Parallel On-the-fly Adaptive Kinetics in Direct Numerical Simulation of Turbulent Premixed Flame

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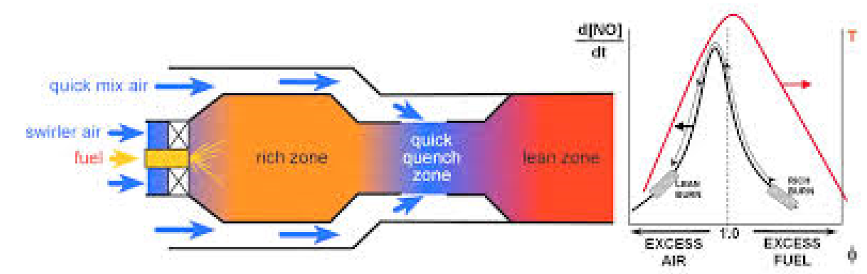
Introduction

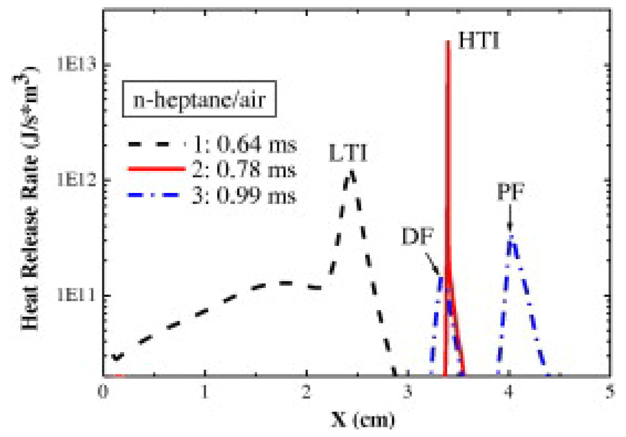
Motivation

Next-generation gas turbines favor lean combustion for high efficiency and low emissions, which suffers from combustion instability, lean blowout (LBO), & related NOx formation [1].



Why Detailed Kinetics?

Detailed kinetics is the key to capture extreme combustion physics like LBO, negative temperature coefficient (NTC)-affected low temperature ignition (LTI) [2] in gas turbines.



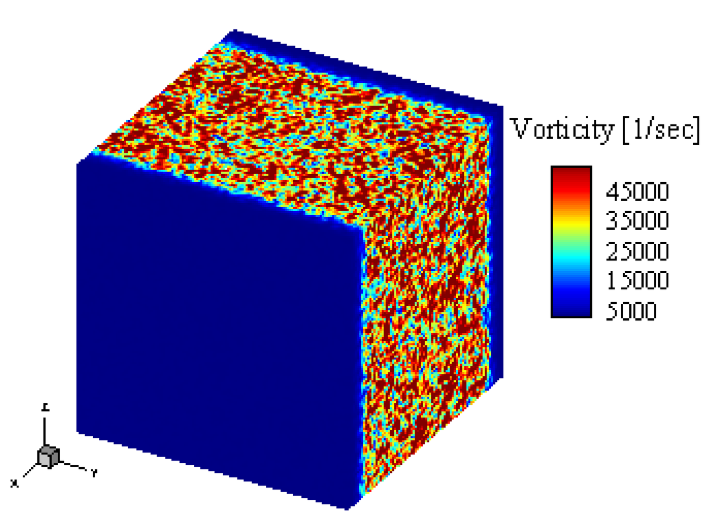
Issues

- Detailed combustion kinetics (e.g. jet fuels of large molecules) have large number of species & high stiffness.
- Globally reduced kinetics mechanisms are still too large for DNS/LES.
- Simple on-line reduction has a very large CPU overhead.
- CPU time of chemistry is the most expensive part.
- CPU time of mixture-averaged transport is the 2nd most expensive part.

