جامعة الملك عبدالله
للعلوم والتقنية
King Abdullah University of Science and Technology

CCRC Winter School 2020

Introduction to Cantera

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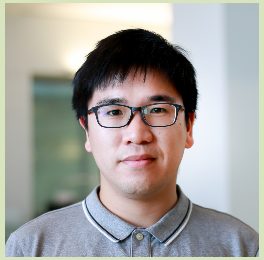

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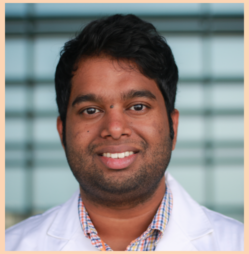

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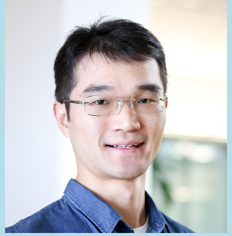


Xiao Shao

What is Cantera?

- Suite of object-oriented software tools for problems involving
  - chemical kinetics,
  - thermodynamics,
  - and/or transport processes
- It offers similar functionality as **Chemkin**, but it is **open-source and free**
- It is a library, not a collection of applications
- The core is written in C++, but it provides interfaces for Fortran, Python, and MATLAB

History of Cantera

- David Goodwin (Caltech, 1957~2012)
- Harry Moffat (Sandia)
- Ray Speth (MIT)

- First workshop was held in July 2004
- Now at version 2.4

Cantera

Useful links

- Project website: https://cantera.org/
  - Documentation
  - Installation instructions for Linux, macOS and Windows (**recommend using Anaconda to install**)
  - Source code repository
  - Tutorials and examples
- User's group: https://groups.google.com/forum/#!forum/cantera-users
- Old materials: http://www.et.byu.edu/~tom/classes/641/Cantera/
- CCRC's CloudFlame: https://cloudflame.kaust.edu.sa/
- Shock/Detonation toolbox: http://shepherd.caltech.edu/EDL/PublicResources/sdt/

Caveat for Chemkin users

- As a library, Cantera provides a collection of objects/functions, not a collection of applications

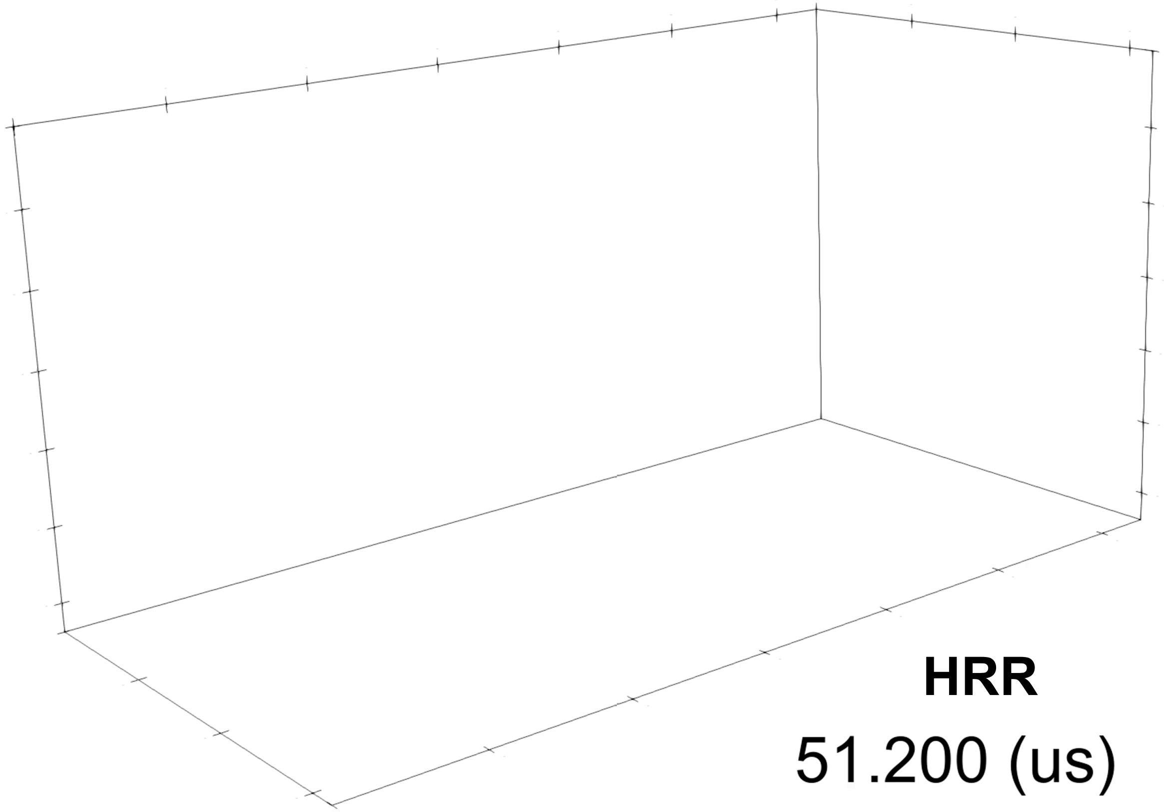
- There is no stand-alone application like PREMIX or OPPDIF

- First an interface among C++/Fortran/Python/MATLAB is chosen, then existing examples and tutorials can be modified to solve our problem

Use in CFD solvers as a library

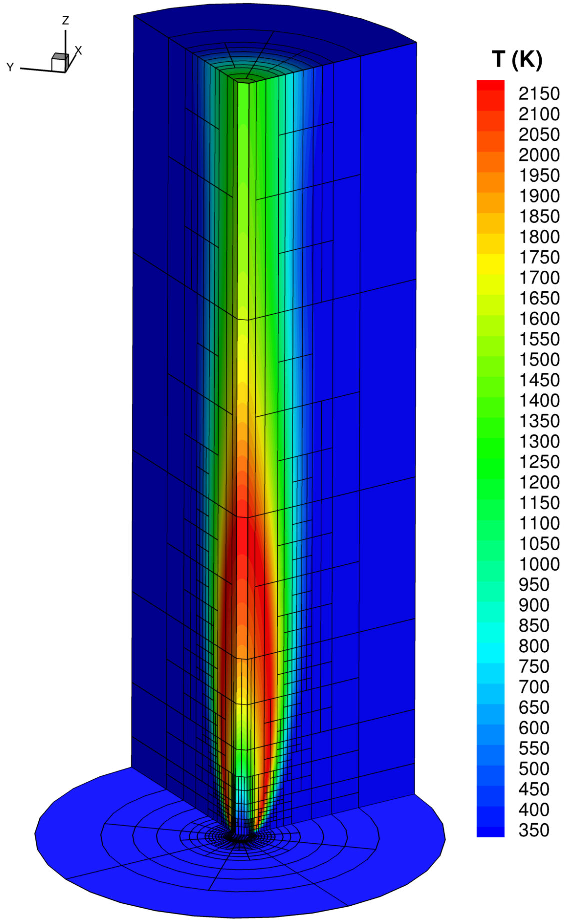
KAUST Adaptive Reacting Flow Solver (KARFS)

- 8^{th} order, finite-difference DNS code
- Performance-portable, designed for hybrid architectures



Computational Framework for Fluids and Combustion (CFFC)

- 2^{nd} order, Godunov-type, finite-volume with adaptive mesh refinement DNS/LES code



Acceleration of Cantera for faster computations

- Topic that is being explored at CCRC
- CPU acceleration using Intel's MKL library (multi-threads)
- GPU acceleration using the MAGMA library

	small	medium	large
number of species / number of reactions	53/325	2192/13927	7172/47157
		wall clock	
sundials CPU 1	0.23 s	2712 s	91583 s
sundials-mkl CPU 16	0.14 s	41 s	722 s
sundials-magma GPU 1	2.0 s	43 s	343 s
		speed-up	
sundials CPU 1	1	1	1
sundials-mkl CPU 16	1.6	66	127
sundials-magma GPU 1	0.1	63	267

- Computation of ignition delay times
- Node with 32 CPU cores (Intel Haswell) and 8 GPUs (Nvidia K80)

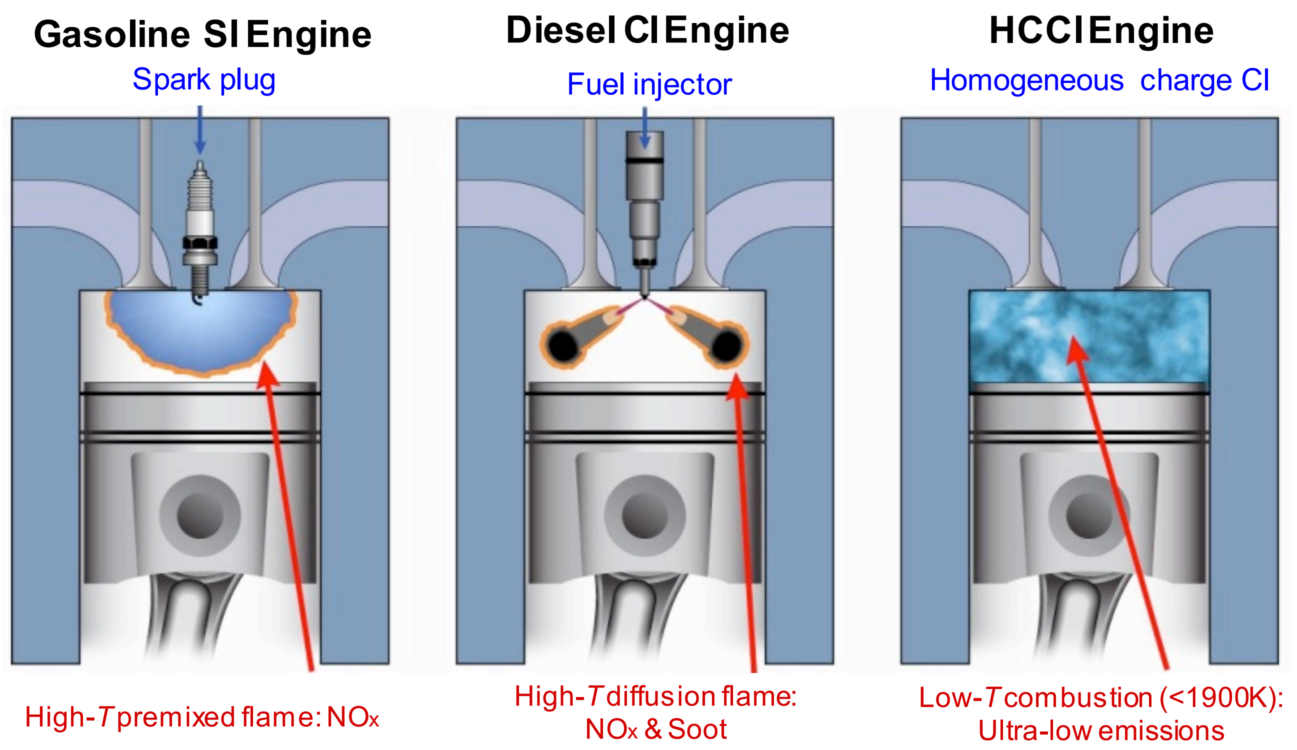
Reaction mechanism files and data

- Community standard: Chemkin format, e.g can found at https://combustion.llnl.gov/archived-mechanisms
  - chem.inp => elements, species, reactions
  - therm.dat => thermodynamic data
  - tran.dat => transport data

