Reduction Methodology for Detailed Kinetic Mechanisms: Application to *n*-Hexane-Air Hot Surface Ignition

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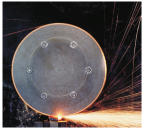
Thermal Ignition Hazards

Motivation: understand thermal ignition hazards present in the aviation, nuclear, mining, and manufacturing sectors.

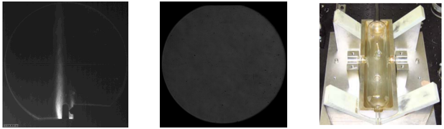


Frictional sparks and hot spots[1]

China Air flight 120, 2007

TWA flight 800, 1996

Previous work: extensive work has been performed at Caltech in the context of aviation safety using ***n*-hexane** as a surrogate for kerosene.



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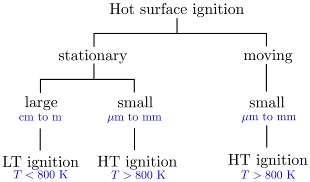
[1] S. Hawksworth et al. Symposium Series No. 150, 2004

Numerical Predictions

Problem: experimental testing is time consuming

- Large number of hot surface geometries and mixture conditions



Hot surface ignition

- stationary
  - large
    cm to m
    - LT ignition
      $T < 800$ K
  - small
    μm to mm
    - HT ignition
      $T > 800$ K
- moving
  - small
    μm to mm
    - HT ignition
      $T > 800$ K

Solution: perform multi-dimensional transient numerical simulations.

- Predictive simulations require the use of detailed chemical mechanisms to predict the ignition and flame propagation events
  - → *n*-Hexane: 531 species and 2628 reactions
  - → Not feasible for modeling real engineering tests or applications

How can computational time be reduced? Mechanism reduction!

Kinetic Mechanism Reduction

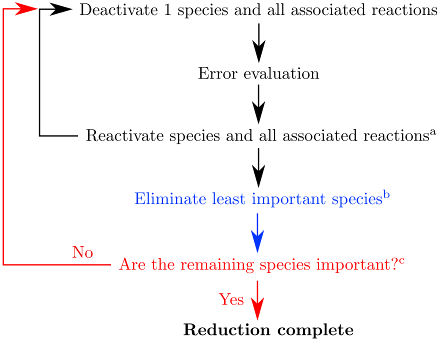
Use modified version of reduction mechanism employed by Davidenko et al.[2] using one target phenomenon: **auto-ignition process**

Evaluated parameters (q): time to peak thermicity, maximum thermicity, equilibrium temperature, equilibrium mean molar mass, and temporal profiles of, thermicity, temperature, and mean molar mass.

a. $s_q = \epsilon_q / \epsilon_q^*$ where $\epsilon_q = |q - q^{\mathrm{ref}}|/q^{\mathrm{ref}}$ q: reduced mechanism, q^{ref}: complete mechanism, ϵ_q^*: error limit; calculate $S = \sum s_q$ across all conditions.

b. $\cancel{S^1} < S^2 < ... < S^k$ where k is species deactivated

c. $S = S^*$ where S^*: error limit



Deactivate 1 species and all associated reactions

Error evaluation

Reactivate species and all associated reactions[a]

Eliminate least important species[b]

No

Are the remaining species important?[c]

Yes

Reduction complete

Final mechanism: 62 species and 223 reactions

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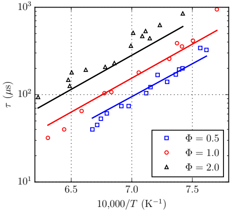
[2] D. Davidenko, R. Mével, and G. Dupré, in Proceedings of the European Combustion Meeting, 2009.

Mechanism Validation (1/3)

Ignition delay time (constant volume adiabatic reactor)



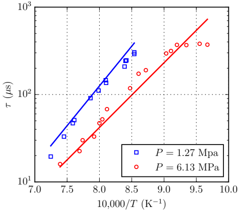
Mével et al.[3]: P = 350 kPa; Y_{Ar} = 0.96 n-hexane-O_2-Ar

RMSE

□ 29 μs

○ 131 μs

△ 132 μs



Data from Zhukov et al.[4] for n-hexane-air at $\Phi = 0.5$

RMSE

□ 47 μs

○ 107 μs

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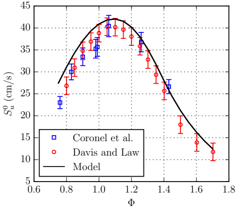
[3] R. Mével, U. Niedzielska, J. Melguizo-Gavilanes, S. Coronel, and J. E. Shepherd, Combustion Science and Technology, 188:2267-2283, 2016.

[4] V. P. Zhukov, V. A. Sechenov, and A. Y. Starikovskii, Combustion and Flame, 136:257-259, 2004.

Mechanism Validation (2/3)

Laminar burning speed (1-D freely propagating flame)



Coronel et al.[5] and, Davis and Law[6]: $P = 100$ kPa, $T = 300$ K
n-hexane-air

RMSE

□ 3.6 cm/s

○ 2.5 cm/s

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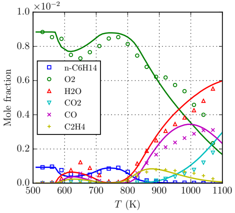
[5] S. Coronel, S. Lapointe, R. Mével and J. E. Shepherd, in preparation for Fuel.

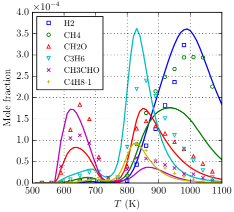
[6] S. G. Davis and C. Law C, Combustion Science and Technology, 140:427-449, 1998.

