PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Improved Chemical Kinetics and Algorithms for More Accurate, Faster Simulations

2021 DOE Vehicle Technologies Office Annual Merit Review Presentation

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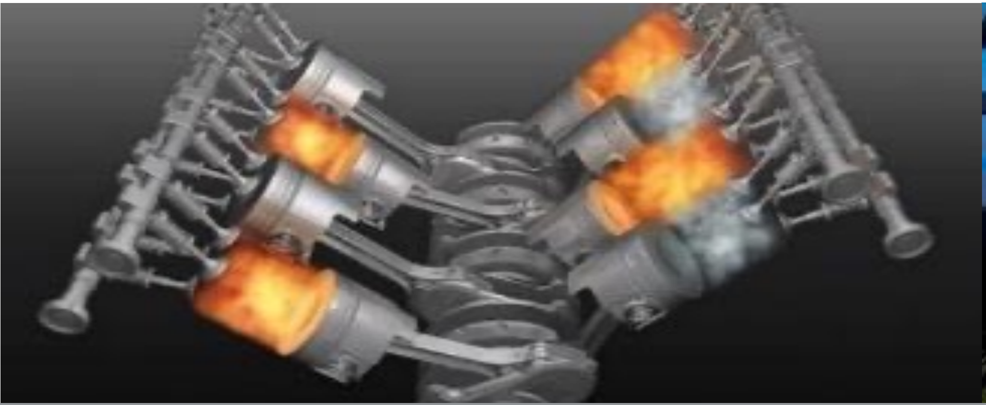
June 22, 2021

Project ID# ace140



This research was conducted as part of the Partnership to Advance Combustion Engines (PACE) sponsored by the U.S. Department of Energy (DOE) Vehicle Technologies Office (VTO). A special thanks to DOE VTO program managers Mike Weismiller and Gurpreet Singh.

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Overview

Timeline

- PACE started in Q3 FY2019*
- PACE will end in Q4 FY2023 (~46% complete)
- Focus and objectives of tasks will be continuously adjusted
- Overall PACE work plan discussed in ace138

FY2019	FY2020	FY21		FY2022	FY2023

*Q, FY = Quarter, Fiscal Year. FY20 begins October 1, 2019.

Barriers

Poor ability to predictively model and control:

- Knock & low speed pre-ignition (LSPI)
- Dilute combustion
- Cold-start emissions

Aligned with USDRIVE ACEC Tech Team
Priority 1: Dilute gasoline combustion

Budget

Tasks (PI)	FY20	FY21
L.M.05.01-07 (Whitesides)	$550K	$750K

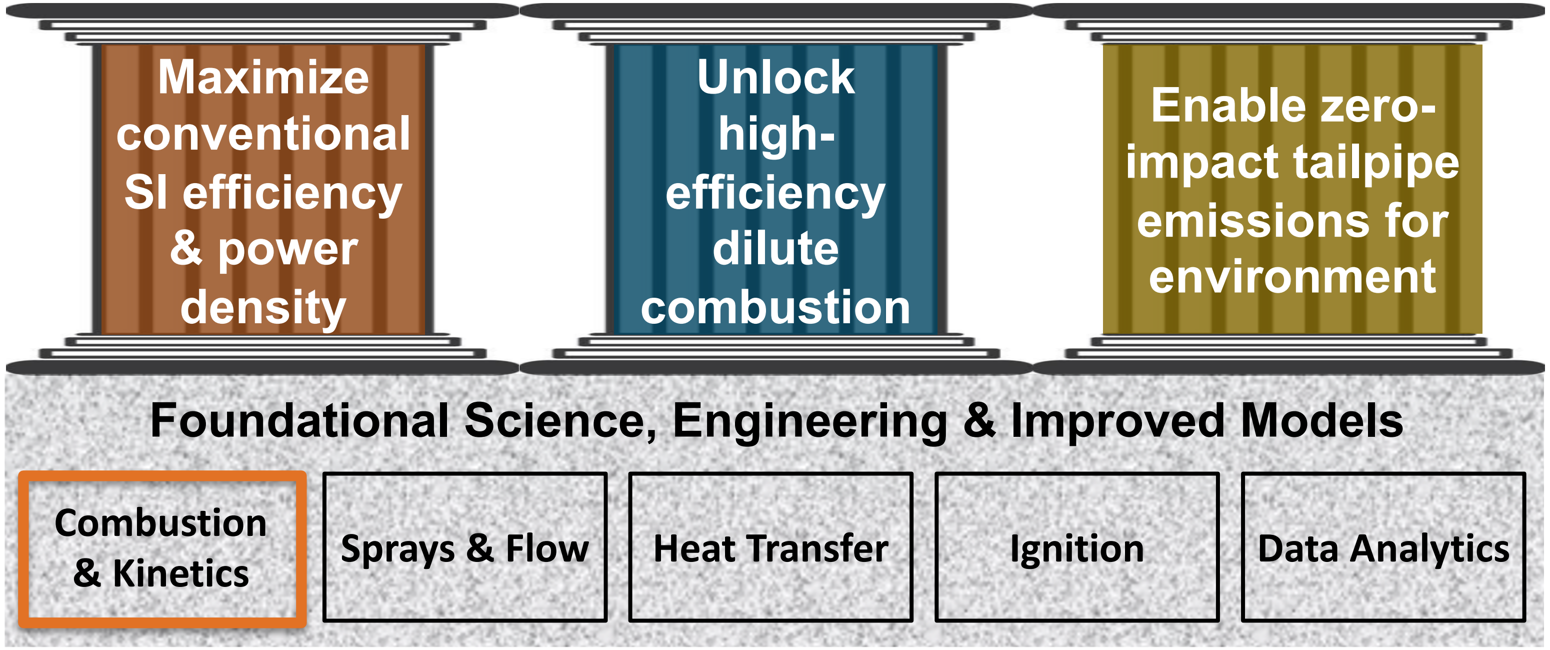
Complete PACE budget included
in reviewer only slides

Partners

- PACE is a DOE-funded consortium of 5 National Labs working toward common objectives (ace138)
  - Goals and work plan developed with input from stakeholders including DOE, ACEC Tech Team, commercial CFD vendors, and others.
- Specific partners on the work shown here:
  - ANL, ORNL, SNL, NREL
  - GM, Convergent Science Inc.

Relevance

PACE Outcomes Require Overcoming Modeling Challenges Related to Kinetically Controlled Phenomena

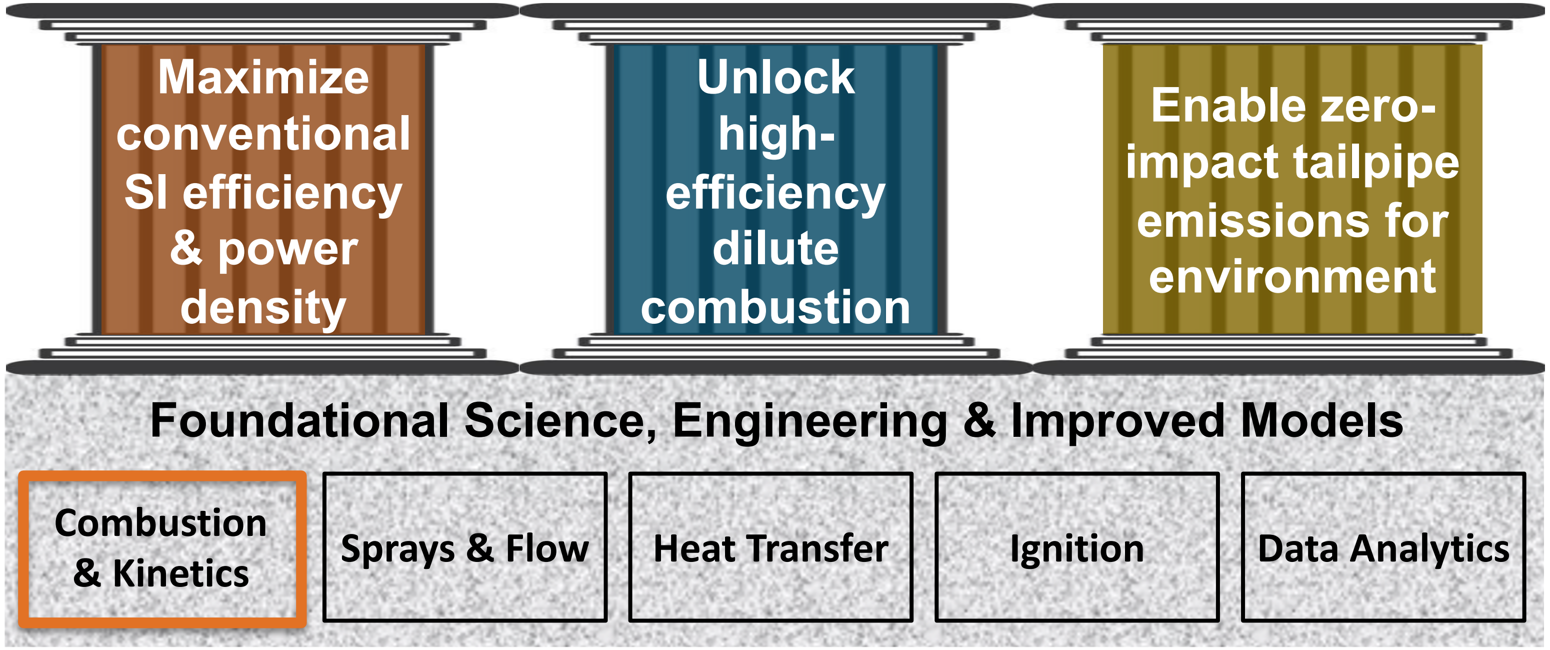


Poor ability to predictively model and control:

- **<u>knock</u> response to design changes and low-speed pre-ignition (LSPI)**
- **lean and/or dilute combustion burn duration and <u>emissions</u>**
- **the impact of injection and spark timing on <u>combustion phasing and emissions</u> during cold-start**

Relevance

PACE Outcomes Require Overcoming Modeling Challenges Related to Kinetically Controlled Phenomena



Project Focus:

- **Advance state-of-the art in combustion simulation**
  - Enable detailed, predictive models
  - Reduce time to solution
- **Use tools to impact industry relevant problems**

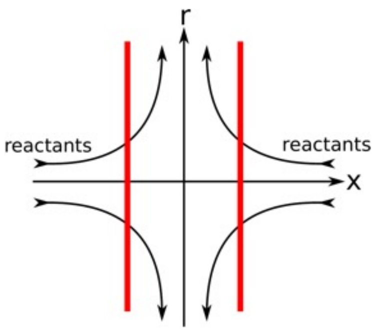
Milestones

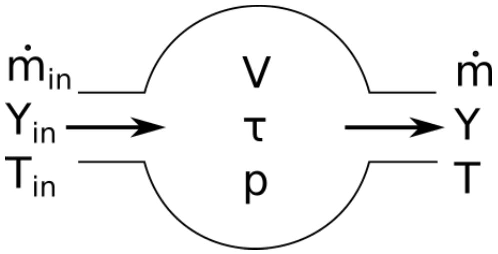
Month Year	Description of Milestone or Go/No-Go Decision	Status	Lab
October 2020	A.02.01. Developed solvers provide >2x reduction in transport time for engine simulations.	**Completed**	LLNL
October 2020	A.02.04. Improvements in performance of Zero-RK coupled to engine CFD on Summit/Sierra.	**Completed**	LLNL
December 2020	L.M.05.04. Zero-RK UDF compiled and tested on ORNL and ANL clusters.	**Completed**	LLNL
March 2021	A.02.04. Preliminary interface design/implementation for high scalability codes.	**Delayed**	LLNL
June 2021	L.M.05.02. New chemical integrators implemented, and data generated for improved solver selector training.	On-target	LLNL
September 2021	L.M.05.01. Transport equation reduction methodology optimized for PACE applications with RD5-87 fuel surrogate.	On-target	LLNL

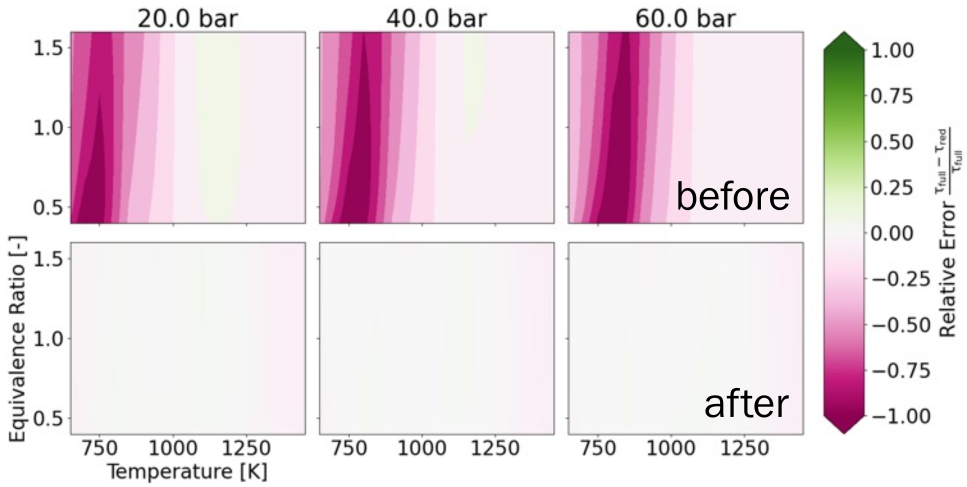
Approach

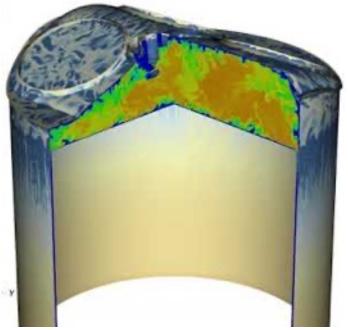
Target Modeling Bottlenecks with Chemical Algorithms to Accelerate Simulations & Increase Predictivity

- **New Accelerated Chemical Kinetics Models**
- **Kinetic Mechanism Reduction & Optimization**
- **Link Zero-RK to Exascale Codes**
- **Deploy Zero-RK to Partner Labs**







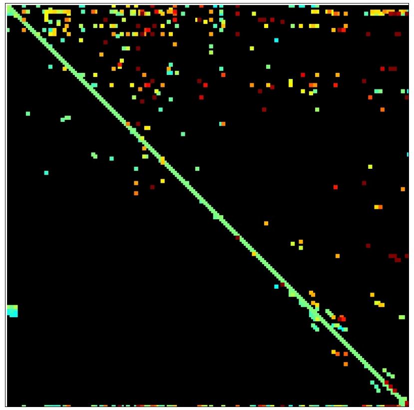


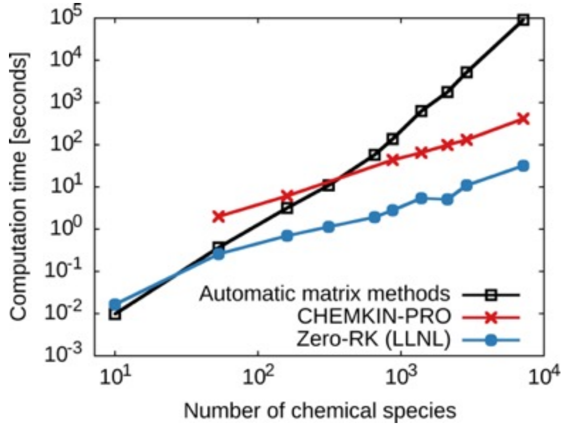
Fast Chemical Tools Developed at LLNL are the Basis of Ongoing Contributions to PACE

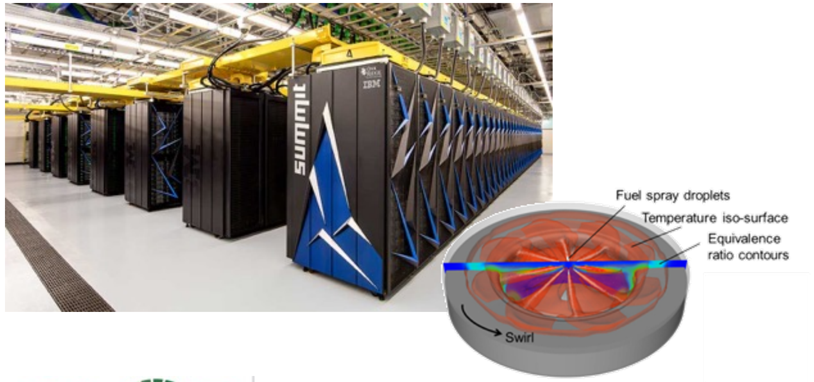
Zero-RK

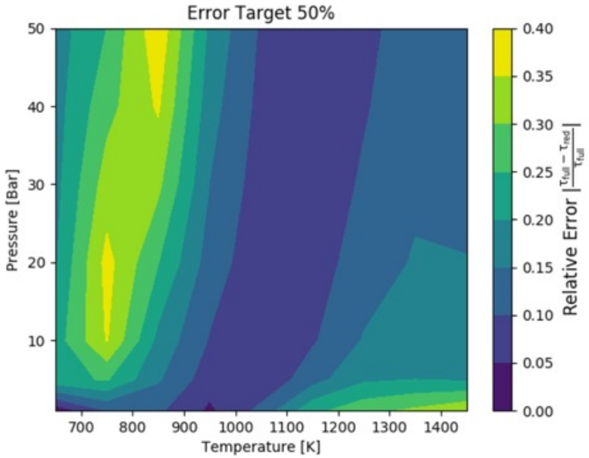
2015 R&D 100 WINNER

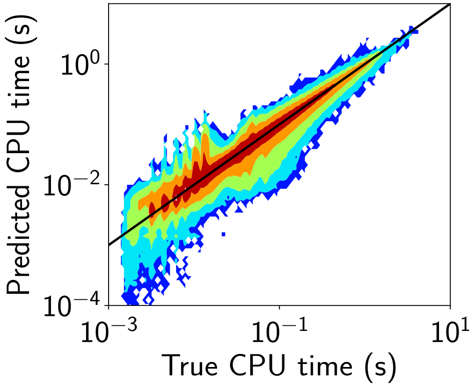
- We have developed algorithms & numerical methods to accelerate detailed chemical model solution
- We have coupled these fast chemistry tools to CFD to enable engine CFD with highly detailed chemical models
- We are applying our chemical tools to mechanism reduction, fitting chemistry model to each application
- We have applied our chemical tools to data generation and machine learning methods to yield further acceleration