- Conversion to Cantera's format: ck2cti
  - $ ck2cti --help
  - Example: $ ck2cti --input=chem.inp --thermo=therm.dat --transport=tran.dat
  - Result: chem.cti

- Conversion to xml: ctml_writer
  - $ ctml_writer chem.cti
  - Result: chem.xml

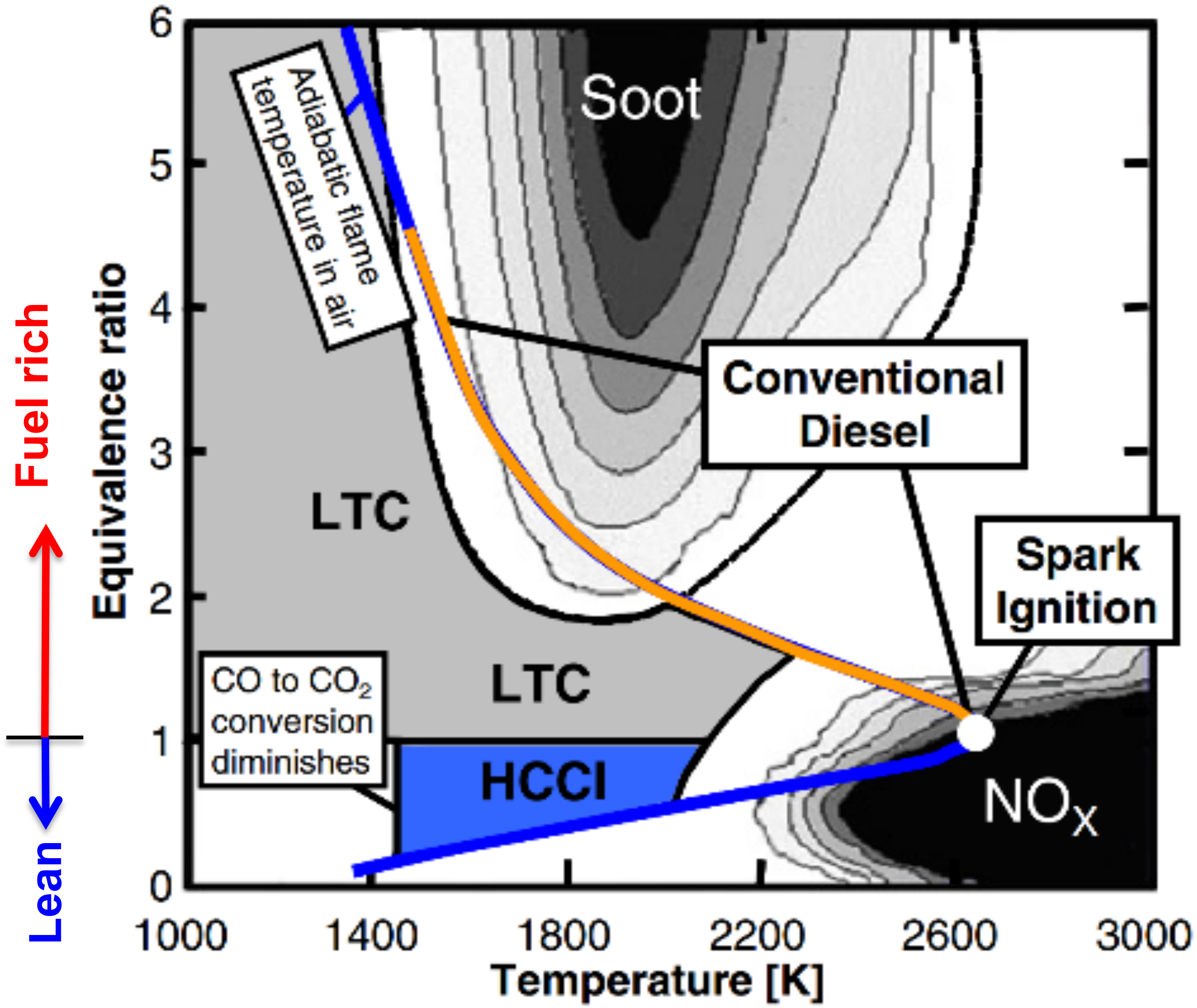
Conventional combustion and advanced combustion modes



- **Spark ignition combustion**: the premixed fuel/air mixture is ignited by a spark plug. A flame propagates out from the spark plug, consuming the reactant mixture.
- **Diesel combustion**: Fuel/air mixtures are non-premixed. Air is inducted into the cylinder during the intake stroke and compressed to a high p & T; followed by fuel direct injection. The charge is compression ignition and burnt in diffusion flame.
- **Homogeneous-charge compression-ignition combustion (HCCI)** is a hybrid combustion strategy.

Homogeneous Charge Compression Ignition (HCCI)

- **Low temperature combustion (LTC)**
  - HCCI is a variant of LTC
- **Alternative to SI and diesel engines**
  - Lean, dilute, low *T*, high pressure
  - High diesel-like efficiency
  - Ultra-low NO_x and soot emissions
- **HCCI combustion**
  - Occurs through volumetric auto-ignition
  - Controlled by chemical kinetics of fuel/air mixture
- **Key issues in HCCI engine development**
  - Prevent excessive combustion rate
  - Tailoring ignition timing



ϕ–temperature ranges for soot and NO_X formation regions*

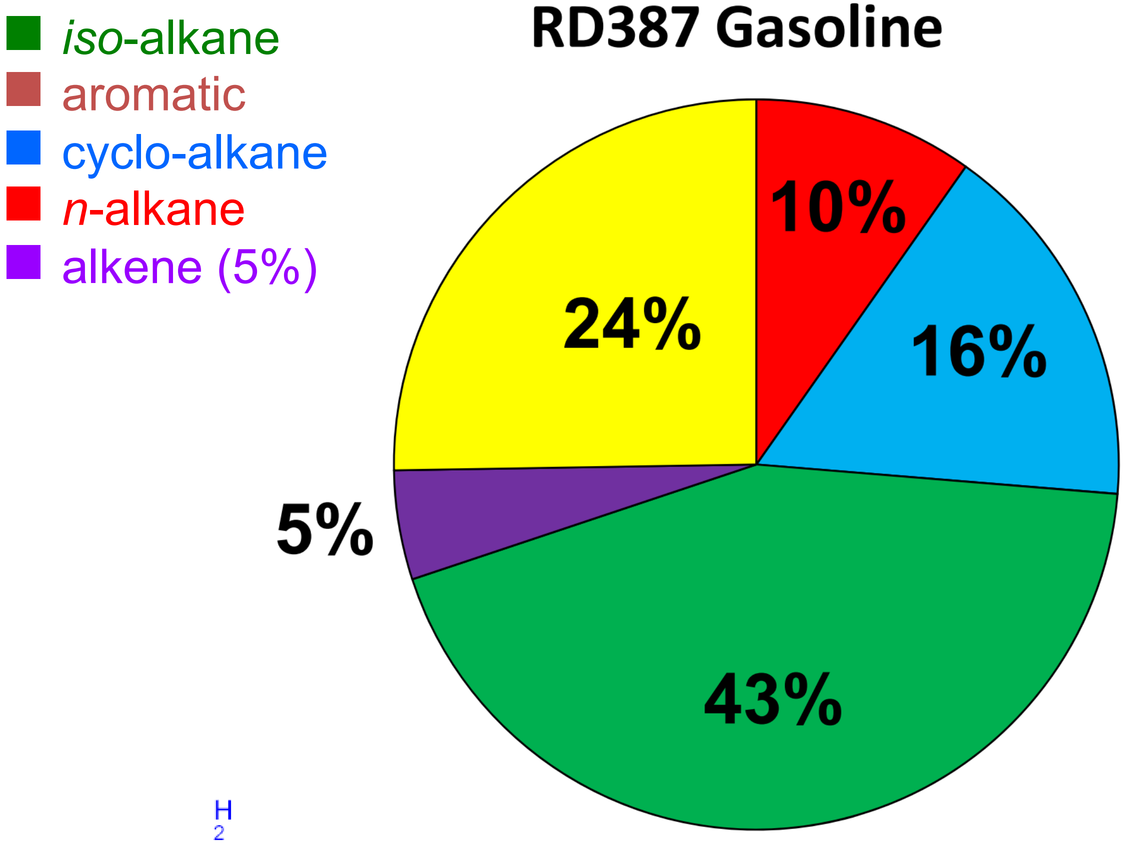
*Dec, Proc. Combust. Inst. 32 (2009) 2727–2742

**Report of the Basic Energy Science Workshop DOI: 10.2172/935428

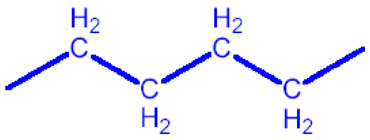
Typical Practical Fuels

- **All petroleum-derived fuels contain a complex mixture of HC molecules**
  - Gasoline 6 < C < 10
  - Jet fuel 9 < C < 13
  - Diesel 13 < C < 22
  - HCCI 1 < C < 22

