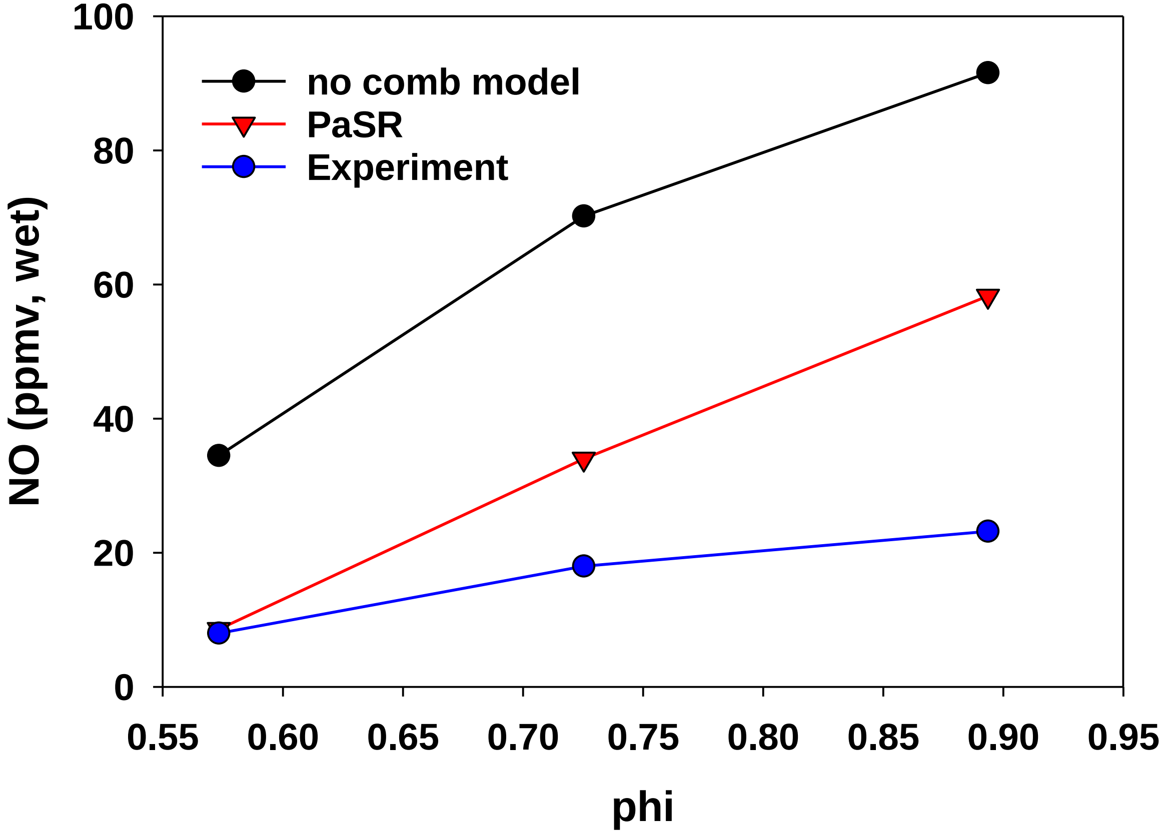
Chemical reaction time

$$\tau_c = max\left(\frac{\rho Y_i}{\omega_i}\right)$$ *i= major species*

PaSR Model Results

NO Formation





- No combustion model results in 4x over-prediction of NO emissions.
- PaSR model significantly reduces NO formation
- Reduction of peak reaction rates and temperatures through kappa

$$\overline{\dot{\omega}_i} = \kappa \frac{\tilde{\rho}(Y_i^* - Y_i^0)}{\tau^*} \qquad \tau_{mix} = C_{mix}\frac{k}{\varepsilon}$$

Calculation of Mixing Timescale

Transported Timescale Approach

$$\tau_{mix} = \frac{\widetilde{Z_V}}{\widetilde{\chi_Z}}$$

Scalar Variance: $\widetilde{Z_V} = C_Z \Delta^2 \left(\nabla \tilde{Z}\right)^2$