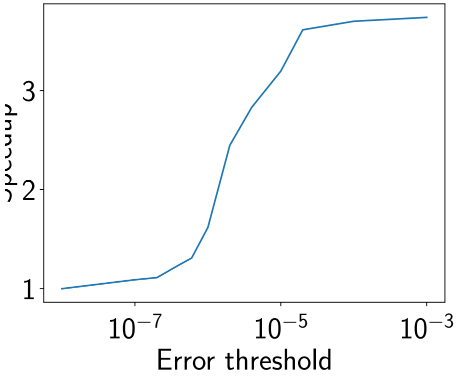






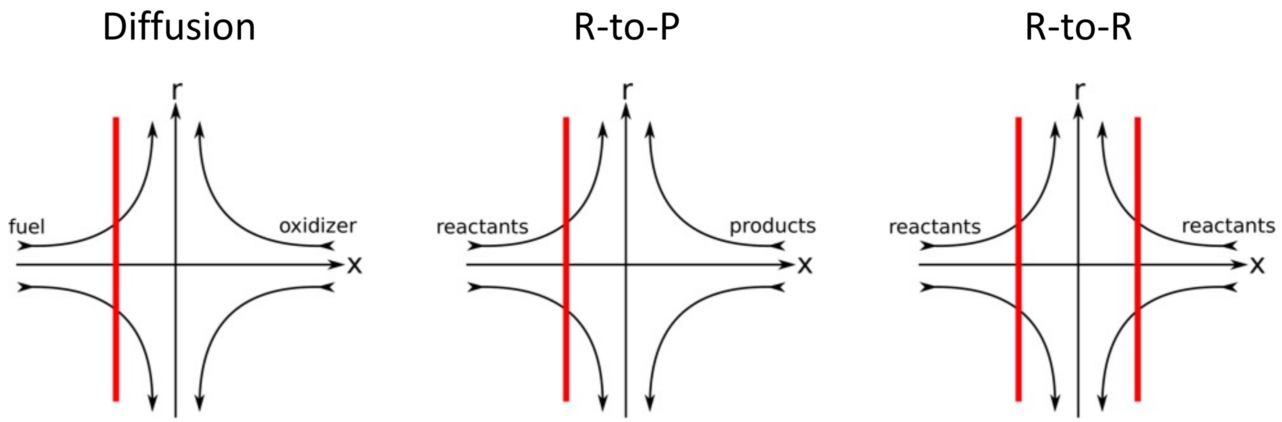


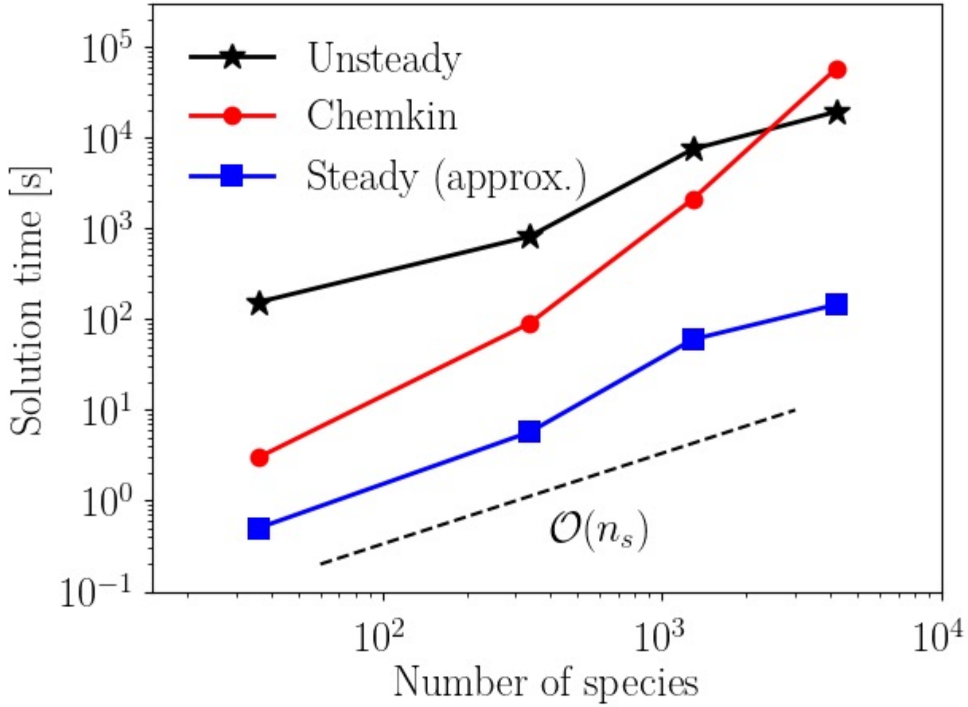




New, Accelerated One-dimensional Solver for Counterflow Flames Developed in Zero-RK

- **Counterflow flame solver allows for direct comparison to experimental measurements**
  - Extension of techniques used previously on laminar premixed and flamelet models
  - Enables direct comparison to more experiments
  - Three flame types:
    - Diffusion flame
    - Single premixed flame (R-to-P)
    - Twin premixed flame (R-to-R)
- **Approximate Jacobian formulation drastically reduces computational cost**
  - CPU time scales linearly with number of species
  - **100x faster** than Chemkin for 3000+ species models
  - Parallelized to exploit high-performance computing

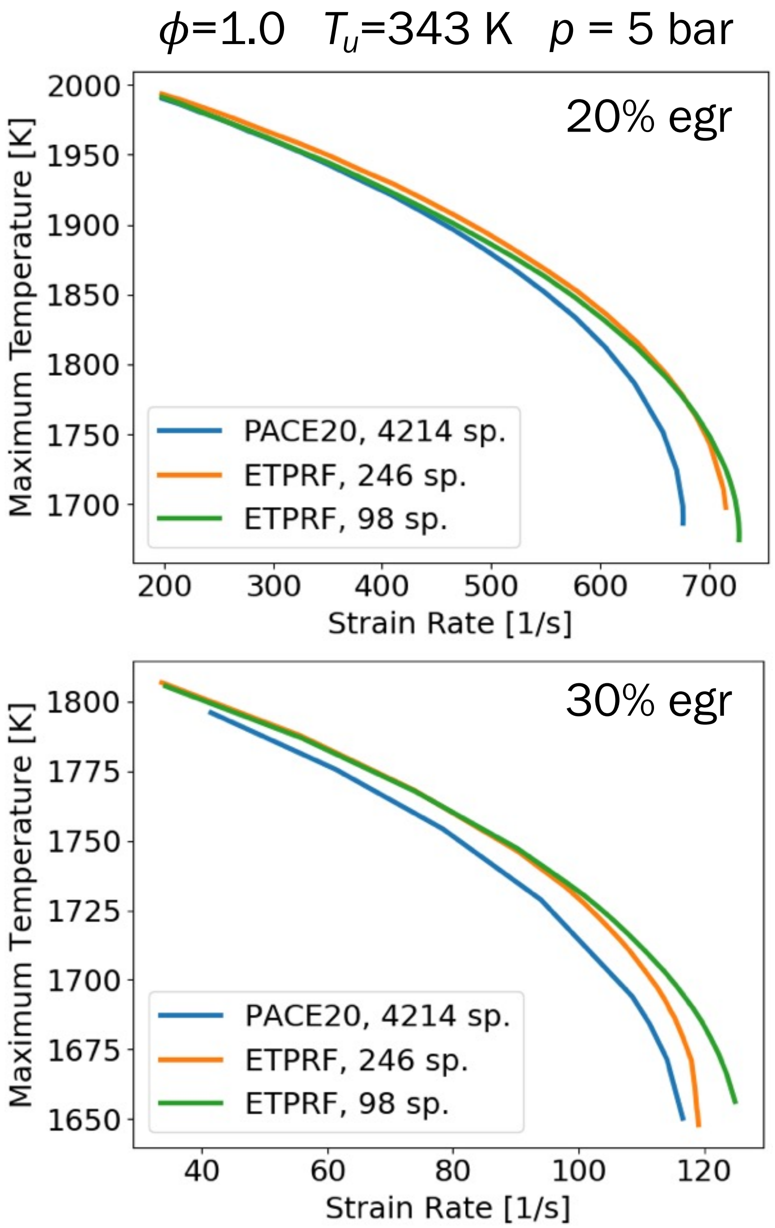




Counterflow Flame Solver Fills Gaps in Our Ability to Evaluate and Improve Chemical Models

- **Strained premixed flames:**
  - Enables previously unattainable computations of extinction strain rates with detailed PACE mechanism (>4000 species)
  - Provides additional data to validate reduced mechanisms for CFD
- **Sooting diffusion flames:**
  - Accelerates evaluation of soot volume fraction with detailed sectional soot model (>1000 species) from ~2h to 5 minutes
  - Opens the door to supervised machine learning in this context through large dataset generation
- **Example PACE Application:**
  - Validation of reduced mechanisms for use in SNL DNS simulations of flame kernel growth (see ace142 - SNL Chen & Soriano)