Methods

Direct Numerical Simulation (DNS)

AVF-LESLIE code of CCL, Georgia Tech



Flow configuration

Premixed flame interaction with decaying isotropic turbulence

Kinetics

Globally reduced jet fuel mechanism with 38 species & 185 elementary reactions

Point Implicit ODE solver (ODEPIM)

Fast semi-implicit stiff ODE solver [3]

On-the-fly adaptive kinetics (OAK)

Use path flux analysis (PFA) method [4] as kernel engine for on-the-fly mechanism reduction. Time and space correlation [5] is applied to reduce the CPU overhead for reduction

Correlated transport (Co Tran) is applied

Compute mixture-averaged transport only once for each time and space correlated group [6]

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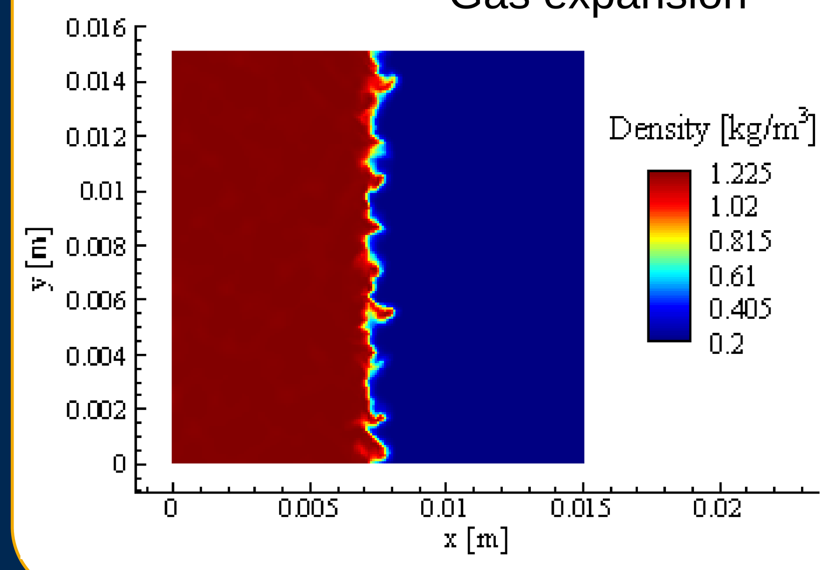
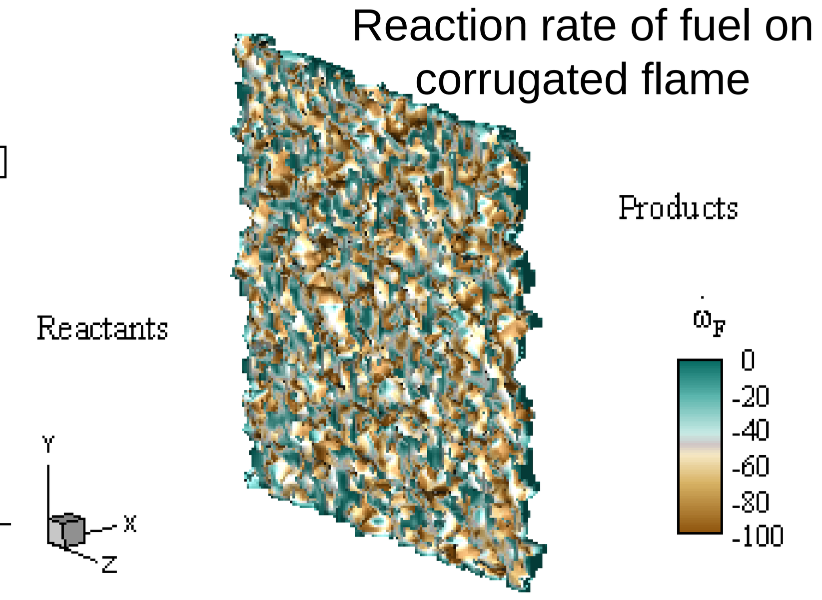
Results