Scalar Dissipation: $\widetilde{\chi_Z} = 2\left(\tilde{D}_Z + D_t\right)\left(\nabla \tilde{Z}\right)^2$

$$\frac{\partial(\bar{\rho}\tilde{Z}_V)}{\partial t} + \frac{\partial \bar{\rho}\widetilde{u_j}\tilde{Z}_V}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\bar{\rho}\left(\tilde{D}_Z + D_t\right)\frac{\partial \tilde{Z}_V}{\partial x_j}\right) + 2\bar{\rho}\left(\tilde{D}_Z + D_t\right)\left(\frac{\partial \tilde{Z}}{\partial x_j}\right)^2 - \bar{\rho}\tilde{\chi}_Z$$

$$\frac{\partial(\bar{\rho}\tilde{\chi}_Z)}{\partial t} + \frac{\partial \bar{\rho}\widetilde{u_j}\tilde{\chi}_Z}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\bar{\rho}\left(\tilde{D}_Z + D_t\right)\frac{\partial \tilde{\chi}_Z}{\partial x_j}\right) - C_1\bar{\rho}\frac{\tilde{\chi}_Z^{\,2}}{\widetilde{Z_V}} - C_2\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\tilde{\chi}_Z - C_3\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\widetilde{u_j'Z'}\frac{\partial \tilde{Z}}{\partial x_j} - C_4\bar{\rho}\frac{\tilde{\chi}_Z}{\tilde{k}}\widetilde{u_i'u_j'}\frac{\partial \tilde{u}_i}{\partial x_j}$$

$C_1 = 2.0$
$C_2 = 0.9$
$C_3 = 1.7$
$C_4 = 1.4$

$$\tau^* = MIN(\tau_c, \tau_{mix})$$

$$\widetilde{u_j'Z'} = -D_t\frac{\partial \tilde{Z}}{\partial x_j} \qquad \widetilde{u_i'u_j'}\frac{\partial \tilde{u}_i}{\partial x_j} = -\nu_t\left|\tilde{S}\right|^2$$

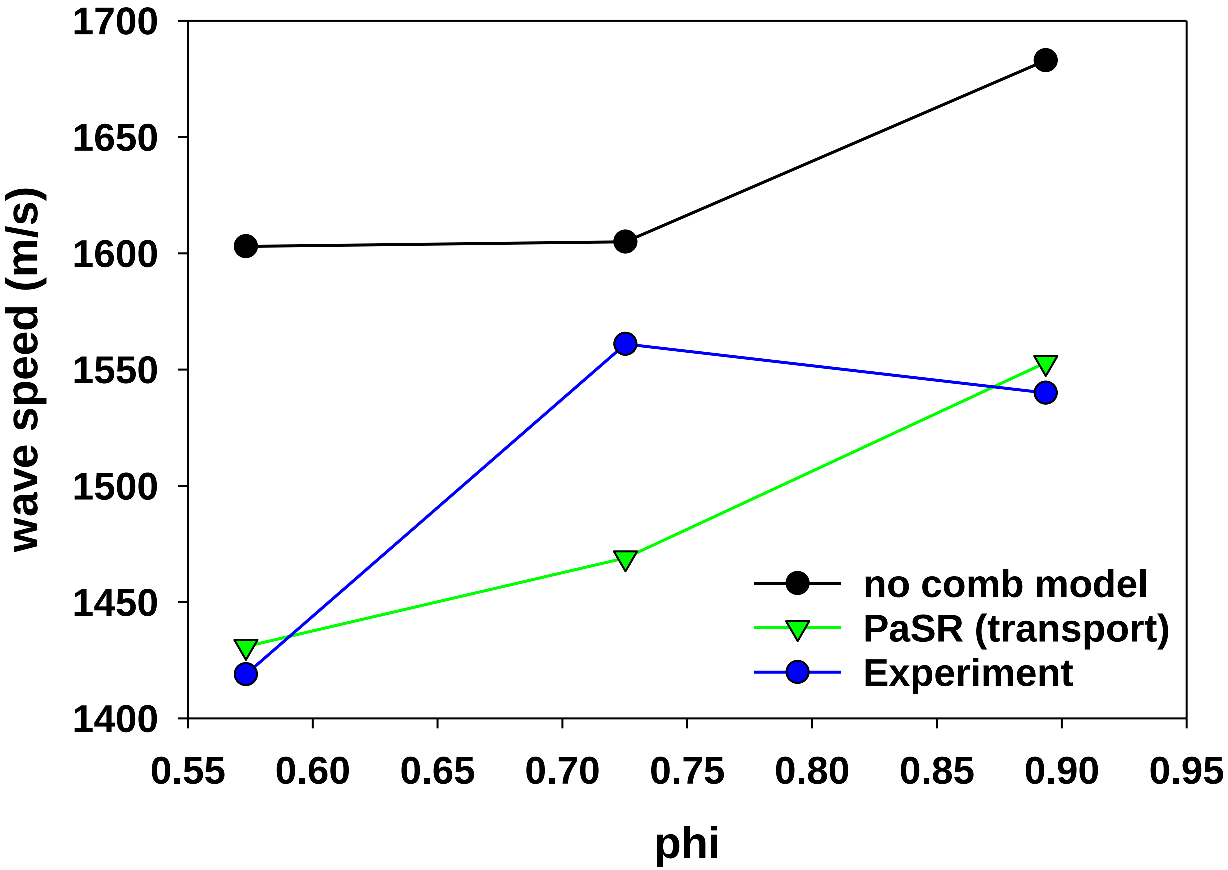
- **Transport equations are solved for scalar variance and scalar dissipation rate.**
- **Accounts for non-equilibrium production and destruction of scalar variance and dissipation.**