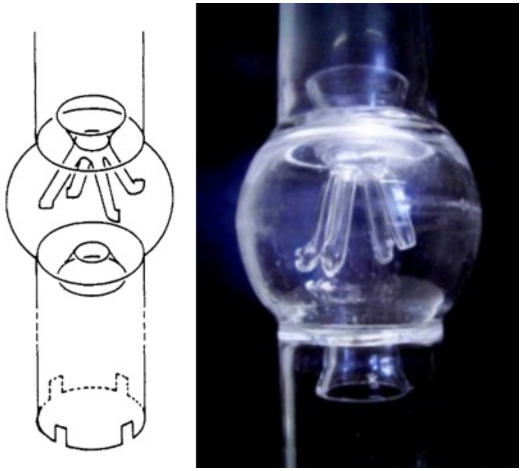
Impact: Confidence in reduced model application to DNS simulations



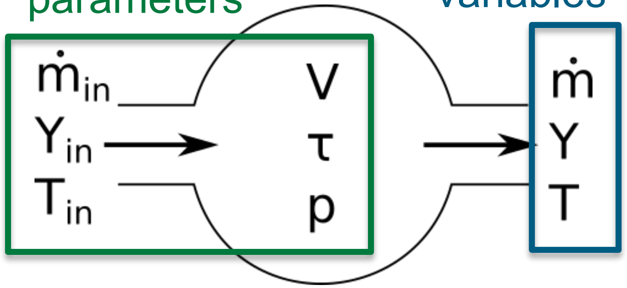
Accelerated Perfectly Stirred Reactor (PSR) Model: New Capability in Mechanism Validation and Tuning

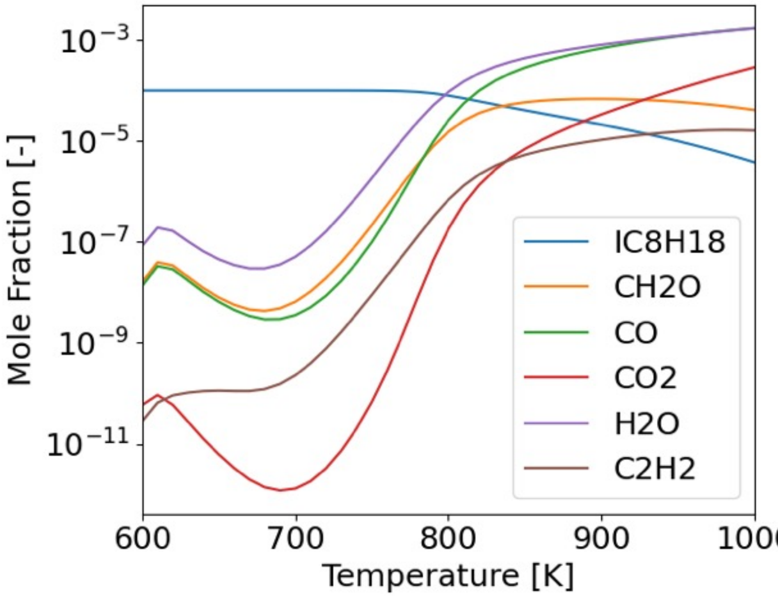
- PSR model closely mimics jet-stirred reactor experiments
- Speciation information can be a **stronger constraint** than ignition delay **on kinetic model performance**
- Model reduction and rate parameter optimization process can benefit from **fast, parallelizable model**
- **>10x faster** than Chemkin and Cantera for large mechanisms

Impact: Rapid validation of chemical mechanisms and improved tools for mechanism reduction and optimization



Cleaner Combustion
Developing Detailed Chemical Kinetic Models
https://doi.org/10.1007/978-1-4471-5307-8





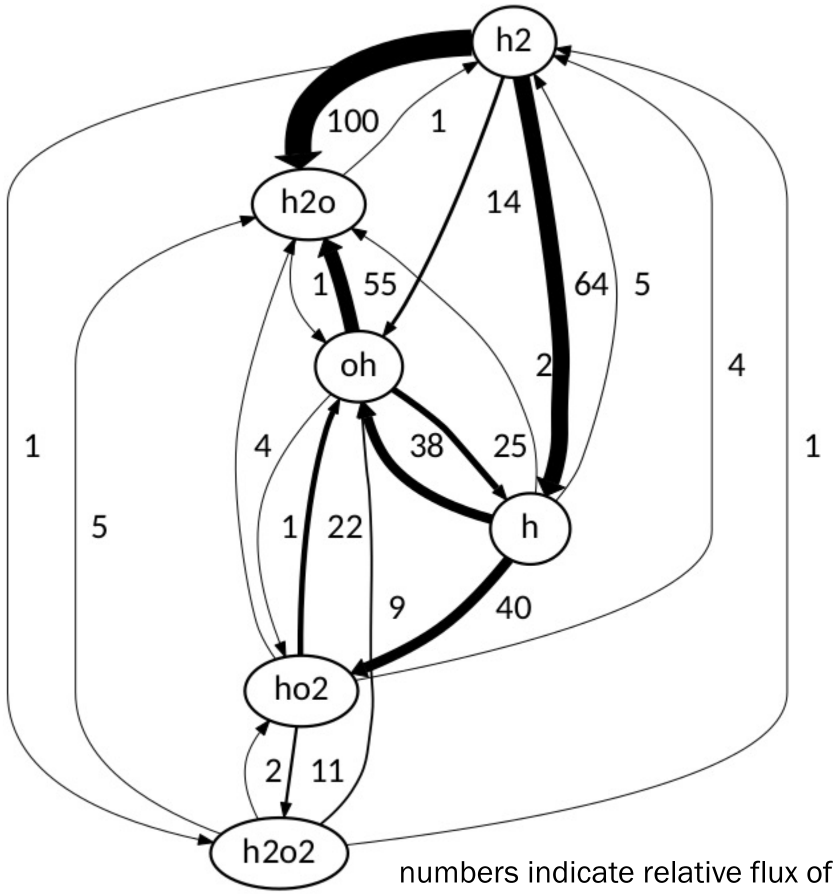
PSR simulations: stoichiometric oxidation of PACE20 surrogate
0.5% mole fraction O_2
N_2 dilution
P=10 atm
Residence time=1 s

Zero-RK Linked to State-of-the-Art Mechanism Reduction Algorithm for More Efficient Combustion CFD

- **Advantages:**
  - More efficient reductions (smaller model size at equivalent error)
  - Better control over sub-models (e.g. NOx, PAH/soot)
- **Challenge:**
  - Inefficient kinetic solution (using dense matrix algebra)
  - Not parallel (doesn't exploit high performance computing)
- **Accomplishment:**
  - Global Pathway Selection (GPS) code adapted for use in VTO run on LLNL computing clusters
  - Calculations at different conditions parallelized:
    16-36x speedup
  - Ignition delay time calculations converted to Zero-RK:
    10-1000x speedup

Impact: We can now perform reduction of full gasoline surrogate mechanism in under 1 hour; previously it would have taken multiple weeks

Global Pathway Selection

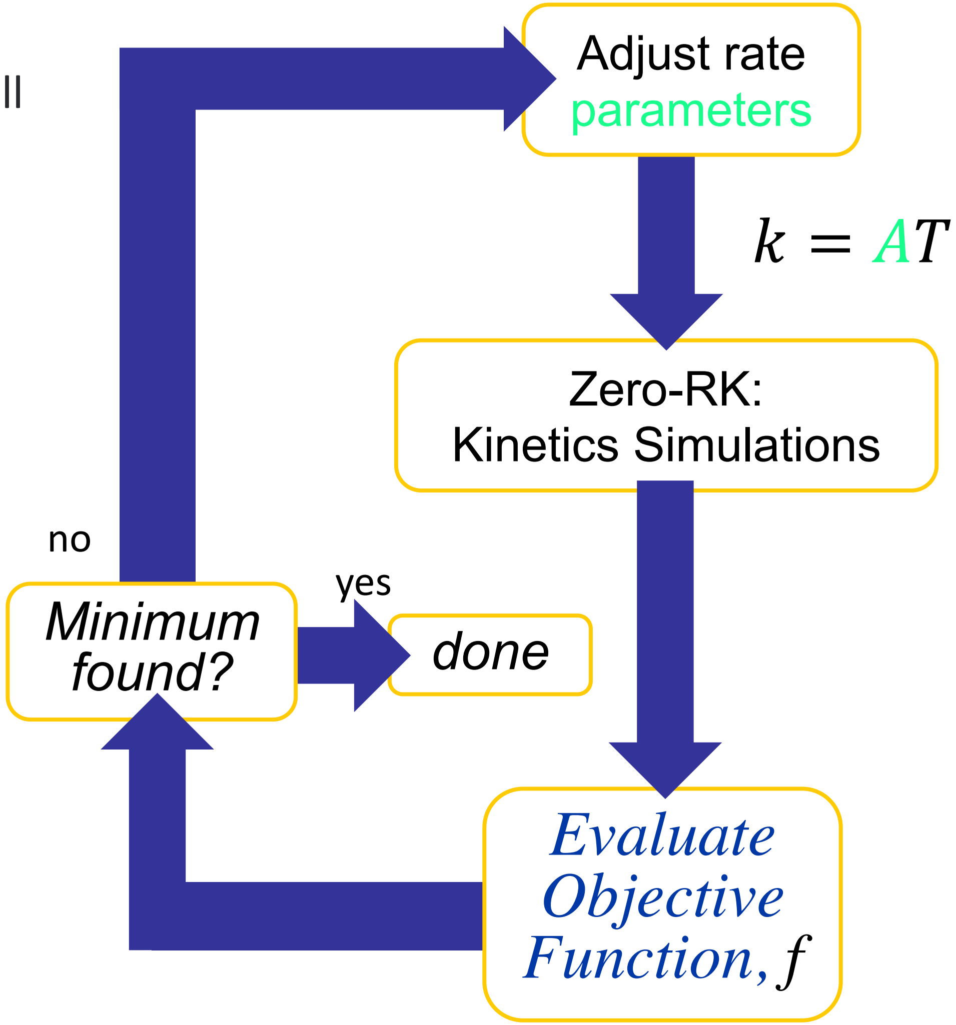


numbers indicate relative flux of H-atom, 100 is maximum relative flux

https://doi.org/10.1016/j.combustflame.2016.02.007
https://doi.org/10.1080/13647830.2018.1560503