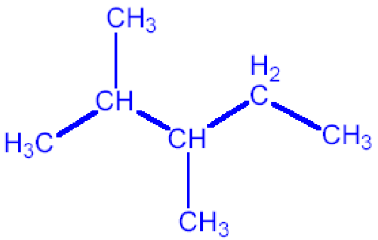
RD387 Gasoline



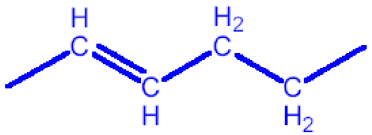
n-paraffin



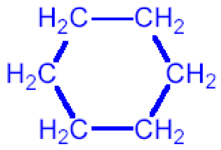
iso-paraffin



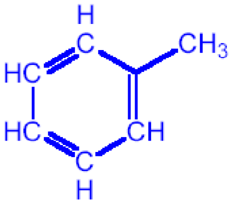
olefin



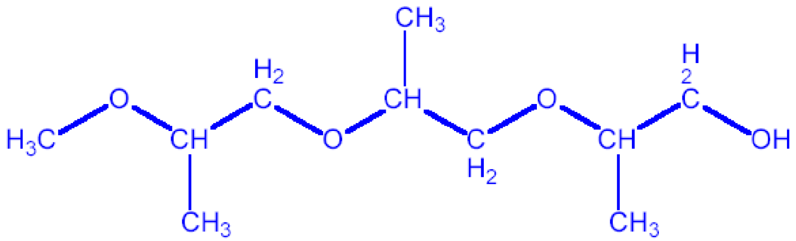
Hydrocarbons in diesel fuel



cyclo-alkane



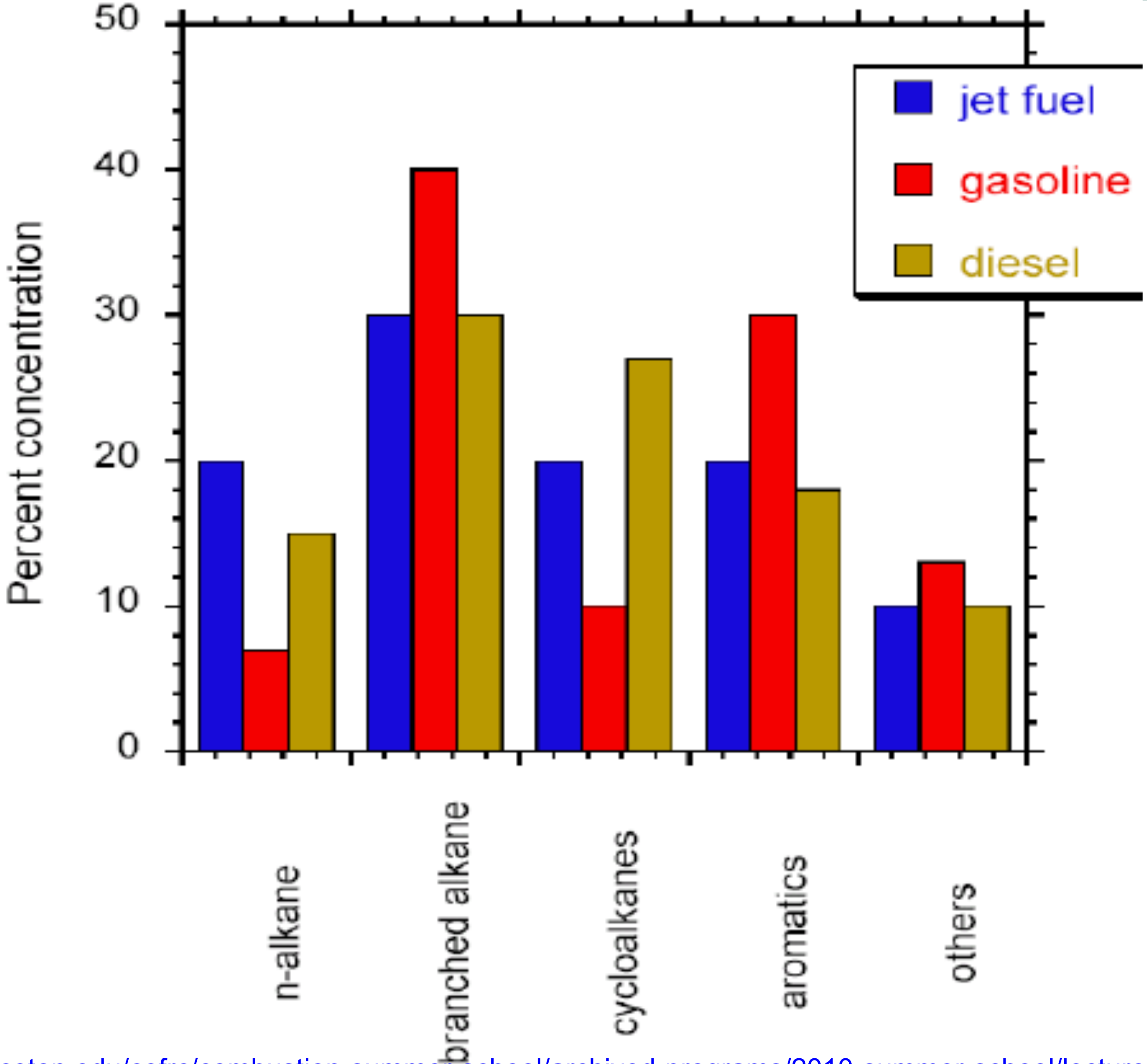
aromatic



oxygenate

C.K. Westbrook's lecture note, http://www.princeton.edu/cefrc/combustion-summer-school/archived-programs/2010-summer-school/lecture-notes/

Chemical Composition Comparison



C.K. Westbrook's lecture note, http://www.princeton.edu/cefrc/combustion-summer-school/archived-programs/2010-summer-school/lecture-notes/

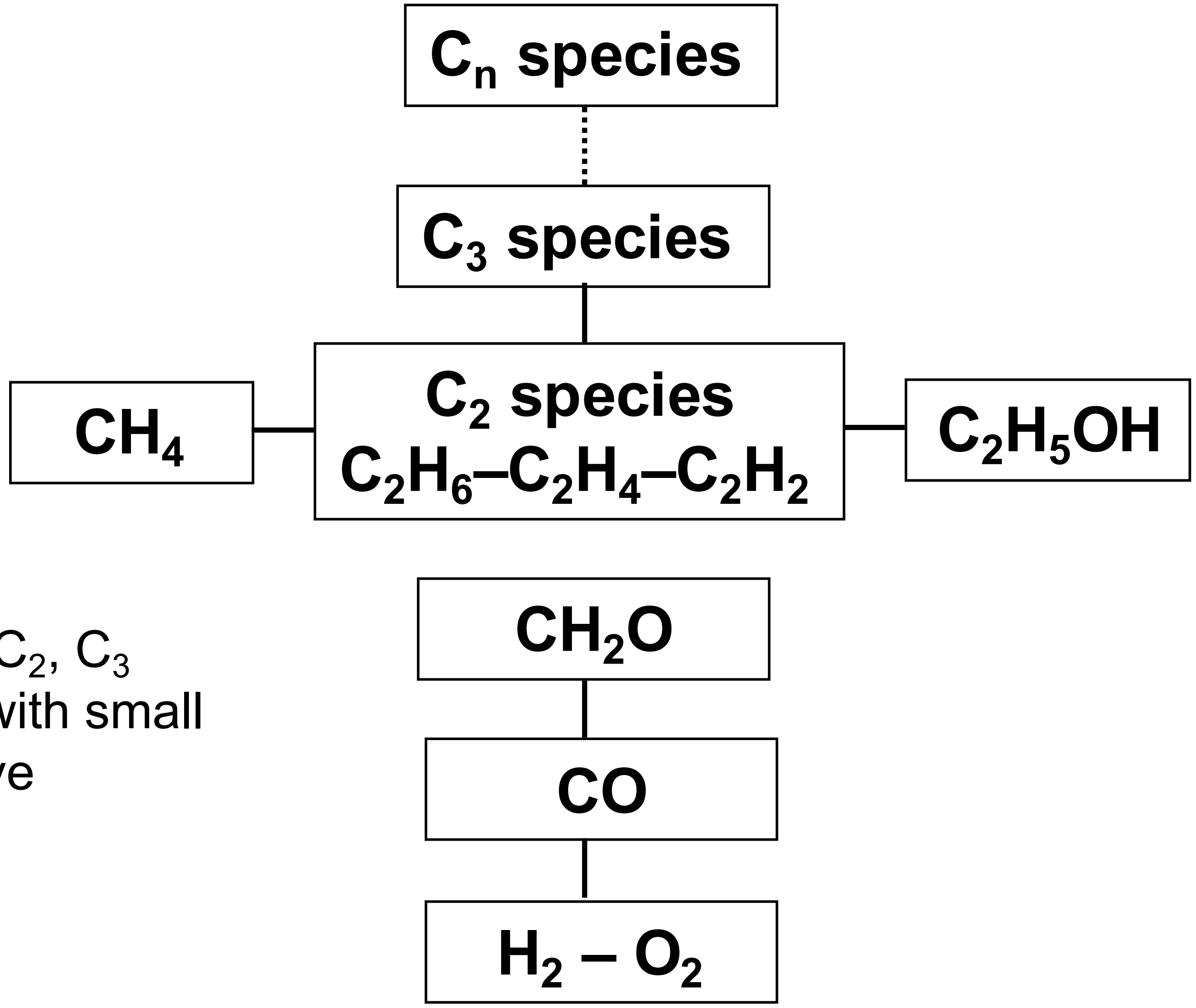
Hydrogen oxidation mechanism

- **Global reaction, $2H_2 + O_2 \rightarrow 2H_2O$ versus actual elementary reactions of $H_2 – O_2$ oxidation mechanism**