Gas expansion

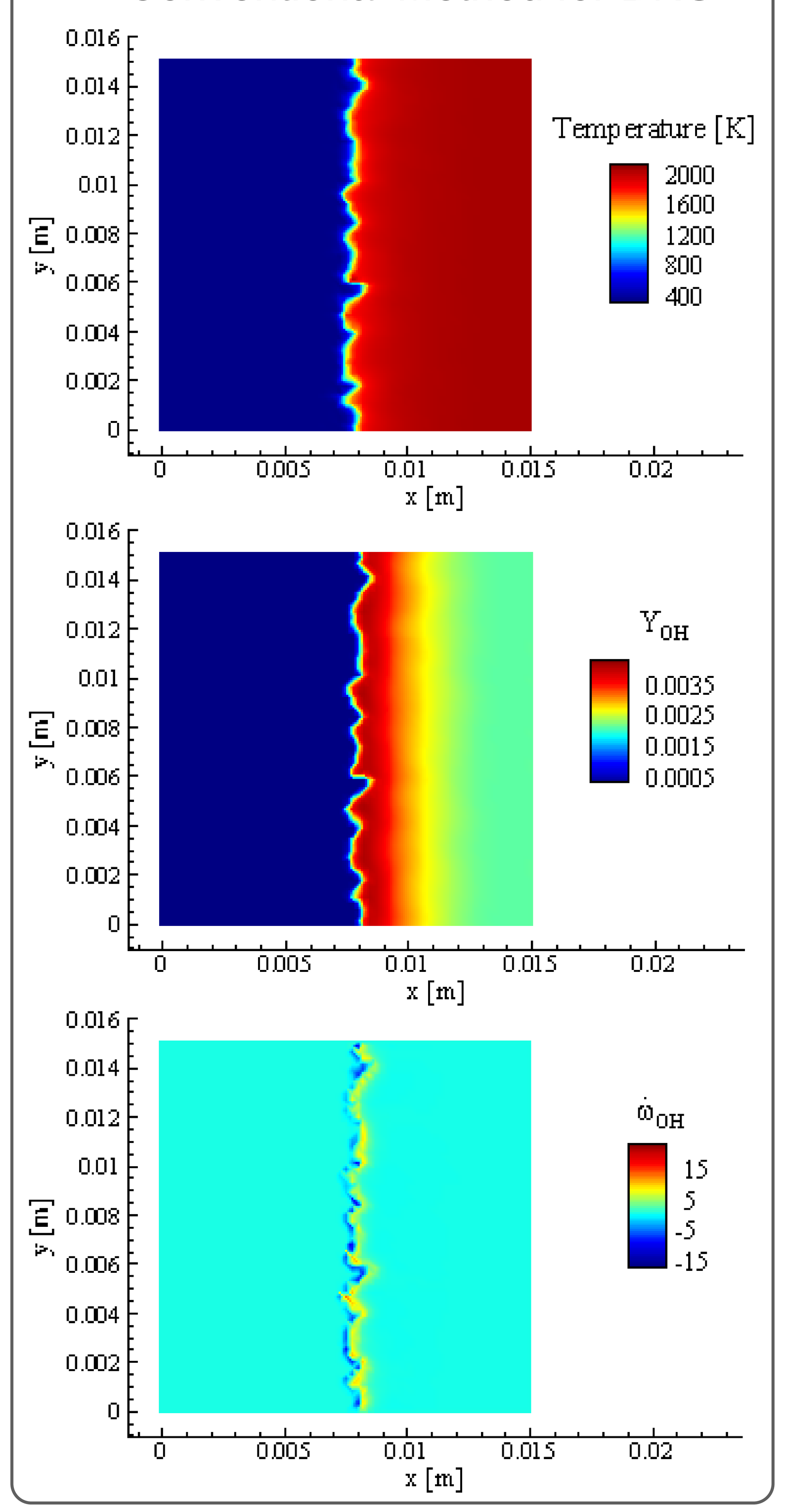


Reaction rate of fuel on corrugated flame

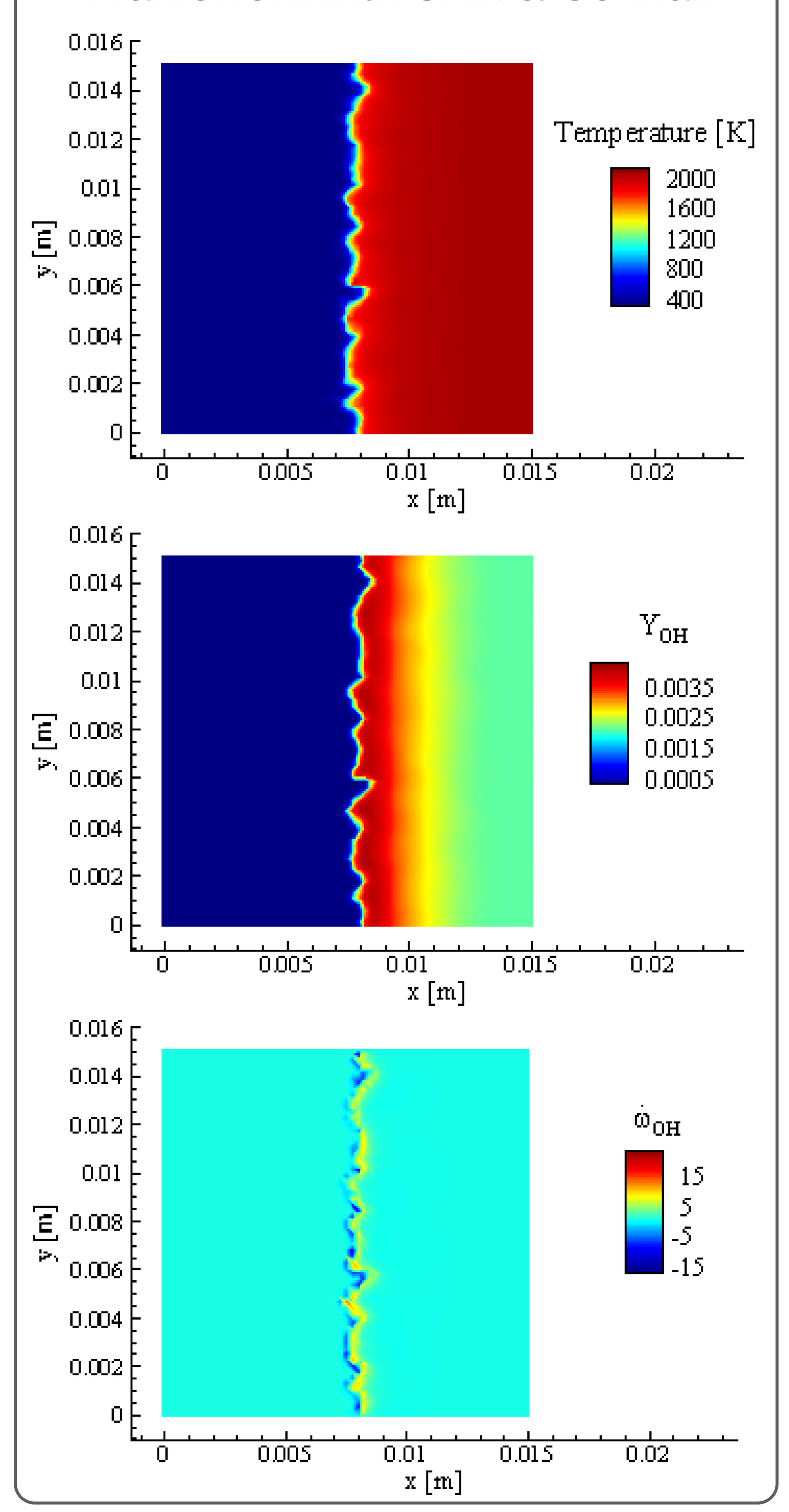


Verification

Conventional Method for DNS



Framework with OAK & Co Tran



Quantified Errors (after 1.5 eddy turn-over time)