New Kinetic Rate Parameter Optimization Framework Created to Achieve Smaller Models with Lower Error

- **Goal:**
  - Smaller reduced mechanisms that still match predictions of full detailed model by adjusting rate parameters
- **Previous practice:**
  - Rates tuned by hand for a limited number of reactions taking days/weeks of expert input
  - Even with such effort, hand-tuned models still less than completely satisfactory in agreement with full model
- **Challenge:**
  - Multi-component fuels (high number of targeted conditions)
  - Large parameter space (curse of dimensionality)
- **Accomplishment:**
  - New framework created linking Zero-RK IDT and PSR simulations with existing optimization routines, including evolutionary and other global algorithms
  - Leverages LLNL models and computing expertise to automate and accelerate process



$$k = AT^n e^{-\frac{E_a}{RT}}$$

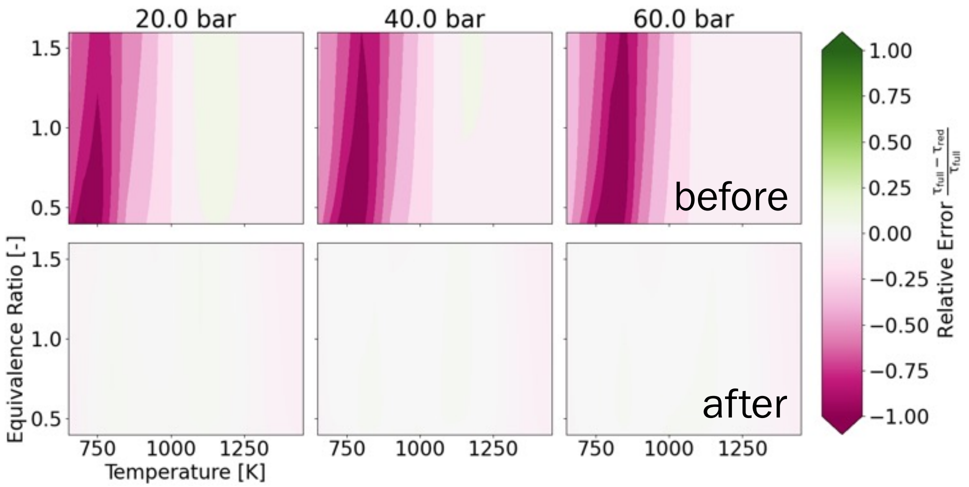
$$f = \sum \left(\log(IDT_{full}) - \log(IDT_{reduced}) \right)^2$$

IDT: Ignition Delay Time

Rate Optimization: Three optimization campaigns provide improved models for transportation fuels

- **PACE-20 (315 species)**
  - 10 component surrogate for RD5-87
  - 70 rate parameters optimized
  - >26,000 models evaluated (>1,800,000 IDT calculations)
  - Max error* before/after optimization: 109/9%
- **Ethanol Toluene Primary Reference Fuel (ETPRF) (246 species)**
  - 4 components (iso-octane, n-heptane, toluene, ethanol)
  - Surrogate with 10% volume of ethanol matching RON/MON of RD5-87 (92.3/84.6)
  - 140 rate parameters optimized
  - >60,000 models evaluated (>20,000,000 IDT calculations)
  - Max error* before/after optimization: 37/16%
- **Diesel surrogate (319 species)**
  - 7 components individually optimized
  - Low and high temperature ignition delays targeted
  - 4 surrogates with varying distillation and cetane properties tested
  - 40-94 rate parameters optimized per component
  - >125,000 models evaluated (>15,000,000 IDT calculations)
  - Max error** before/after optimization: 90/25%

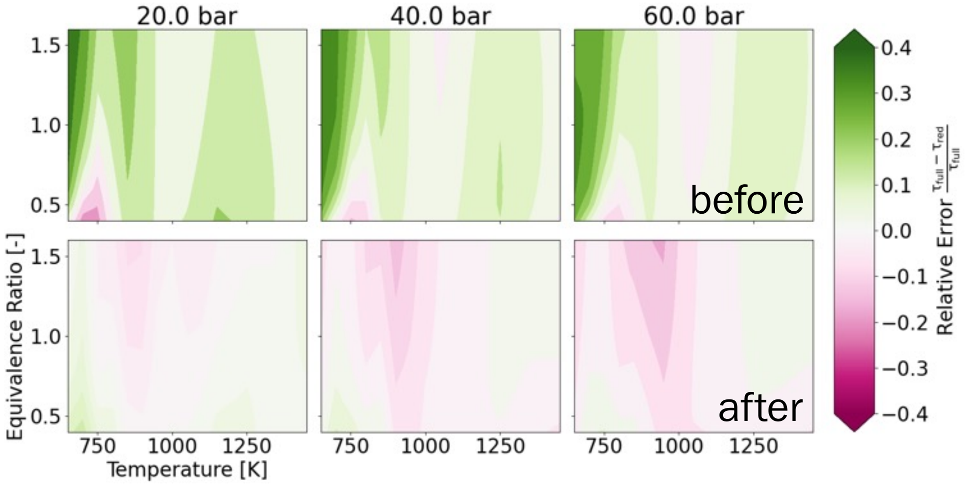
PACE-20 Model Performance Improvement



red is slow
green is fast
white is matching

More details on PACE-20 and ETPRF models shown in ace139

ETPRF Model Performance Improvement



* Relative error in ignition delay for surrogate fuel comparing full 4212 species gasoline mech. to un-/optimized reductions

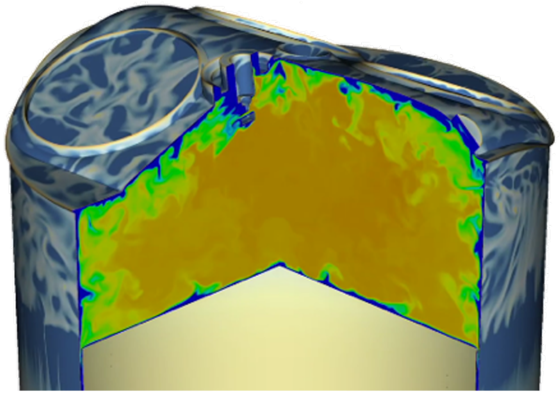
** Relative error in ignition delay for n-hexadecane comparing full 6507 species diesel mech. to un-/optimized reductions

Impact: Significant increase in chemical model fidelity for CFD-relevant mechanisms. Models in use across VTO programs and available to industry users

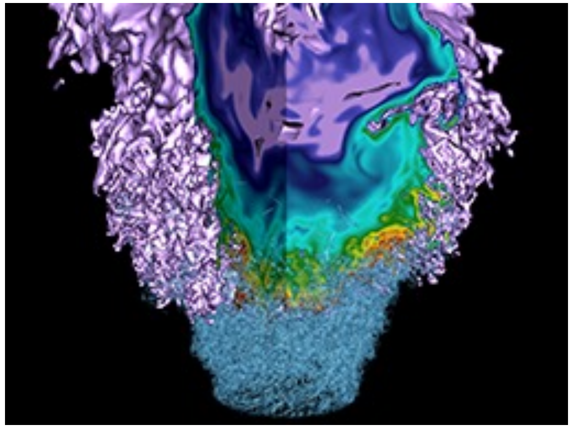
PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

New Prototype Implementations of Zero-RK Linked to Nek5000 and Pele will Enable Exascale Simulations with More Detailed Chemistry

- DOE scalable CFD codes allow the PACE program to investigate turbulence chemistry interactions at highly resolved scales
- Both Pele and Nek5000 include chemistry solvers, however current implementations can be improved for detailed chemistry
- We are implementing interfaces between Zero-RK and both Pele and Nek5000
- Our current prototypes are showing good performance and we are working with PACE partners at ANL and SNL to validate and apply the combined solvers to problems of interest