Wave Speed Results

Hydrogen-Air

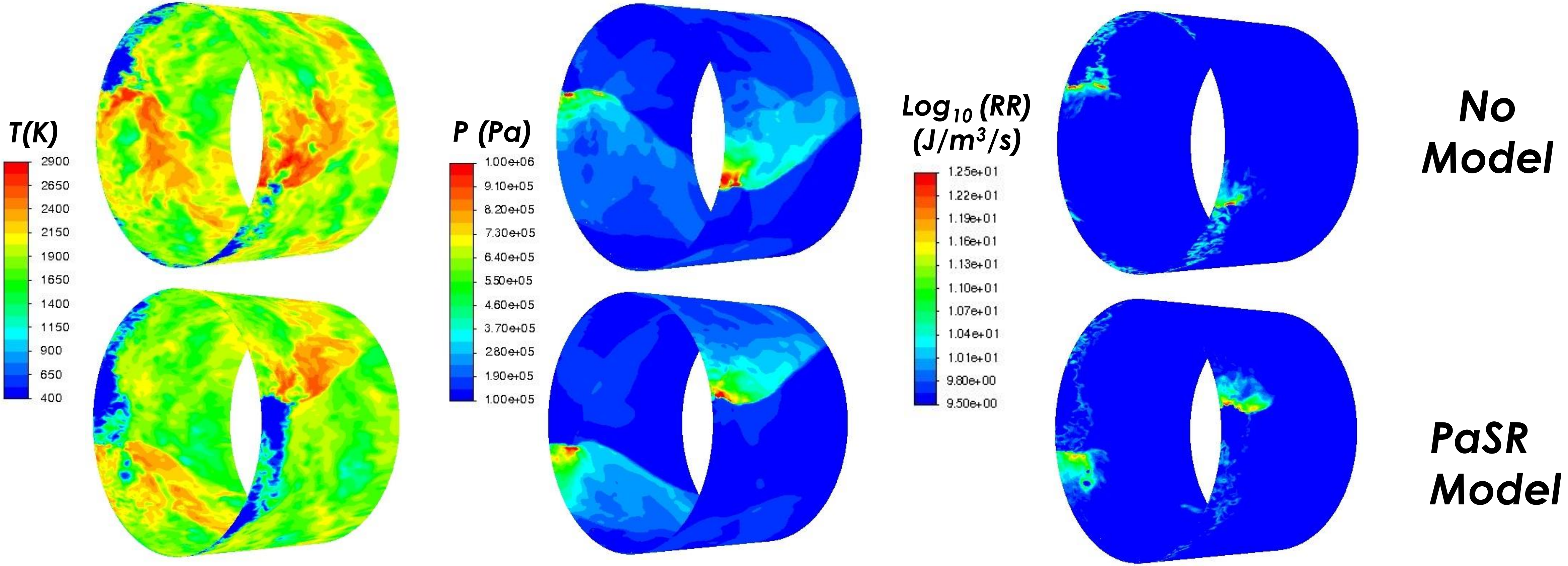
Case	ϕ	Wave Speed Experimental (m/s)	Wave Speed No Comb Model (m/s)	Wave Speed PaSR Model (m/s)
Run 4	.573	1419	1603	1431
Run 12	.725	1561	1605	1469
Run 15	.894	1540	1683	1553