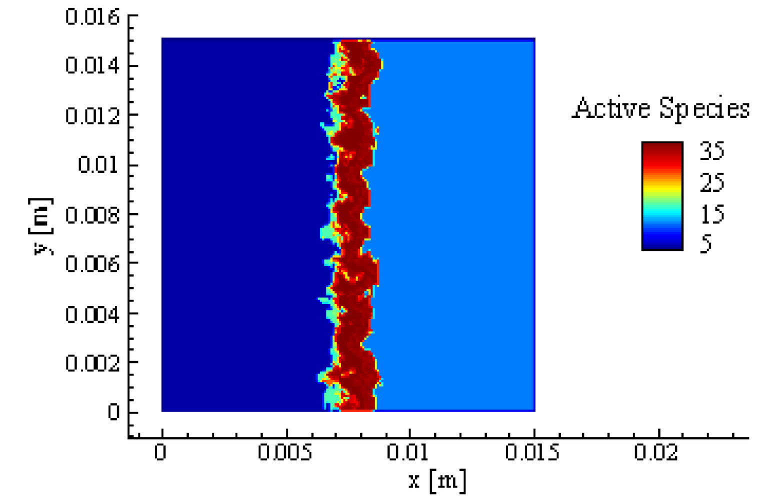
Average L_2 error	Tgas (K)	Y_{fuel}	Y_{OH}	$\dot{\omega}_{fuel}$	$\dot{\omega}_{OH}$
ODEPIM	1.19E-4	5.91E-09	9.50E-10	1.3E-4	1.01E-05
ODEPIM+OAK	1.27E-4	6.46E-09	1.09E-09	1.36E-4	2.77E-05
ODEPIM+OAK+CoTran	3.52E-4	1.02E-08	1.59E-09	1.62E-4	2.85E-05