No.	Reaction	B[cm, mol, s]	α	E_a(kcal/mol)
	$H_2–O_2$ Chain Reactions			
(1)	$H + O_2 \rightleftharpoons O + OH$	1.9×10^{14}	0	16.44
(2)	$O + H_2 \rightleftharpoons H + OH$	5.1×10^{04}	2.67	6.29
(3)	$OH + H_2 \rightleftharpoons H + H_2O$	2.1×10^{08}	1.51	3.43
(4)	$O + H_2O \rightleftharpoons OH + OH$	3.0×10^{06}	2.02	13.40
	$H_2–O_2$ Dissociation/Recombination			
(5)	$H_2 + M \rightleftharpoons H + H + M$	4.6×10^{19}	−1.40	104.38
(6)	$O + O + M \rightleftharpoons O_2 + M$	6.2×10^{15}	−0.50	0
(7)	$O + H + M \rightleftharpoons OH + M$	4.7×10^{18}	−1.0	0
(8)	$H + OH + M \rightleftharpoons H_2O + M$	2.2×10^{22}	−2.0	0
	Formation and Consumption of HO_2			
(9)	$H + O_2 + M \rightleftharpoons HO_2 + M$	6.2×10^{19}	−1.42	0
(10)	$HO_2 + H \rightleftharpoons H_2 + O_2$	6.6×10^{13}	0	2.13
(11)	$HO_2 + H \rightleftharpoons OH + OH$	1.7×10^{14}	0	0.87
(12)	$HO_2 + O \rightleftharpoons OH + O_2$	1.7×10^{13}	0	−0.40
(13)	$HO_2 + OH \rightleftharpoons H_2O + O_2$	1.9×10^{16}	−1.00	0
	Formation and Consumption of H_2O_2			
(14)	$HO_2 + HO_2 \rightleftharpoons H_2O_2 + O_2$	4.2×10^{14}	0	11.98
		1.3×10^{11}	0	−1.629
(15)	$H_2O_2 + M \rightleftharpoons OH + OH + M$	1.2×10^{17}	0	45.50
(16)	$H_2O_2 + H \rightleftharpoons H_2O + OH$	1.0×10^{13}	0	3.59
(17)	$H_2O_2 + H \rightleftharpoons H_2 + HO_2$	4.8×10^{13}	0	7.95
(18)	$H_2O_2 + O \rightleftharpoons OH + HO_2$	9.5×10^{06}	2.0	3.97
(19)	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$	1.0×10^{12}	0	0
		5.8×10^{14}	0	9.56

General Considerations of Hydrocarbon Oxidation

- **HC oxidation is hierarchical**
  - H_2/O_2 is the foundation
  - CO/CO_2 is the next level
  - $CH_4/CH_2O/CH_3OH$ is the next level
  - $C_2H_6/C_2H_4/C_2H_2$ is next
  - This pattern continues to C_{10} and C_{20}
  - There are many side branches to this tree

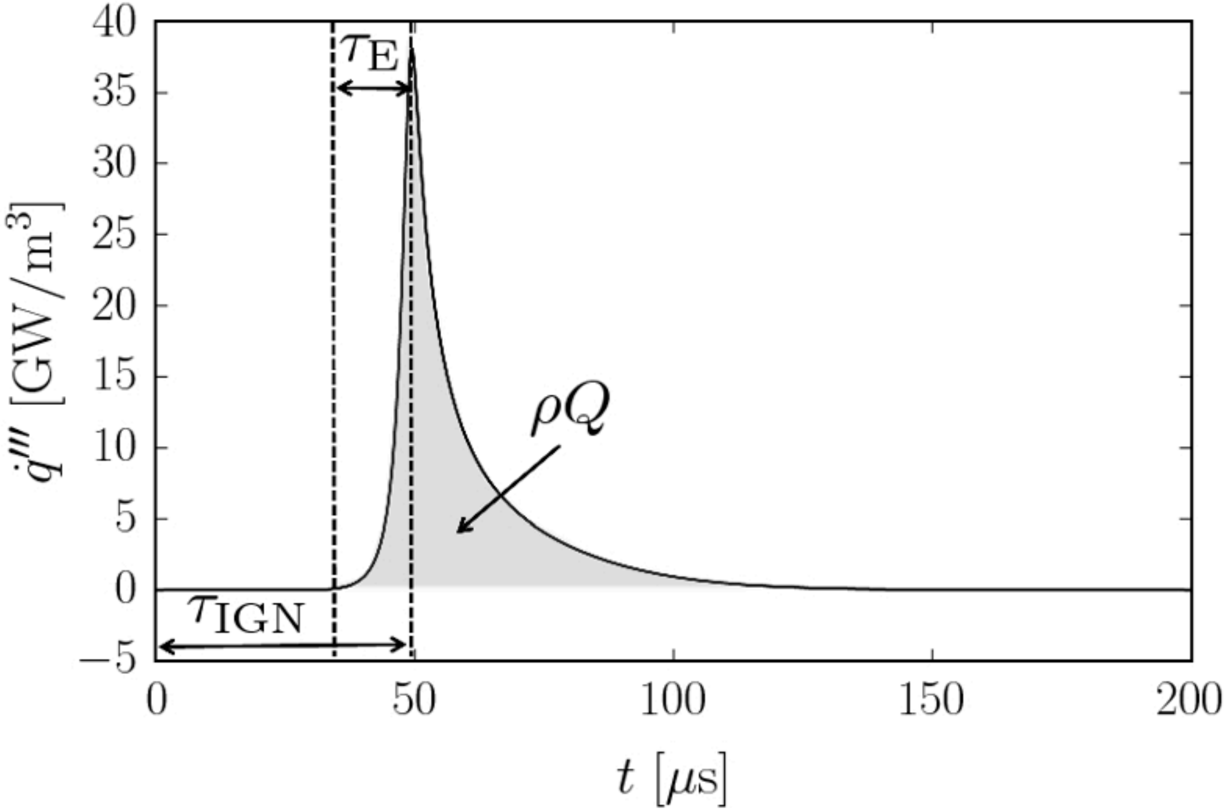


- Large HC molecule breaks down into smaller C_1, C_2, C_3 fragments in the low-temperature region/regime, with small heat release, which subsequently undergo massive oxidation with large heat release

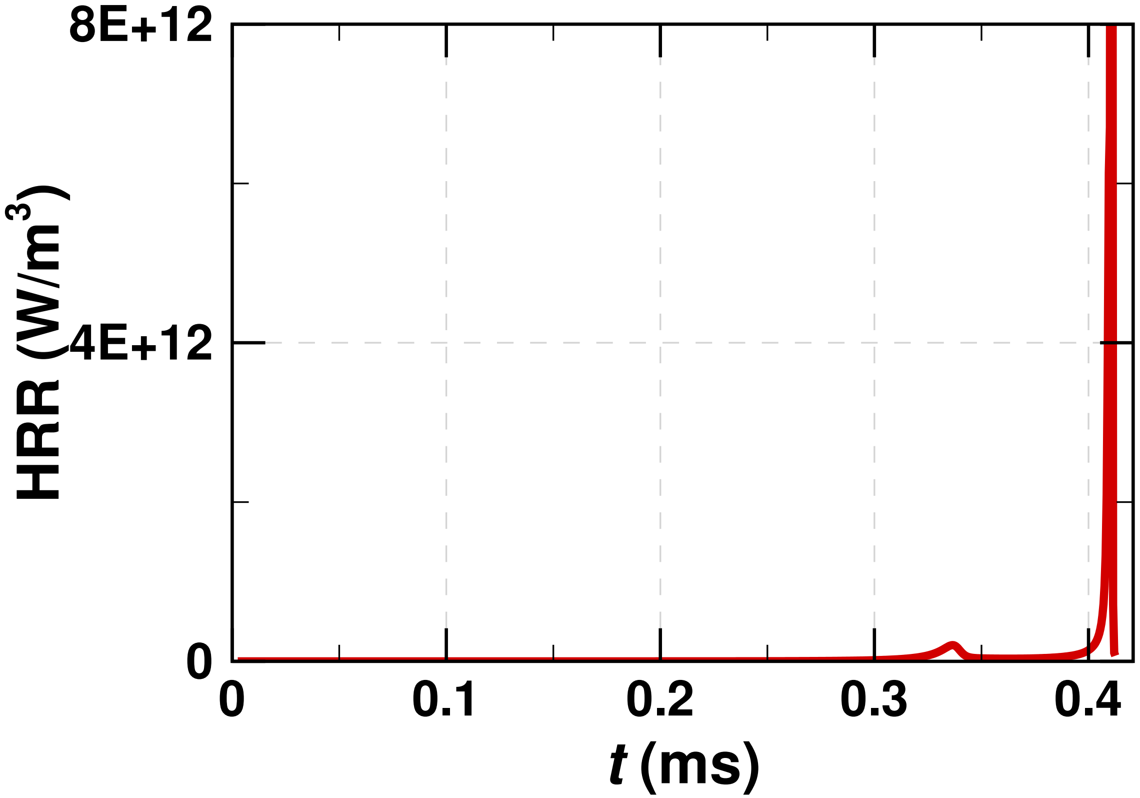
C.K. Westbrook's lecture note, http://www.princeton.edu/cefrc/combustion-summer-school/archived-programs/2010-summer-school/lecture-notes/

Ignition delay time

τ_{ig}: ignition delay time (s)
τ_e : excitation time (s)