- **Wave speed prediction generally improved with PaSR model**
- Two waves observed at ϕ=.725 and ϕ=.894 and two/three waves at ϕ=.573



Temperature, Pressure, Reaction Rate

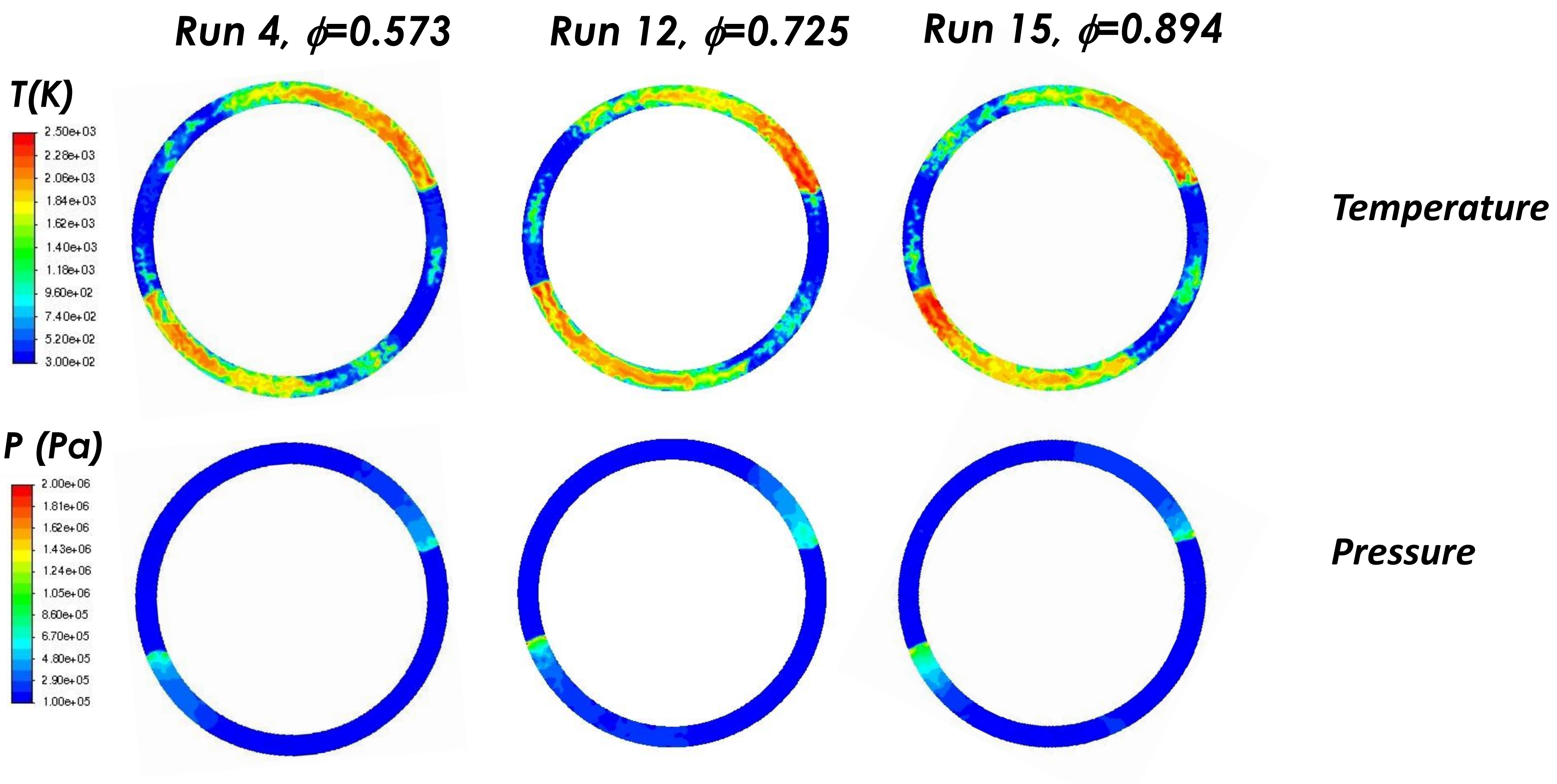
Contours through mid-plane, run12, $\phi = .725$