References
[1] M. Khosravy el_Hossaini (**2013**). Review of the New Combustion Technologies in Modern Gas Turbines, *Progress in Gas Turbine Performance*, Dr. Ernesto Benini (Ed.), ISBN: 978-953-51-1166-5, InTech, DOI: 10.5772/54403. Available from: http://www.intechopen.com/books/progress-in-gas-turbine-performance/review-of-the-new-combustion-technologies-in-modern-gas-turbines
[2] Sun, W., Won, S. H., Gou, X., and Ju, Y., "Multi-scale modeling of dynamics and ignition to flame transitions of high pressure stratified n-heptane/toluene mixtures," *Proceedings of the Combustion Institute* Vol. *35*, No. 1, **2015**, pp. 1049-1056.
[3] Katta, V.R., Roquemore, W.M., **2008**, Calculation of multidimensional flames using large chemical kinetics, *AIAA Journal*, *46*, 1640-1650.

Performance Analysis

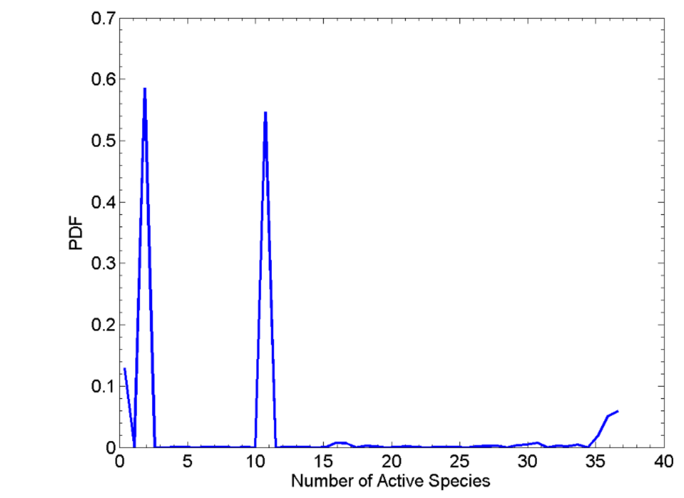
Number of Active Species

- Large number of active species only exist near the flame.
- No-flame regions only have 2 (cold reactants) or 10 (hot products) active species.
- Buffer layers b/w flame and no-flame regions have intermediate number of active species.