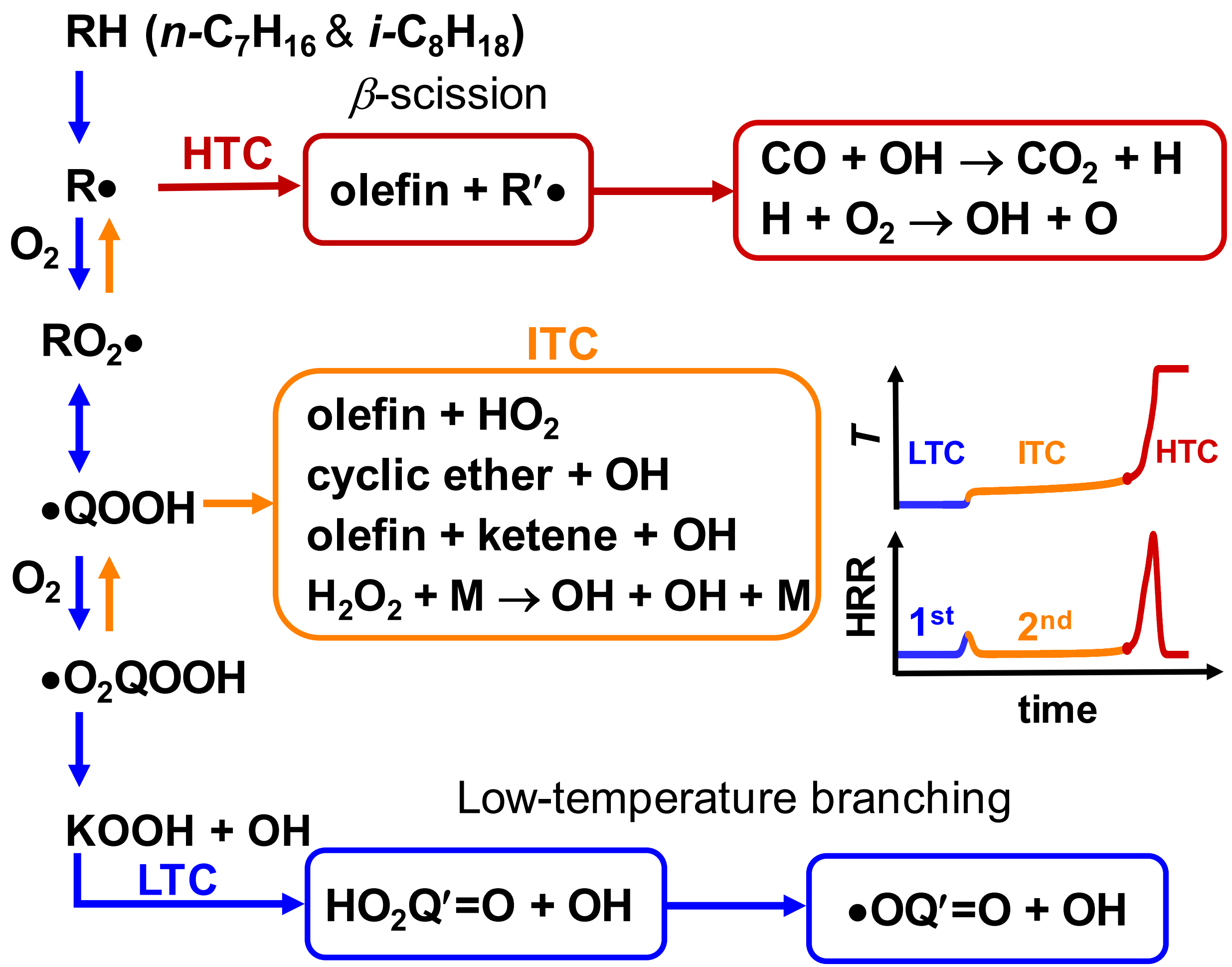
Single-stage ignition



Two-stage ignition

General Considerations of Hydrocarbon Oxidation

1. Hierarchical structure with H_2–CO–O_2, CH_4–O_2, and C_2H_x–O_2 are core submechanisms
2. Temperature-dependent reaction pathways



Matryoshka hierarchy
(nesting doll)

C.K. Westbrook's lecture note, http://www.princeton.edu/cefrc/combustion-summer-school/archived-programs/2010-summer-school/lecture-notes/

Overall Hydrocarbon Oxidation

Three distinct chain branching pathways

Low *T*, *T* < 850 K

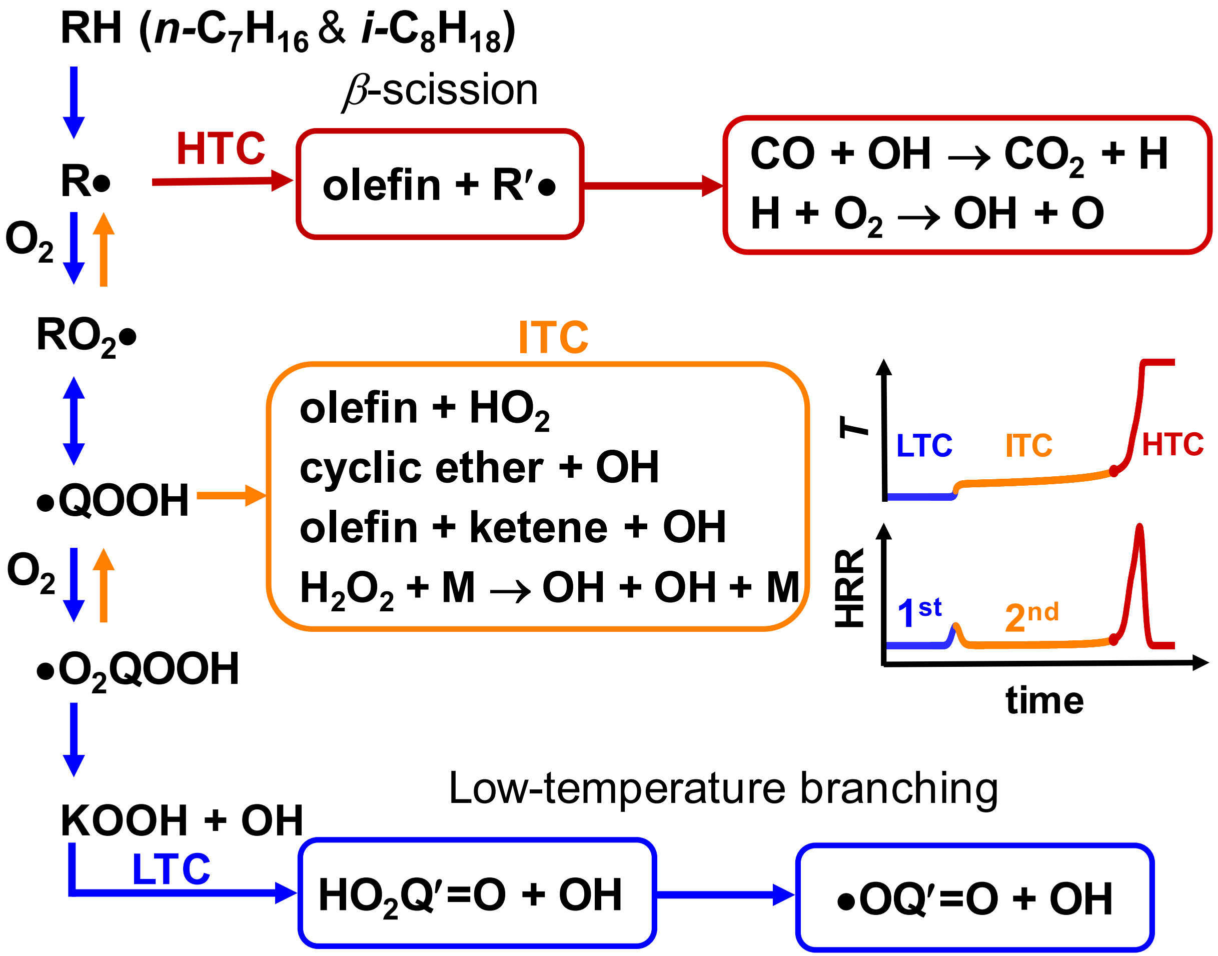
$R + O_2 \rightarrow RO_2$
$RO_2 \rightarrow QOOH \rightarrow O_2QOOH \rightarrow$ radicals

Intermeadiate *T*, 850 K < *T* < 950 K

$H + O_2 + M \rightarrow HO_2 + M$
$RH + HO_2 \rightarrow R + H_2O_2$
$H_2O_2 + M \rightarrow OH + OH + M$

High *T*, *T* > 1100 - 1150 K

$H + O_2 \rightarrow OH + O$

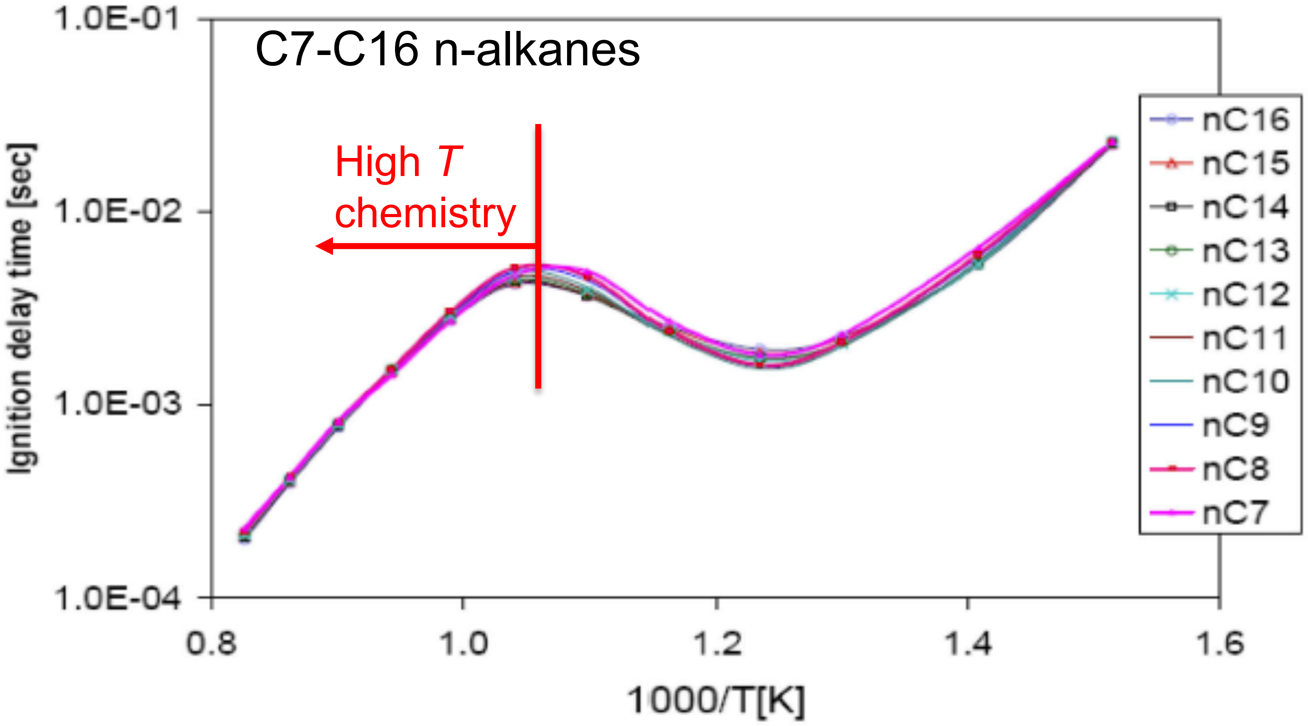


Note: The temperature ranges listed here are just for reference, which is typical in a practical IC engine. The exact temperature ranges for the low-, intermediate-, and high-temperature chemistry are varied for each specific system.