- PaSR model reduces deflagrative (parasitic) combustion in fill region.
- Peak pressures and temperatures also reduced.

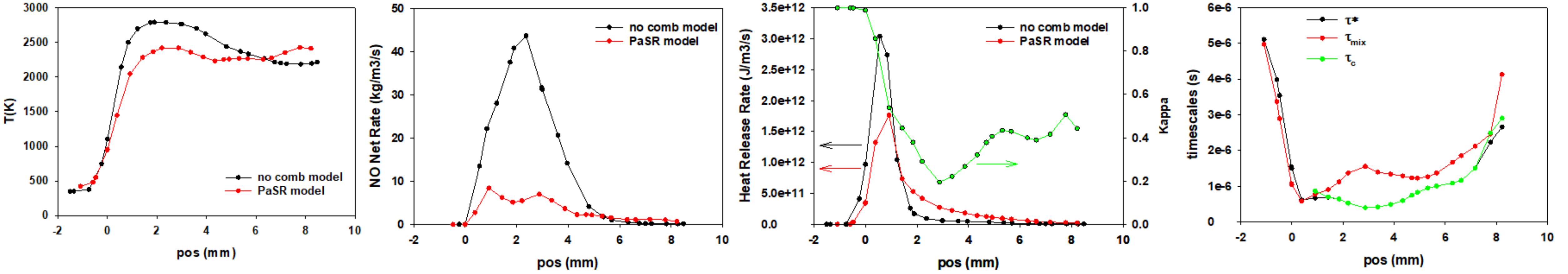
Cutting Plane at Z=5 mm

Single Snapshots



Line Plot Through One Wave

Line plots through one wave, run12, $\phi = .725$



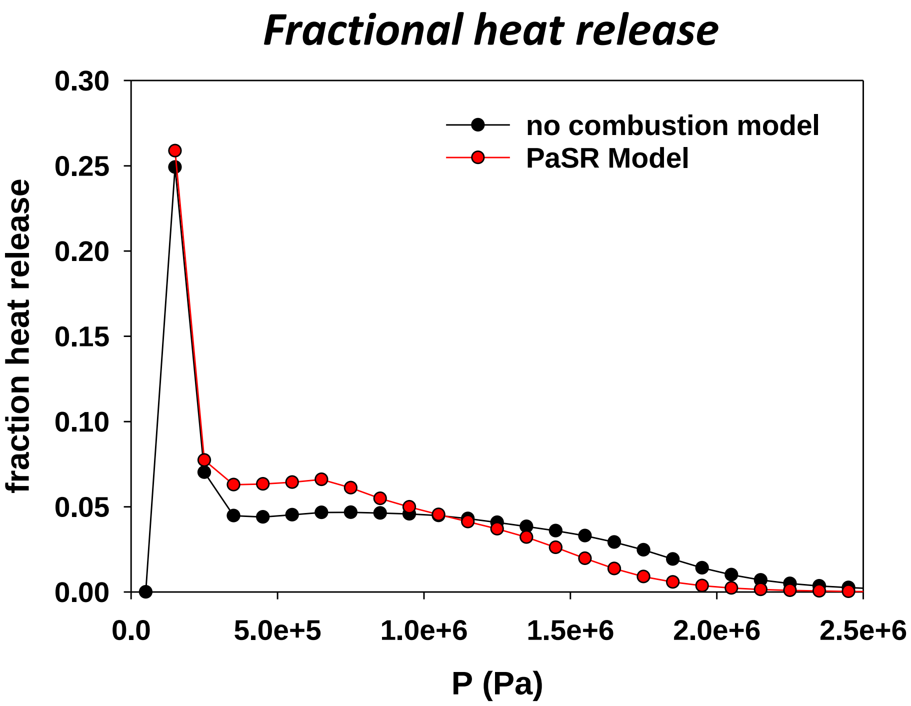
- **Peak temperature reduced by almost 400 K.**
- **Fine scale mass fraction in NO formation region between 0.2 and 0.4.**
- **Reactor residence time τ*, order of magnitude longer than solver time step (dt=1e-7s).**