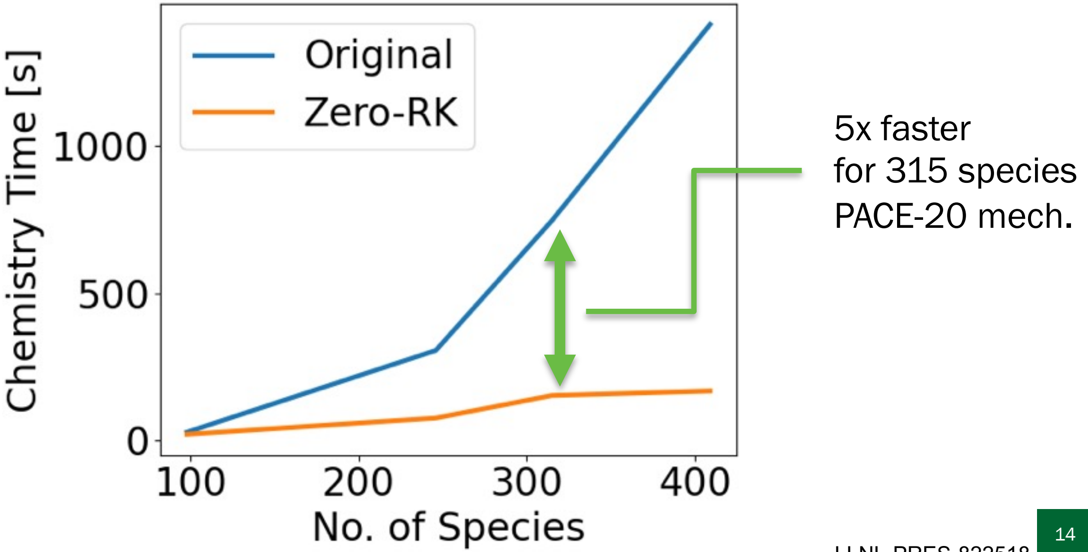


DNS of Motored Engine in NEK5000
Credit: Giannakopoulos (ETH Zurich)
https://nek5000.mcs.anl.gov/category/gallery/



PeleLM simulation of low swirl burner
Credit: Day et al.
https://doi.org/10.1016/j.combustflame.2015.01.013
https://amrex-combustion.github.io/gallery.html

Closed-reactor simulation in Nek5000



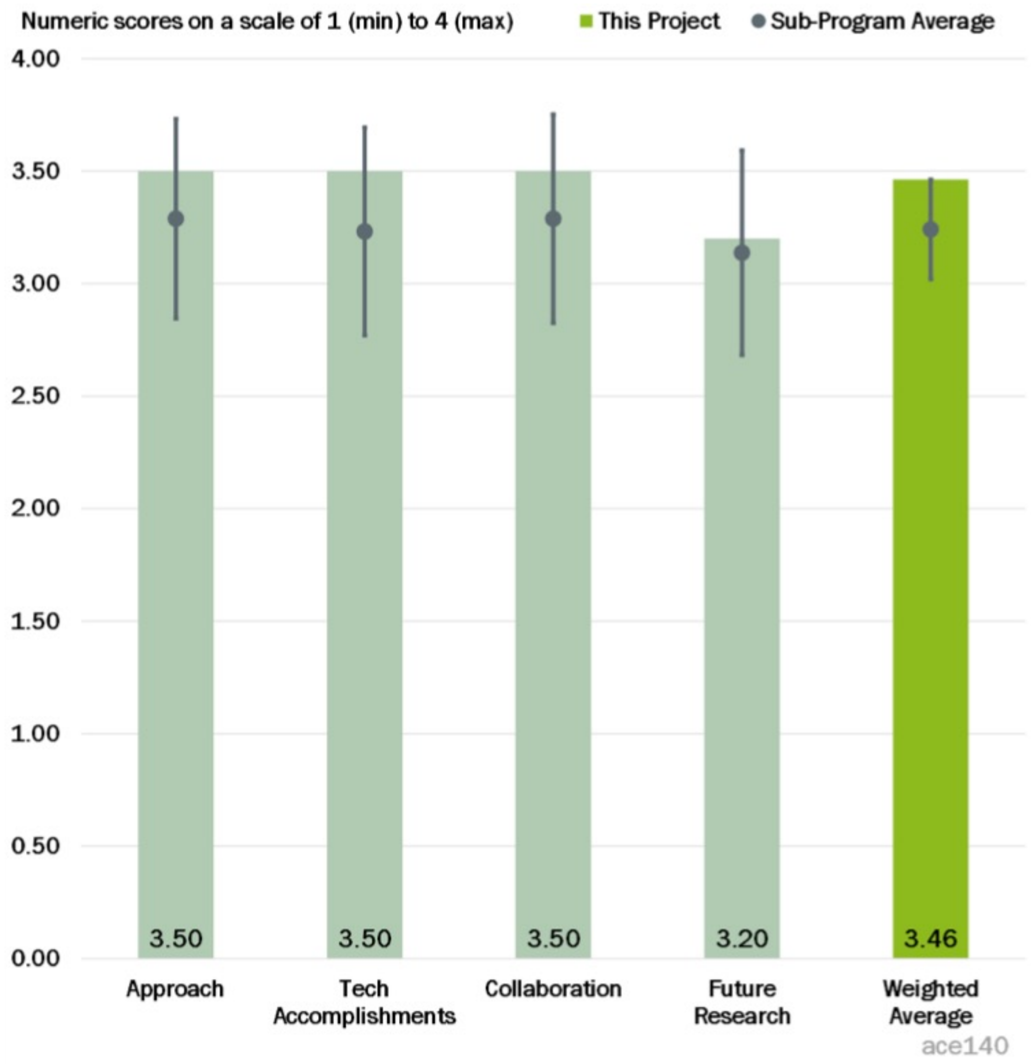
Deploying Zero-RK for use in CFD and Kinetics Research at other PACE Laboratories

- We have helped the other PACE labs install and use Zero-RK for PACE and Co-Optima related kinetics and CFD simulations
- At **Sandia**: Working towards using Zero-RK in Converge and Pele CFD simulations
- At **Argonne**: Zero-RK has been used for flame-speed table generation and rapid compression machine calculations. Future use will include CFD simulations in Converge and Nek5000
- At **Oak Ridge**: Zero-RK coupled to Converge is used on the Summit supercomputer and CADES cluster
- At **NREL**: Zero-RK is being used to compute ignition delay time calculations for phi-sensitivity and Livengood-Wu integrals under the Co-Optima program

FY2020 Reviewer Comments & Our Responses

Mostly positive comments and above average scores

- **A reviewer highlighted issues with reduced model fidelity for ignition delay at low temperature and suggested exploring impact of reduction on flame speeds**
  - Reduction/optimization work done in this year is directly addressing reduced model fidelity at low temperature. Flame speeds have been tested and results shown in ace139.
- **A reviewer suggested that acceleration of non-chemistry areas of simulation should be explored**
  - This remains a task in this project and results will be shown in future reviews.
- **A reviewer requested that automated mechanism reduction tools be made available to other researchers**
  - Past reduction methods were difficult to release due to licensing issues. We are planning to release the new reduction and optimization tools later this fiscal year.



Collaboration

Foundational Nature of Work in this Project Leads to Wide Interaction Across VTO Research Programs

- PACE is a collaborative project of multiple national laboratories combining unique experiments with world-class DOE computing and machine learning expertise to speed discovery, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions.
- The work plan for PACE is developed in coordination with the USDRIVE Advanced Combustion and Emission Control (ACEC) Tech Team
- **Collaboration highlights for this project:**
  - **PACE**:
    - Mechanism Reduction/Optimization
    - Mechanism validation
    - Surrogate formulation
    - CFD with detailed chemistry
  - **Co-Optima**:
    - LBNL (Muller)
    - SNL (Monroe)
    - ANL (Goldsborough)
    - NREL (Martin)
  - **DOE Technology Commercialization Fund Partnerships:**
    - Convergent Science Inc. – Zero-RK GPU accelerated chemistry in CONVERGE CFD
    - Gamma Technologies Inc. – Zero-RK 0- and 1-dimensional solvers for chemical kinetics in GT-SUITE

Remaining Challenges and Barriers

PACE-wide barriers discussed in ACE138

- **Road to exascale**
  - Position PACE to benefit from DOE investment in world-leading computing platforms
- **Industry adoption**
  - Ensure industry users have what they need to succeed in these areas
- **Rate tuning for detailed mechanism**
  - Give kineticists more leverage in evaluating and improving model performance
- **Soot model coupling with core fuel chemistry**
  - Bridge the largest remaining gap in transportation fuel kinetics

Continuing to Deliver on Milestones and Releasing New Zero-RK Capabilities in FY2021

- **Nek5000/Pele Verification and Applications**
  - Work with partner labs to prove Zero-RK is working properly coupled to Nek5000 and Pele
  - Move toward full-scale simulations
- **Transport reduction**
  - Apply data-driven methodology to accelerate multi-species transport in CFD
  - Expect 2x reduction in wall-clock time for solving transport equations
- **Zero-RK 3.0 Release (targeted for August 2021)**
  - Counter-flow flame solver
  - Perfectly-stirred reactor
  - Reaction rate parameter optimization
  - Interface to Global Pathway Selection (GPS) code

*Any proposed future work is subject to change based on funding levels

Proposed Future Research

FY2022 and beyond: Continuing to advance state-of-the art in combustion simulation