C.K. Westbrook's lecture note, http://www.princeton.edu/cefrc/combustion-summer-school/archived-programs/2010-summer-school/lecture-notes/

Overall Hydrocarbon Oxidation at High *T*

- **General rules**
  - Fuel + (O, H) $\rightarrow$ Alkenes + H
  - Alkenes $\rightarrow$ (CO, H_2) $\rightarrow$ H_2O
  - CO + OH $\rightarrow$ CO_2 + H, primary reaction converting CO into CO_2 and key heat release step of the overall mechanism



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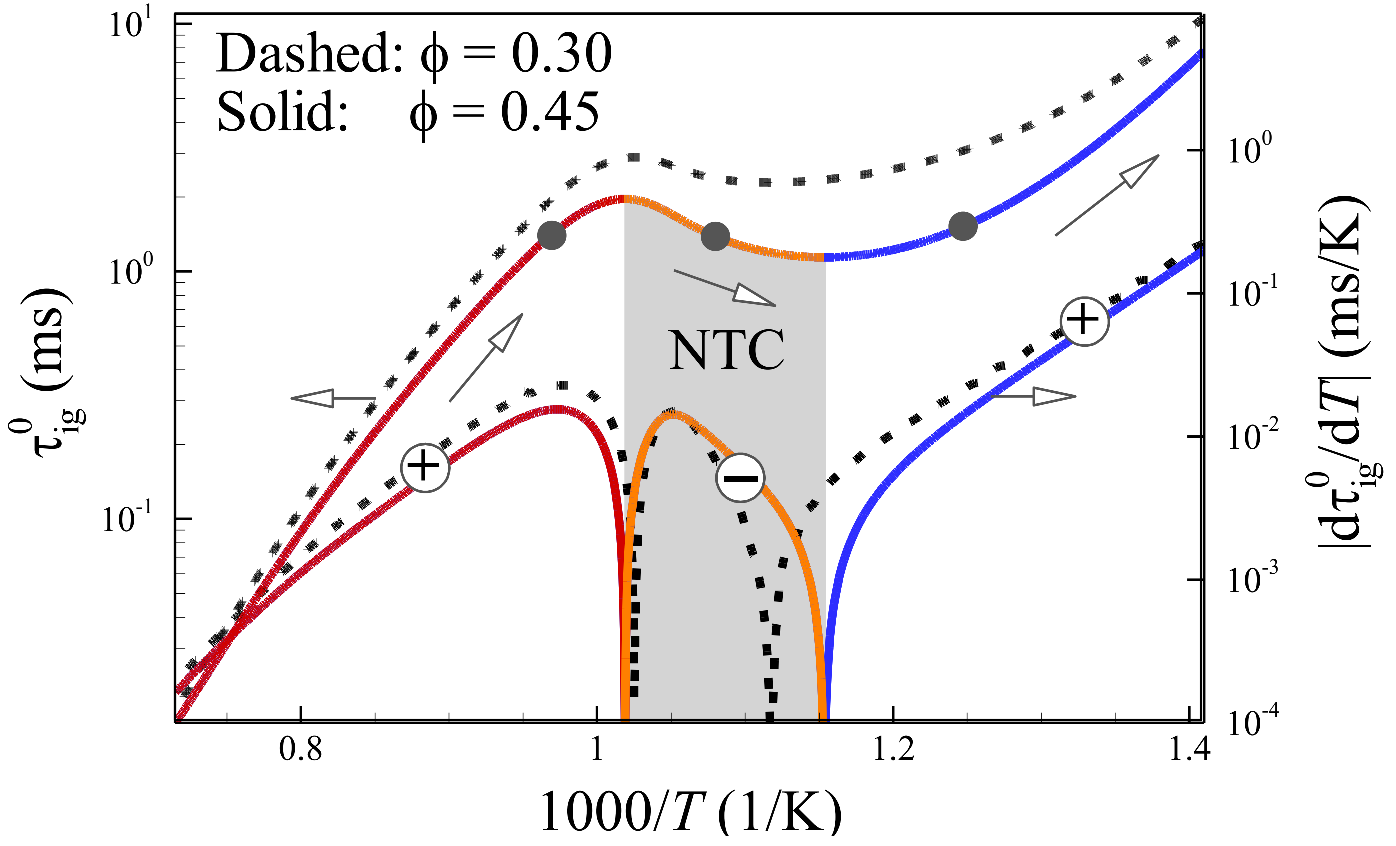
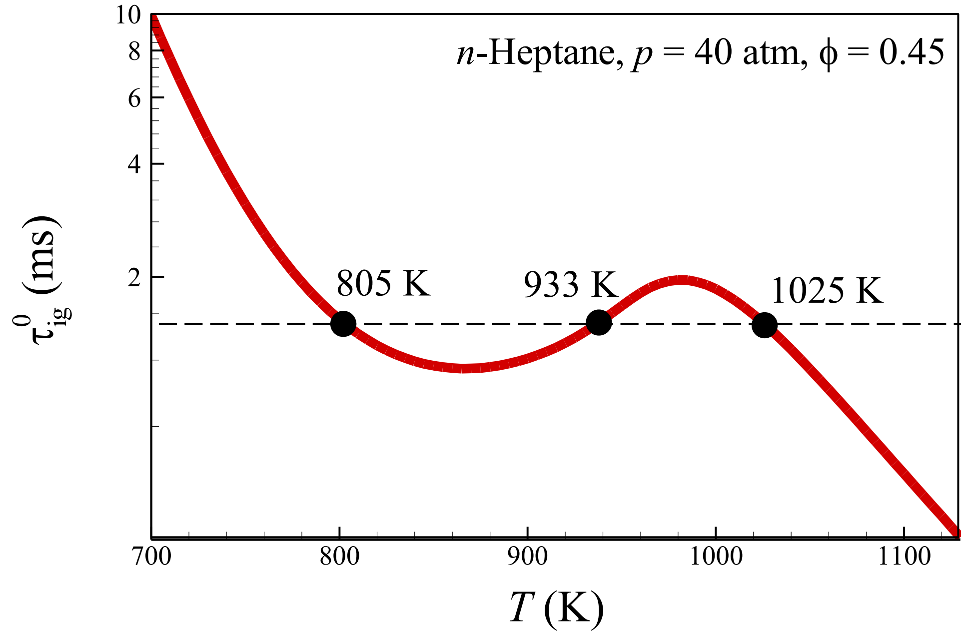
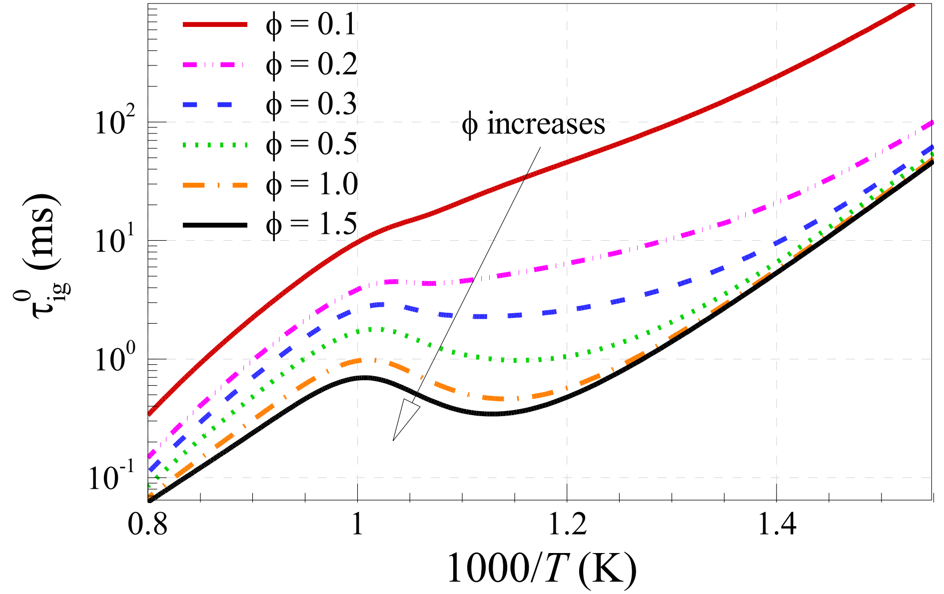
0-D Ignition of *n*-heptane