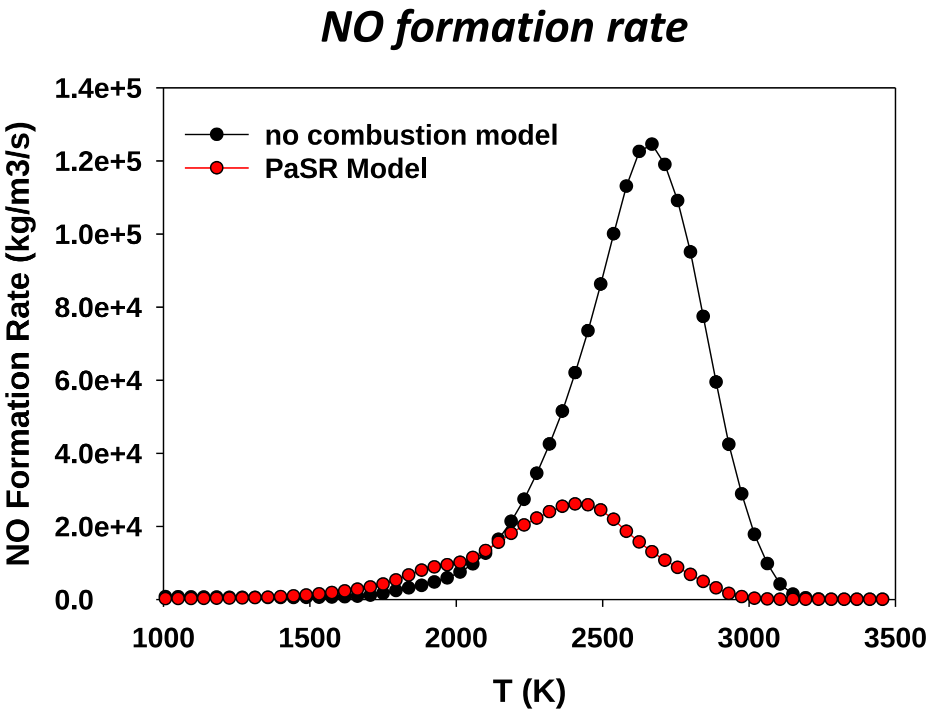
$$\kappa = \frac{\tau_c}{\tau_c + \tau_{mix}}$$

$$\overline{\dot{\omega}_i} = \kappa \frac{\tilde{\rho}(Y_i^* - Y_i^0)}{\tau^*}$$