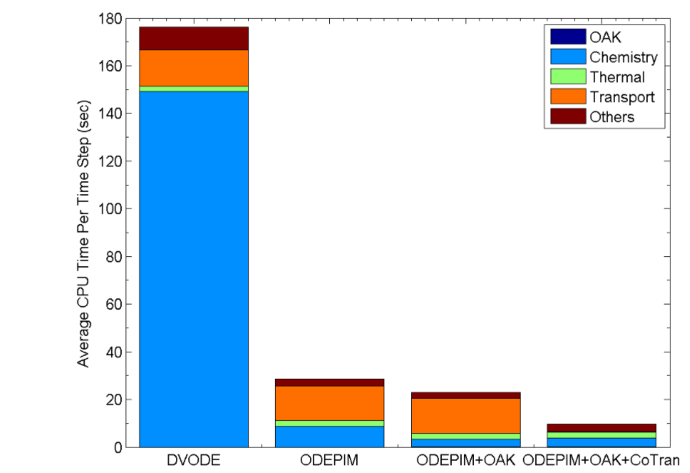
Speed-Up

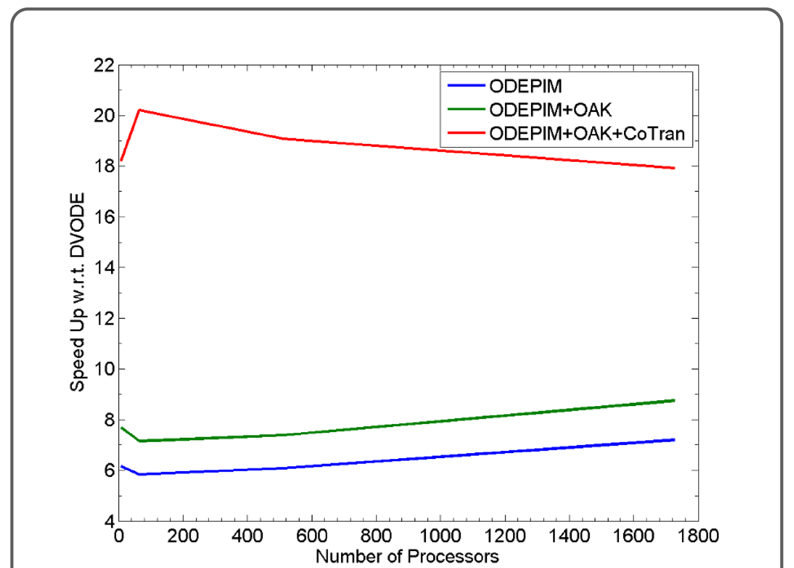
- ODEPIM: ~6 times in total, ~17 times in chemistry.
- OAK: ~8 times in total, further ~2.7 times in chemistry w/ negligible overhead.
- Co Tran: ~20 times in total, transport time become negligible w/ no overhead.



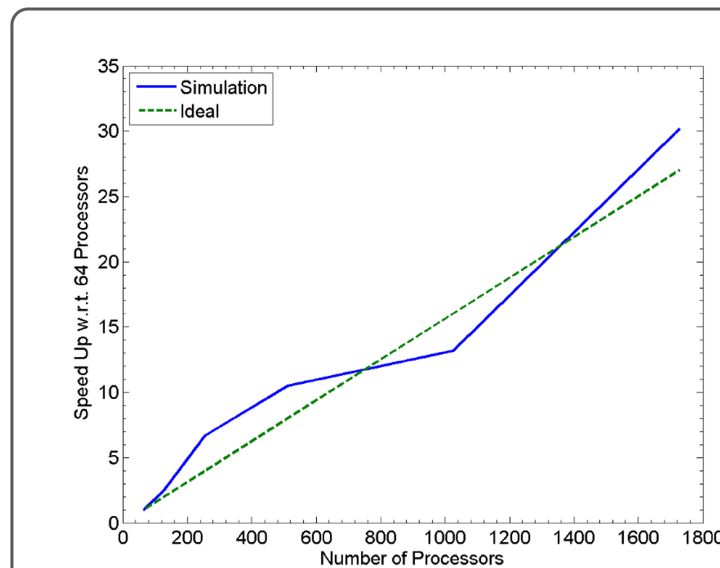
Parallel Scaling

- ODEPIM, OAK, Co Tran all show a good weak scaling of speed-up.
- Good strong scaling: no new communication overhead introduced by ODEPIM, OAK, Co Tran.





Weak scaling of speed-up



Strong scaling

Conclusions

1. New framework with OAK & Co Tran provides highly accurate results.
2. New framework with OAK & Co Tran has speed-up ~20 times in total, and ~46 times in chemistry, which enables DNS w/ detailed kinetics.
3. New framework shows good parallel weak & strong scaling.

[4] Sun, W., Chen, Z., Gou, X., and Ju, Y., "A path flux analysis method for the reduction of detailed chemical kinetic mechanisms," *Combustion and Flame* Vol. *157*, No. 7, **2010**, pp. 1298-1307.
[5] Sun, W., Gou, X., El-Asrag, H. A., Chen, Z., and Ju, Y., "Multi-timescale and correlated dynamic adaptive chemistry modeling of ignition and flame propagation using a real jet fuel surrogate model," *Combustion and Flame* Vol. *162*, No. 4, **2015**, pp. 1530-1539.
[6] Sun, W., and Ju, Y., "Multi-timescale and Correlated Dynamic Adaptive Chemistry and Transport Modeling of Flames in n-Heptane/Air Mixtures," *53rd AIAA Aerospace Sciences Meeting*. Kissimmee, Florida, **2015**, pp. AIAA 2015-1382.