Flame speed and adiabatic temperature as a function of ϕ

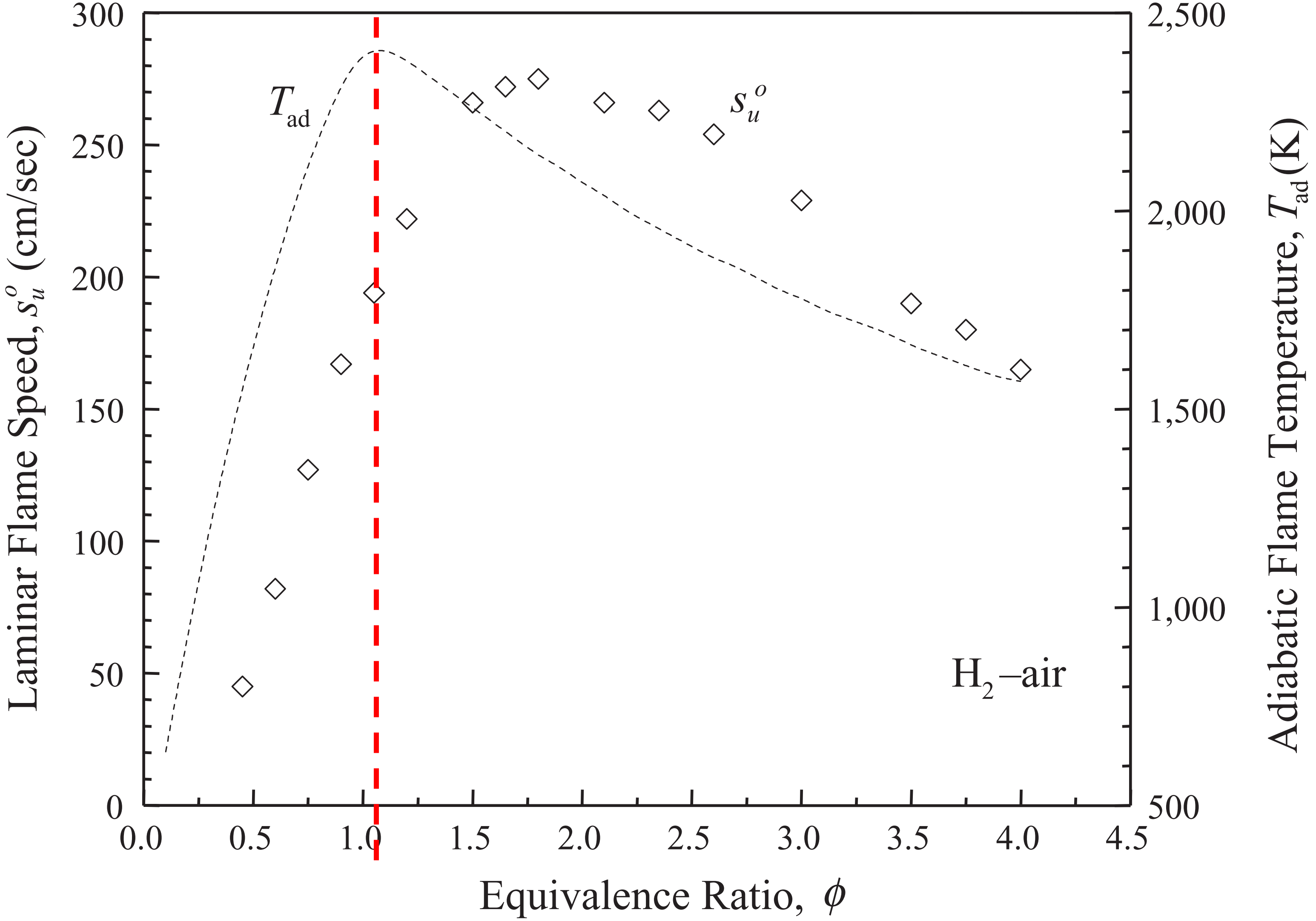


Figure 7.7.2. Calculated adiabatic flame temperatures and measured laminar flame speeds of atmospheric hydrogen–air mixtures.

Adiabatic temperature as a function of ϕ for different fuels

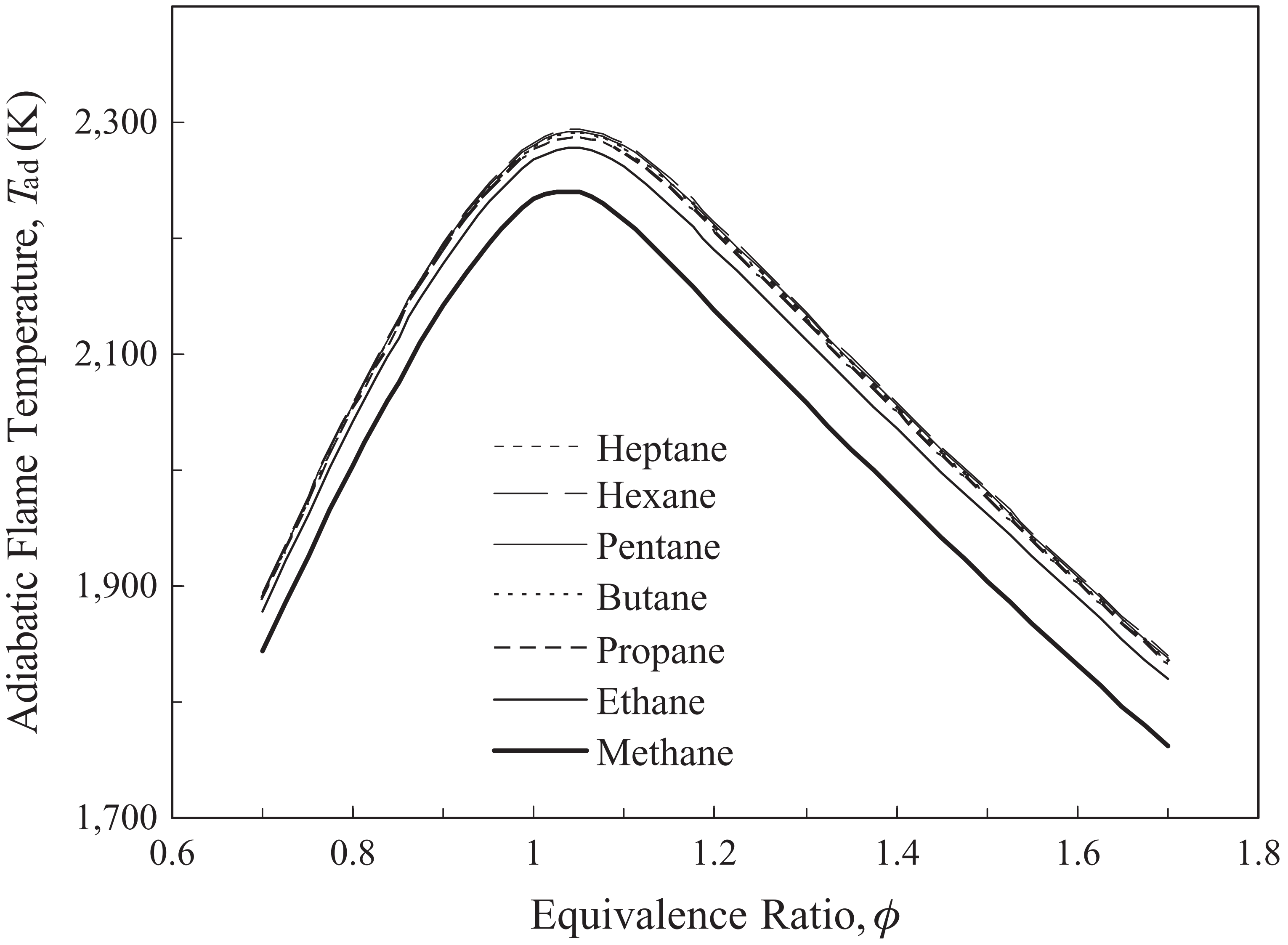


Figure 7.7.5. Calculated adiabatic flame temperatures for varies alkanes.

Objectives

How to use Cantera to

- **Calculate thermal properties as a function of temperature**
  - Heat capacities, thermal conductivity, thermal diffusivity, mass diffusivity, etc.
- **Calculate 0-D ignition as a function of temperature**
  - **Cool flame**: two-stage ignition fuels with negative temperature coefficient (NTC)
  - Effect of pressures and equivalence ratios
- **1-D premixed laminar flame speed**
  - Different fuels
  - Domain length (induction length)
  - Look at the structure of a premixed flame

Hands-on

From the command line of the terminal, type

- Load Cantera

```
source /opt/cantera-2.4/bin/setup_cantera
```

- List the examples provided by Cantera

```
ls /opt/cantera-2.4/lib/python3.5/site-packages/cantera/examples/
```

>> kinetics/   multiphase/   onedim/   reactors/   surface_chemistry/   thermo/   transport/

- **Run an example test**

```
cd $HOME
git clone
https://github.com/minhbau/cantera_tutorial_CCRC_winterSchool.git
cd cantera_tutorial_CCRC_winterSchool
source /opt/cantera-2.4/bin/setup_cantera
python3 example.py
```

SIMULATE 1-D PREMIXED FLAME

1D flame computations

Examples available from Cantera’s installation:

$ ls $HOME/ anaconda3/envs/cantera_py3/lib/python3.X?/site-packages/cantera/examples/onedim

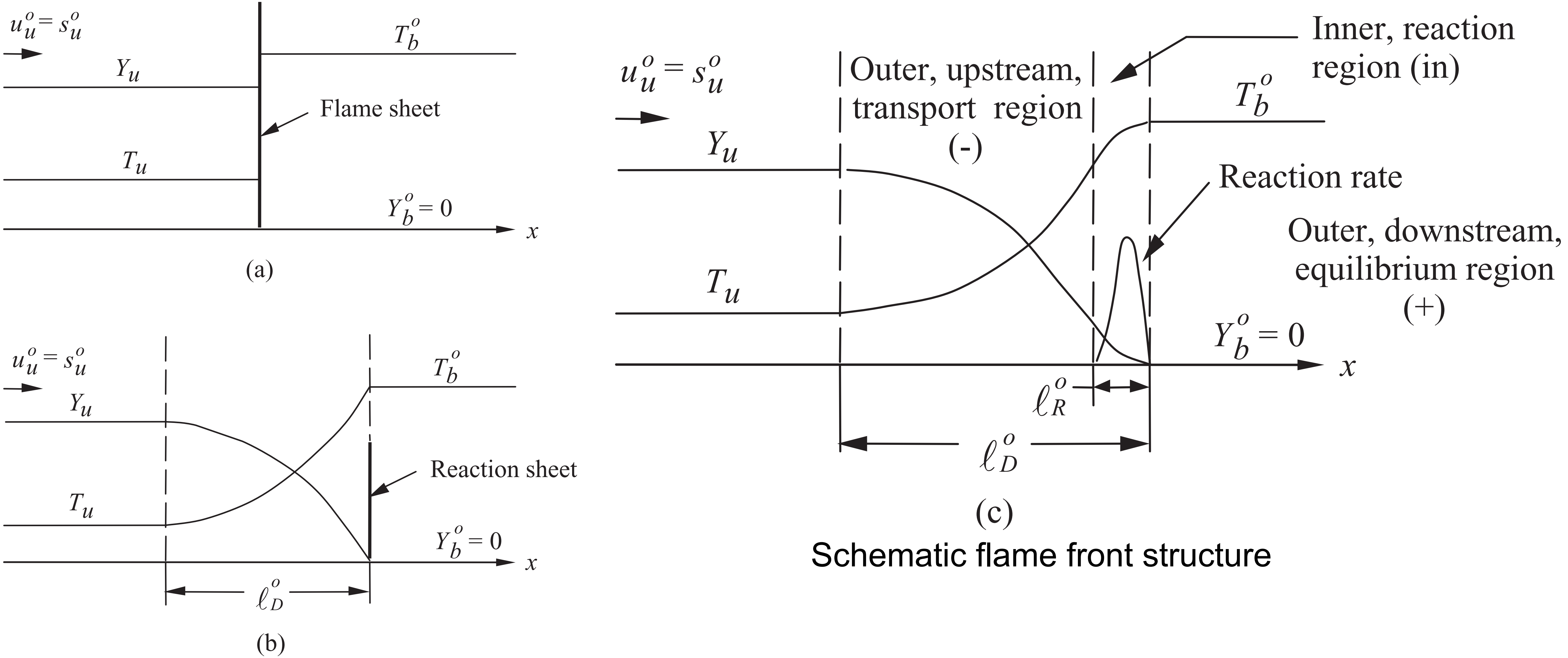
adiabatic_flame.py ➔ **freely propagating premixed flame**
burner_flame.py ➔ **burner-stabilized premixed flame**
premixed_counterflow_flame.py ➔ **counterflow premixed flame**
diffusion_flame.py ➔ **counterflow diffusion flame**
diffusion_flame_batch.py ➔ **batch of counterflow diffusion flames at different conditions**
diffusion_flame_extinction.py ➔ **extinction point of counterflow diffusion flame**