Histogram Analysis

NO formation rate



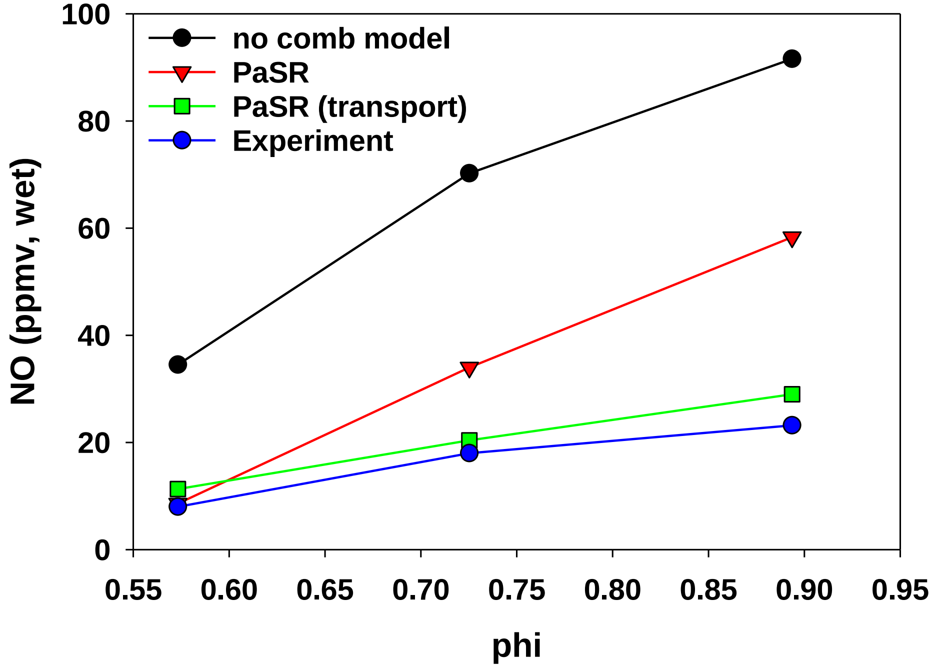


- **Heat release and NO formation rate binned by pressure or temperature through entire domain and averaged in time.**
- **Shows shift to lower pressures and temperatures.**

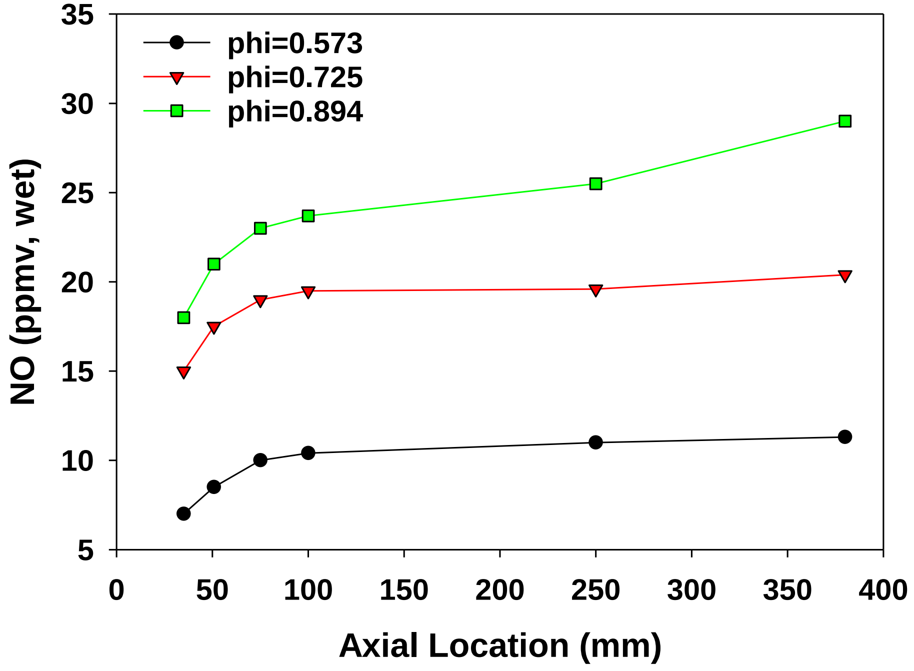
Integrated NO Emissions

Averaged in time and space at domain exit

NO vs. ϕ



NO vs. axial location



- Current treatment of timescale results in significant improvement in NO prediction.
- Bulk of NO is formed in the detonation region.