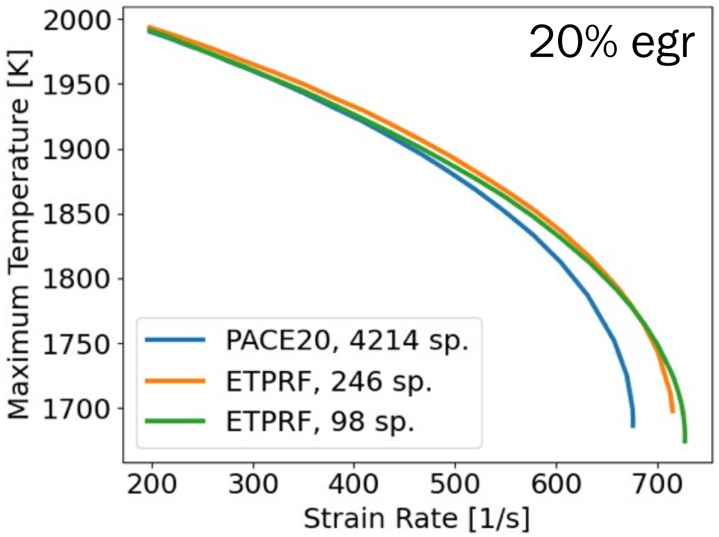
- **Kinetic Rate Parameter Optimization**
  - Refine best practices for detailed models with multiple components
  - Add new model targets (variable volume and flame speeds)
  - Target experimental measurements with uncertainty in targets and parameters
  - Optimize soot and aromatic sub-models
- **Comprehensive Platform for Detailed Kinetics in Scalable Combustion CFD**
  - Hardware acceleration (GPU/CPU)
  - Optimal, on-the-fly solver selection
  - Efficient load-balancing with fast stiffness estimator
  - Transport solver acceleration

*Any proposed future work is subject to change based on funding levels

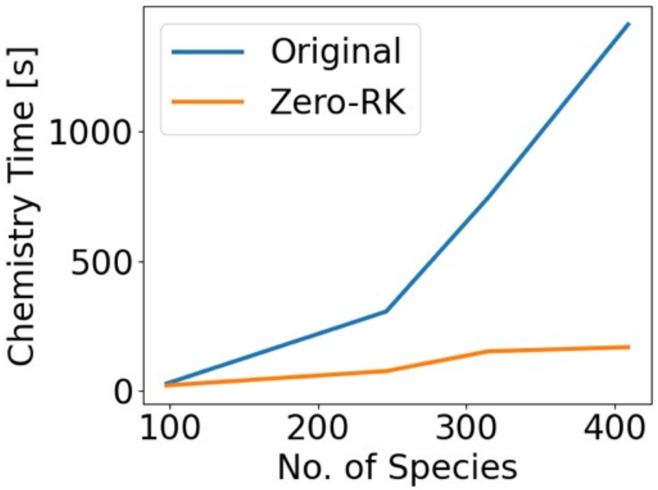
Summary

- **Accelerating chemical kinetics applications for the PACE program**
    - Accelerated counterflow flame and perfectly stirred reactor models
    - New mechanism reduction and optimization tools
    - Supporting PACE CFD efforts at partner labs
    - Integrating fast chemistry solver with DOE exascale capable CFD codes

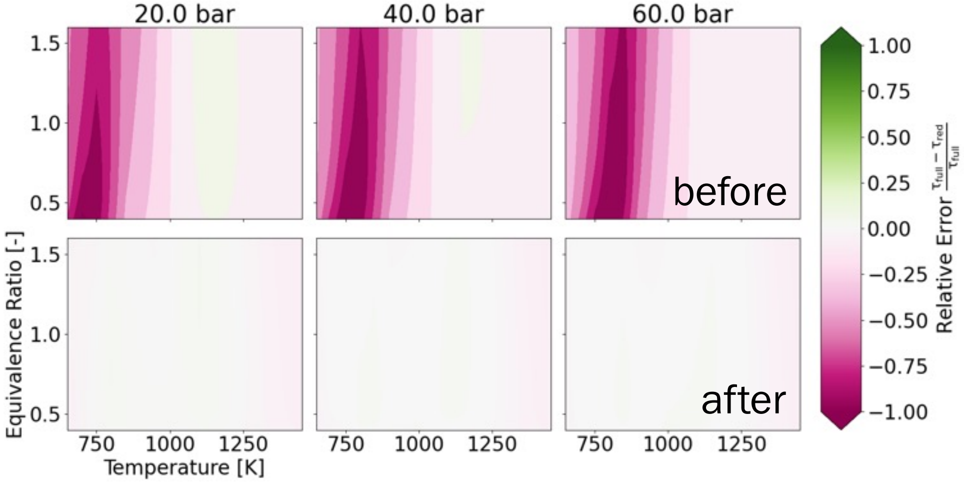
Counterflow flame simulation results for extinction strain rate of gasoline surrogates



Closed-reactor simulation in Nek5000



PACE-20 Model Performance Improvement

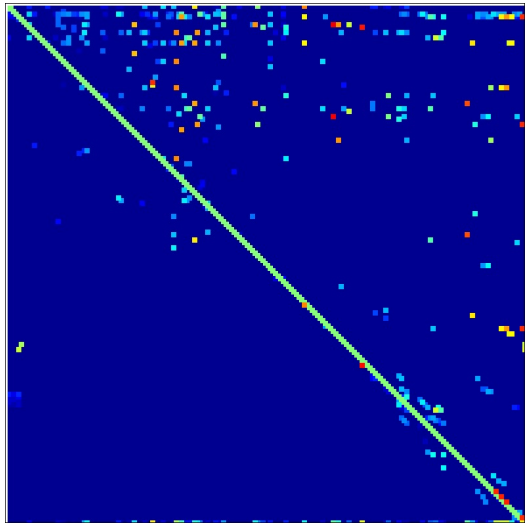


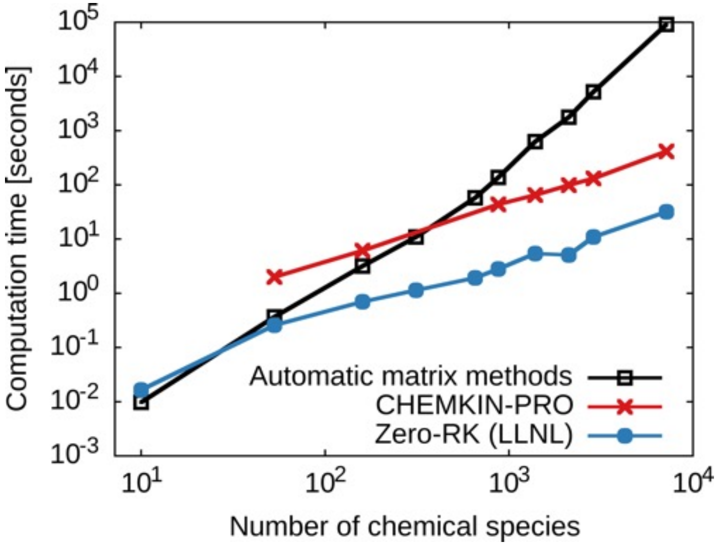
Technical Back-up Slides

Zero-RK: Accelerated Solution for Chemically-Reacting Systems

- Combustion chemistry is stiff,
- Implicit solvers /Jacobians are needed
- We pioneered methods to accelerate solutions of these systems:
  - Fast computation of chemical derivatives
  - Semi-analytic Jacobian formulation
  - Iterative solutions with adaptive preconditioning
- For isolated systems, solutions scale linearly with system size (n_s)

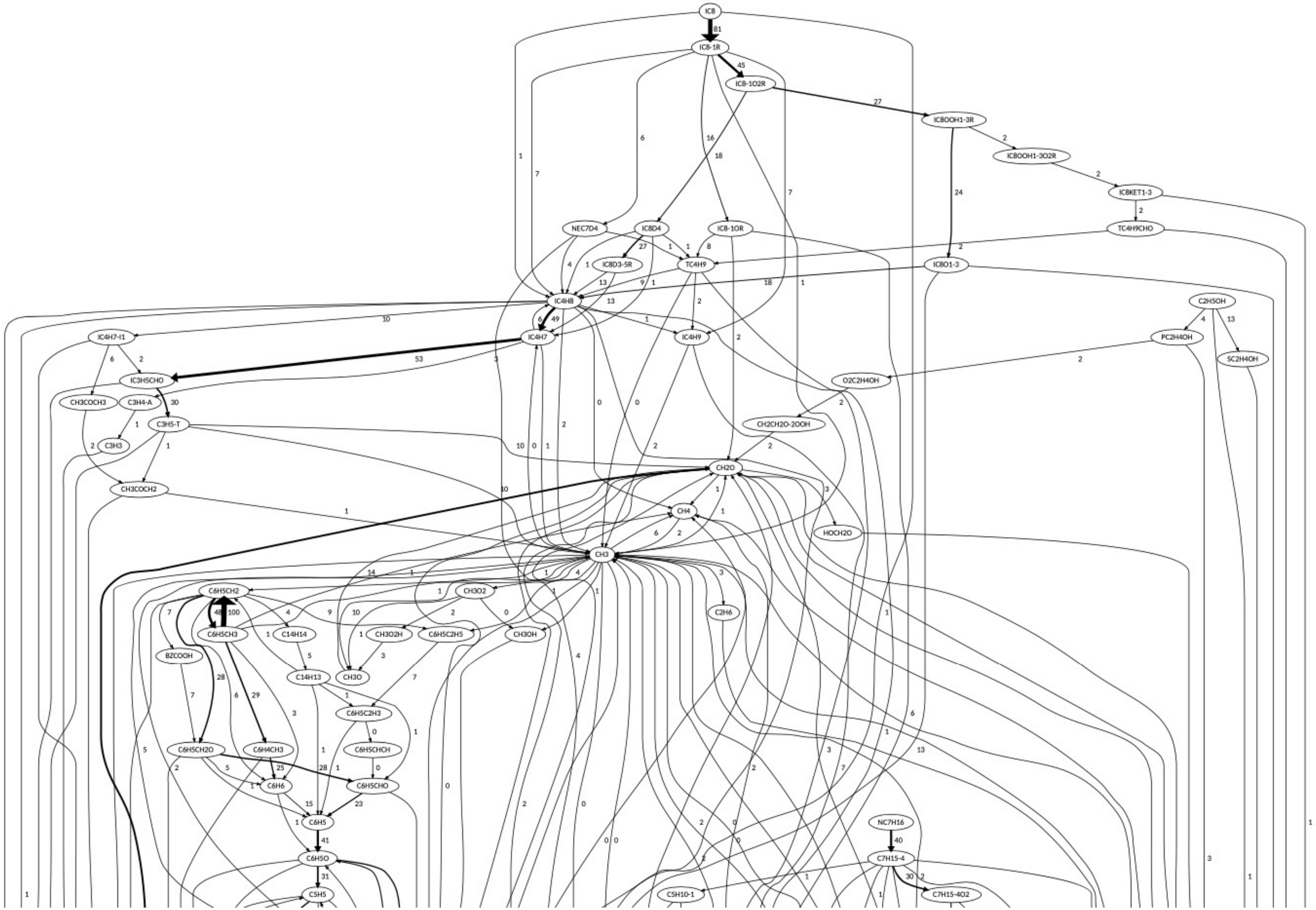
$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & & \frac{\partial f_2}{\partial x_N} \\ \vdots & & \ddots & \vdots \\ \frac{\partial f_N}{\partial x_1} & \frac{\partial f_N}{\partial x_2} & \cdots & \frac{\partial f_N}{\partial x_N} \end{pmatrix}$$