Mechanism Validation (3/3)

Jet-stirred reactor[7] (perfectly-stirred reactor–PSR)



Major species



Minor species

Normalized root-mean-square error

Species	NRMSE	Species	NRMSE
n-C_6H_{14}	0.35	H_2	0.5
O_2	0.15	CH_4	1.4
H_2O	0.48	CH_2O	0.4
CO_2	0.7	C_3H_6	1.2
CO	1.2	CH_3CHO	0.6
C_2H_4	10.6	C_4H_8-1	0.4

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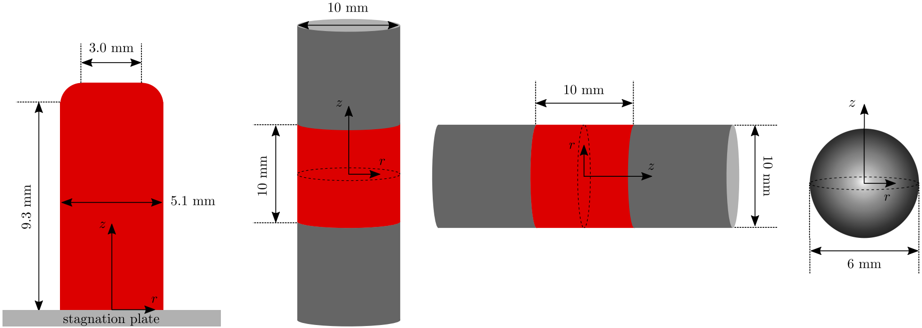
[7] K. Zhang, C. Banyon, C. Togbé, P. Dagaut, J. Bugler, and H. J. Curran, Combustion and Flame, 162:4194-4207, 2015.

Multi-Dimensional Numerical Calculations

Hot surface geometries



Commercial glow plug **stationary**

Vertical cylinder **stationary**

Horizontal cylinder **stationary**

Sphere **moving**

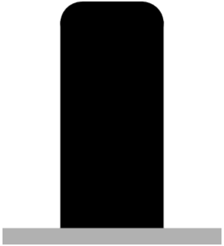
Mesh Geometry Setup

Mesh geometry

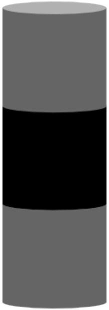
	Glow plug	Vertical cylinder	Horizontal cylinder	Sphere
Config.	2D axisymmetric about z	2D axisymmetric about z	2D planar normal to z	2D axisymmetric about z
Cells	180,000	80,000	60,000	300,000
Cell size (μm)	80	40	40	60

Numerical Solution

- → Variable-density, reactive Navier-Stokes
- → Temperature dependent transport and thermodynamic properties
- → Differential diffusion included using constant non-unity Lewis numbers
- → n-Hexane-air: $\Phi = 0.9$, $T_0 = 300$ K, and $P_0 = 100$ kPa



Temperature ramp: 220 K/s



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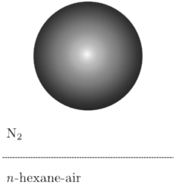
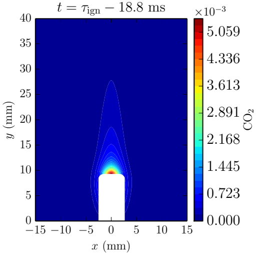


Temperature ramp and then drop

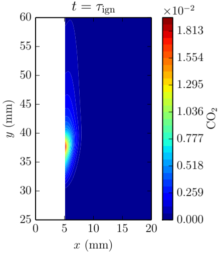
CO_2 Mass Fraction

Glow plug



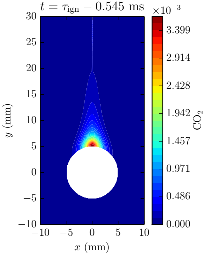
Ignition occurs above glow plug in stagnation region

Vertical cylinder



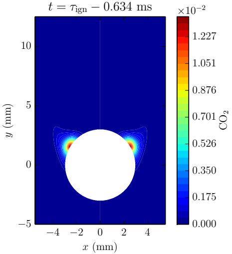
Ignition occurs along the top limit of the hot surface

Horizontal cylinder



Ignition occurs in the rear stagnation point

Moving sphere



Ignition occurs in region of flow separation

Ignition Predictions

Minimum surface temperature required for ignition

Geometry	Exp. (K)	Calc. (K)	$\Delta T/T_{\mathrm{exp}}$	% Diff.
Hor. Cyl[8]	1180	1093	0.07	7%
Vert. Cyl.[8]	1270	1191	0.06	6%
Sphere[9]	1224	1300	0.06	6%
Glow Plug[10]	1275	1162	0.09	9%

Experimental and numerical results for all geometries tested

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[8] L. Boeck, M. Meijers, A. Kink, R. Mével, and J. E. Shepherd, Combustion and Flame, 185:265-277, 2017.

[9] S. A. Coronel, J. Melguizo-Gavilanes, R. Mével, and J. E. Shepherd, submitted to Combustion and Flame.

[10] J. Melguizo-Gavilanes, A. Nové-Josserand, S. A. Coronel, R. Mével, and J. E. Shepherd, Combustion Science and Technology, 188:2060-2076, 2016

Conclusions

- The reduced mechanism performs well when applied to 1D freely propagating flames
- Ignition predictions within 10% of measured experimental thresholds
  - → Natural and forced convection
  - → Flows with stagnation and separation points
  - → Do not account for surface chemistry
- Largest temperature difference observed for commercial glow plug (9%)
  - → Surface temperature inhomogeneities observed experimentally
  - → Experimental measurement is made at the top edge of glow plug and not at ignition location
- Significant decrease in computational time
  - → Maybe Josue can put a rough estimate of the savings in computational time?
- Rigorous validation of reduced mechanism and solver indicates that simulations of real-engineering geometries and flow configurations can be performed