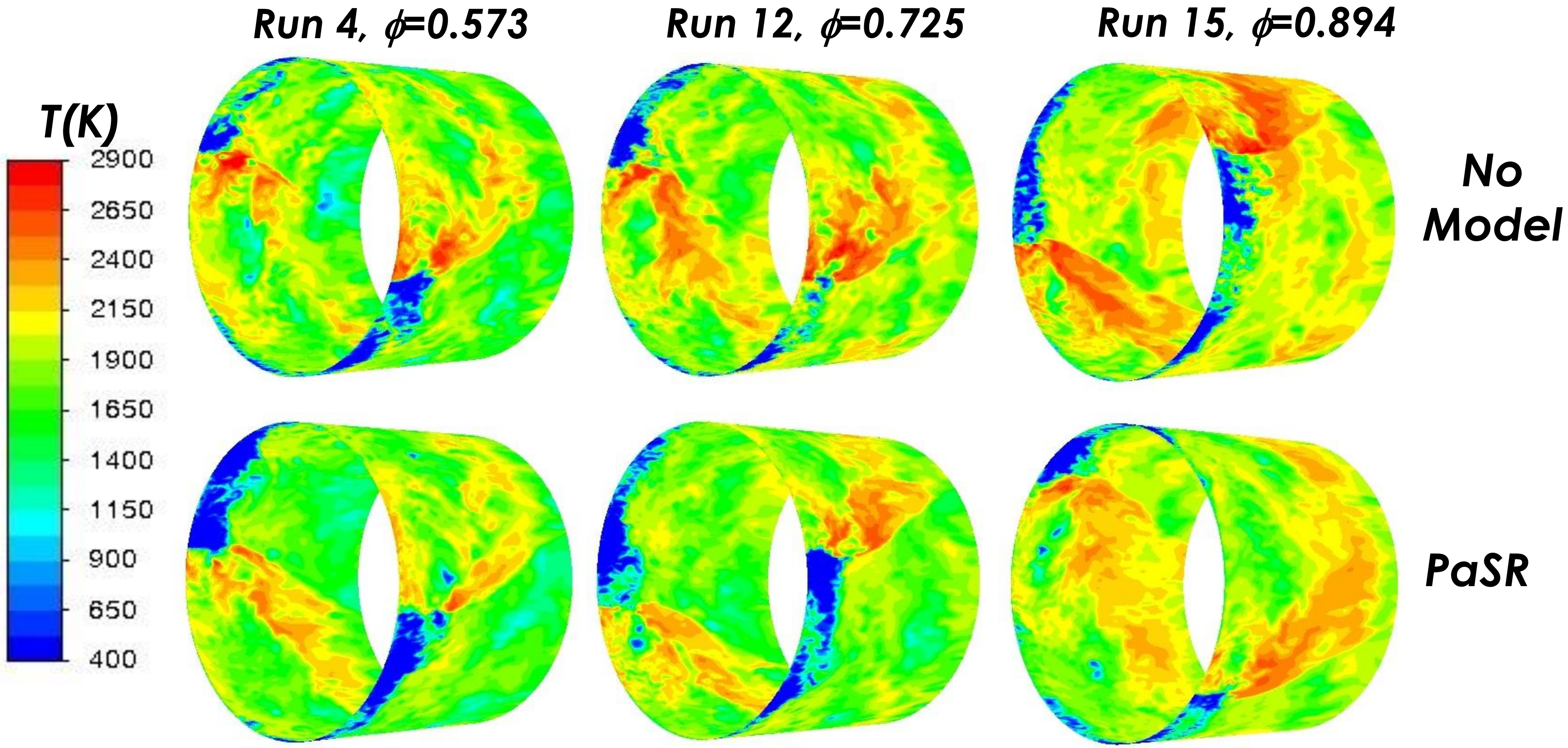
Conclusions

- **Ignoring turbulence-chemistry interaction results in significant (4x) over-prediction of NOx while the PaSR model seems to improve results.**
  - **Constant C_{mix} approach likely contributing to limitations.**
  - **Dynamic approach using transport equations for scalar variance and dissipation rate to determine mixing timescale results in significant improvement.**
- **Bulk of NOx formation occurs in or directly behind the detonation wave.**
- **NOx emissions very reasonable, some single digit, over wide range of equivalence ratios and up to 4 atm back pressure.**

Backup Slides

Temperature Contours

Contours through mid-plane



- PaSR model reduces deflagrative (parasitic) combustion in fill region.
- Peak pressures and temperatures also reduced.

NOx Formation

Run 15, ϕ=0.894