https://doi.org/10.1016/j.proci.2014.05.113

Global Pathway Selection: Flux Graph for C-atoms in ETPRF Mech.



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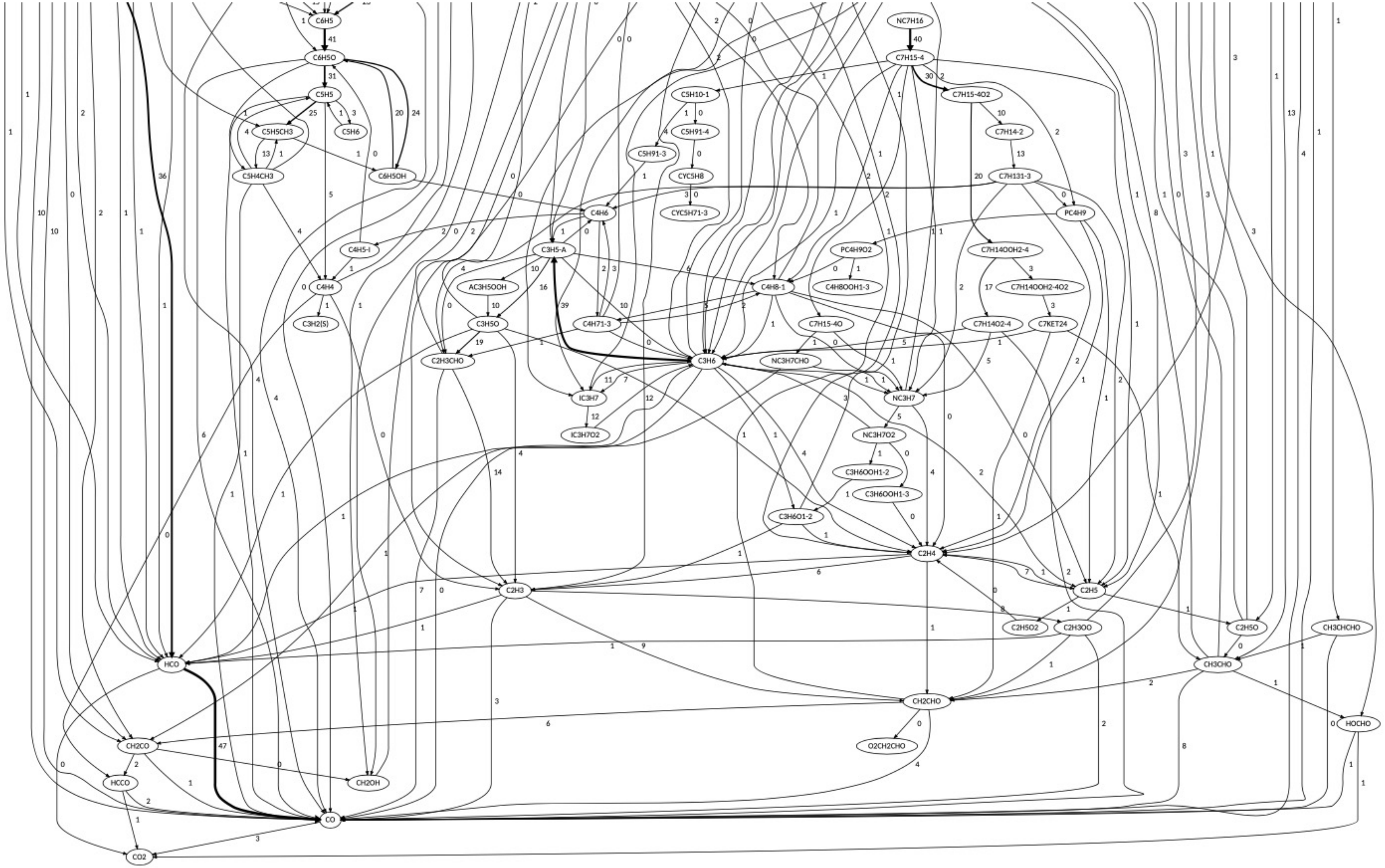
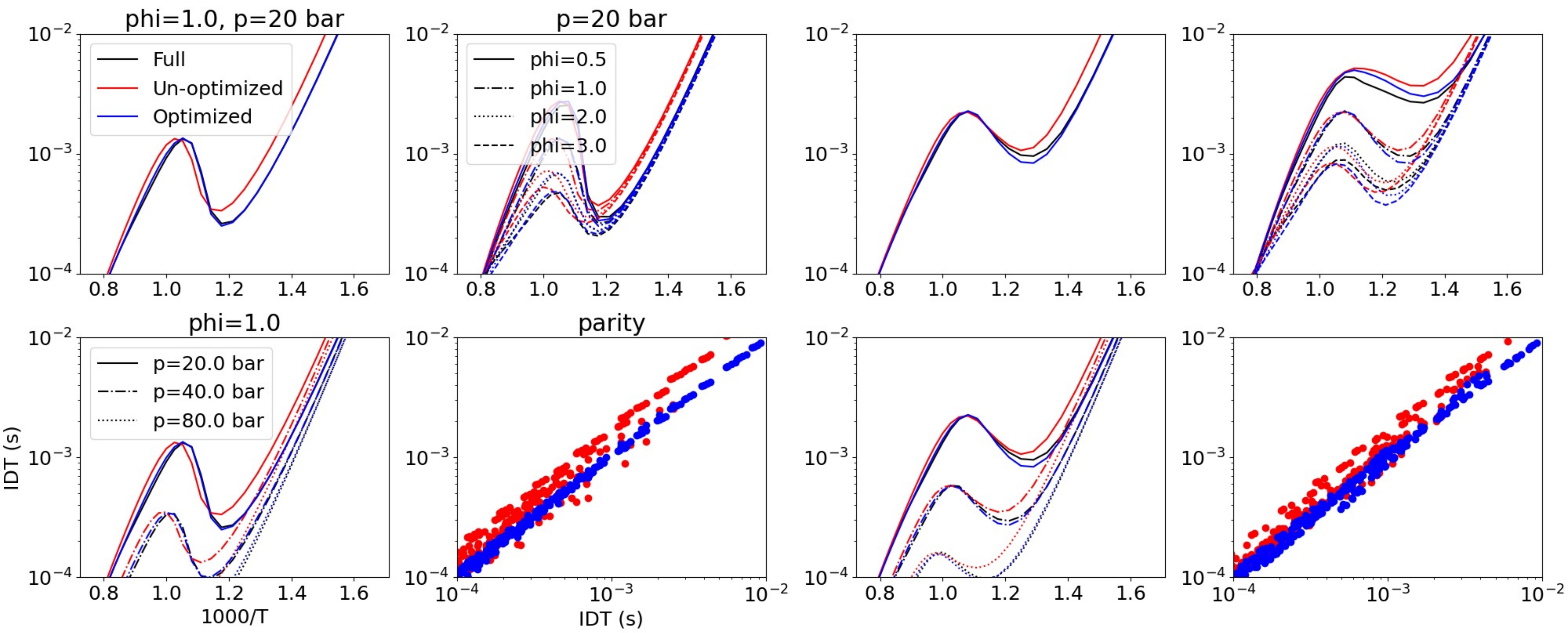


Diesel surrogate reduced mechanism optimization: low and high temperature ignition delays for n-hexadecane



Low temperature ignition (ΔT = 50 K)

High temperature ignition (ΔT = 500 K)

Zero-RK/Nek5000 Coupling: Validation

- Ignition of PACE-20 surrogate with 315 species mechanism in constant volume chamber
  - Equivalence ratio: 1.0
  - Initial temperature: 1600 K
  - Initial pressure: 1 atm

- Zero-RK matches very closely the predicted temperature and pressure (not-shown) history