and more…

Python scripts are also available from Cantera’s website (current version):
https://cantera.org/examples/python/index.html

Structure of 1-D Premixed Flame

- **Fuel & oxidizers are on the same side of the flame, i.e. premixed**



Schematic flame front structure

Governing equations, transport models, and schemes

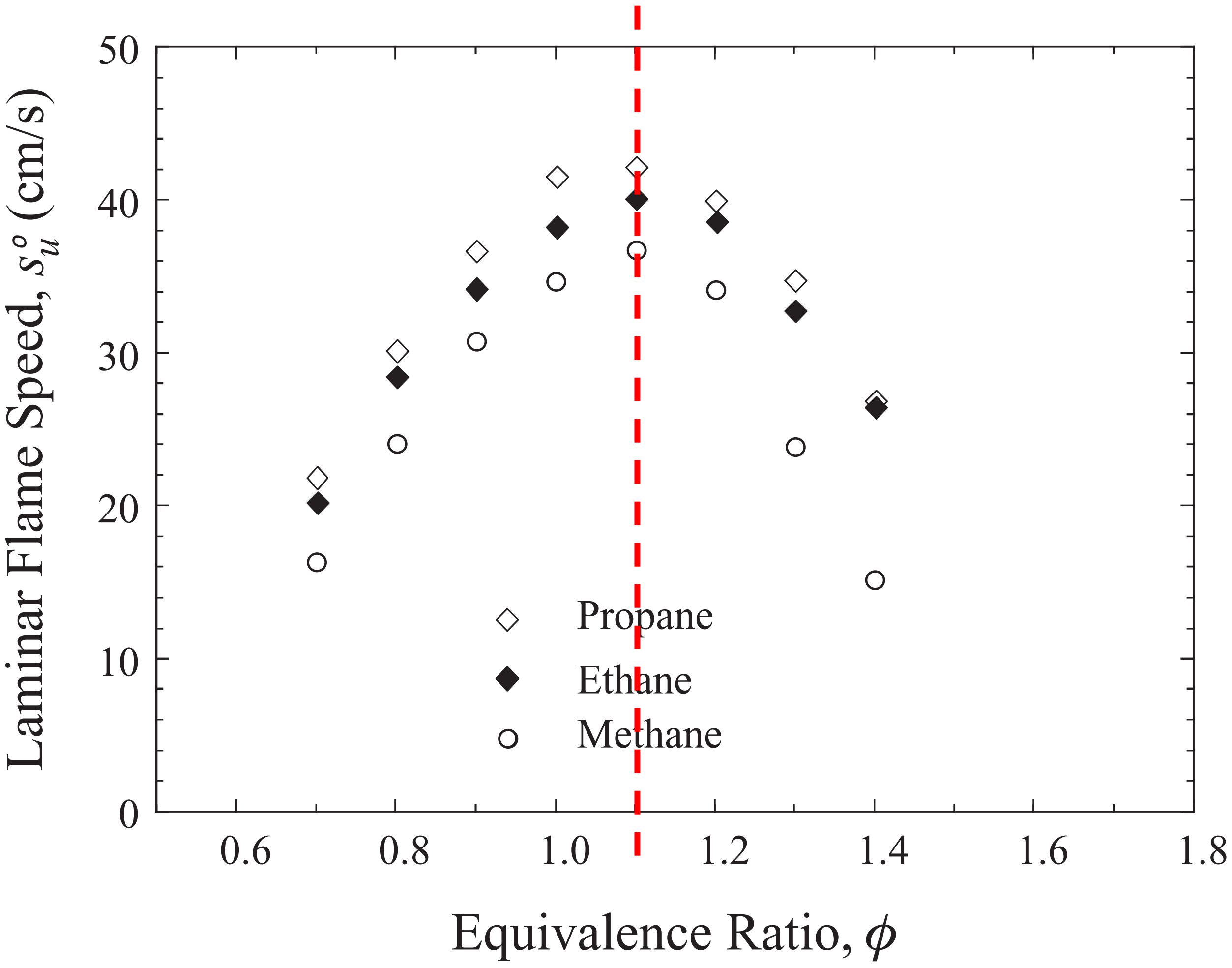
- **Cantera models flames that are stabilized in an axisymmetric flow and computes the steady-state solution along the centerline (r=0)**

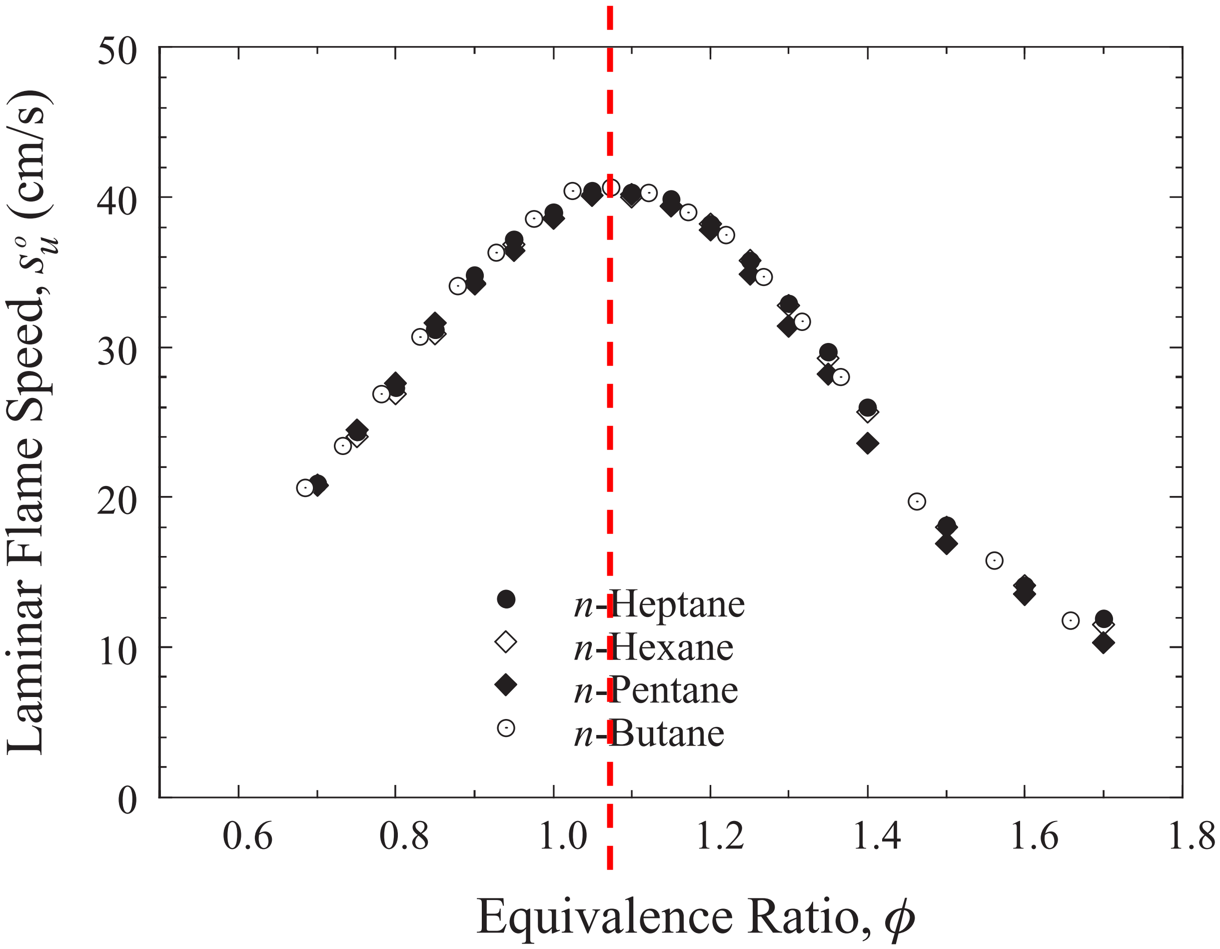
- **Governing equations: continuity, momentum, energy, species mass fractions**

- **Transport models:**
  - mixture-averaged: mixture-averaged diffusion coefficients, Mathur's mixing rule for thermal conductivity, no thermal diffusion
  - multicomponent: multicomponent diffusion coefficients, including thermal diffusion (Soret effect)
  - both mixture-averaged and multicomponent models use Wilke's mixing rule for the mixture viscosity

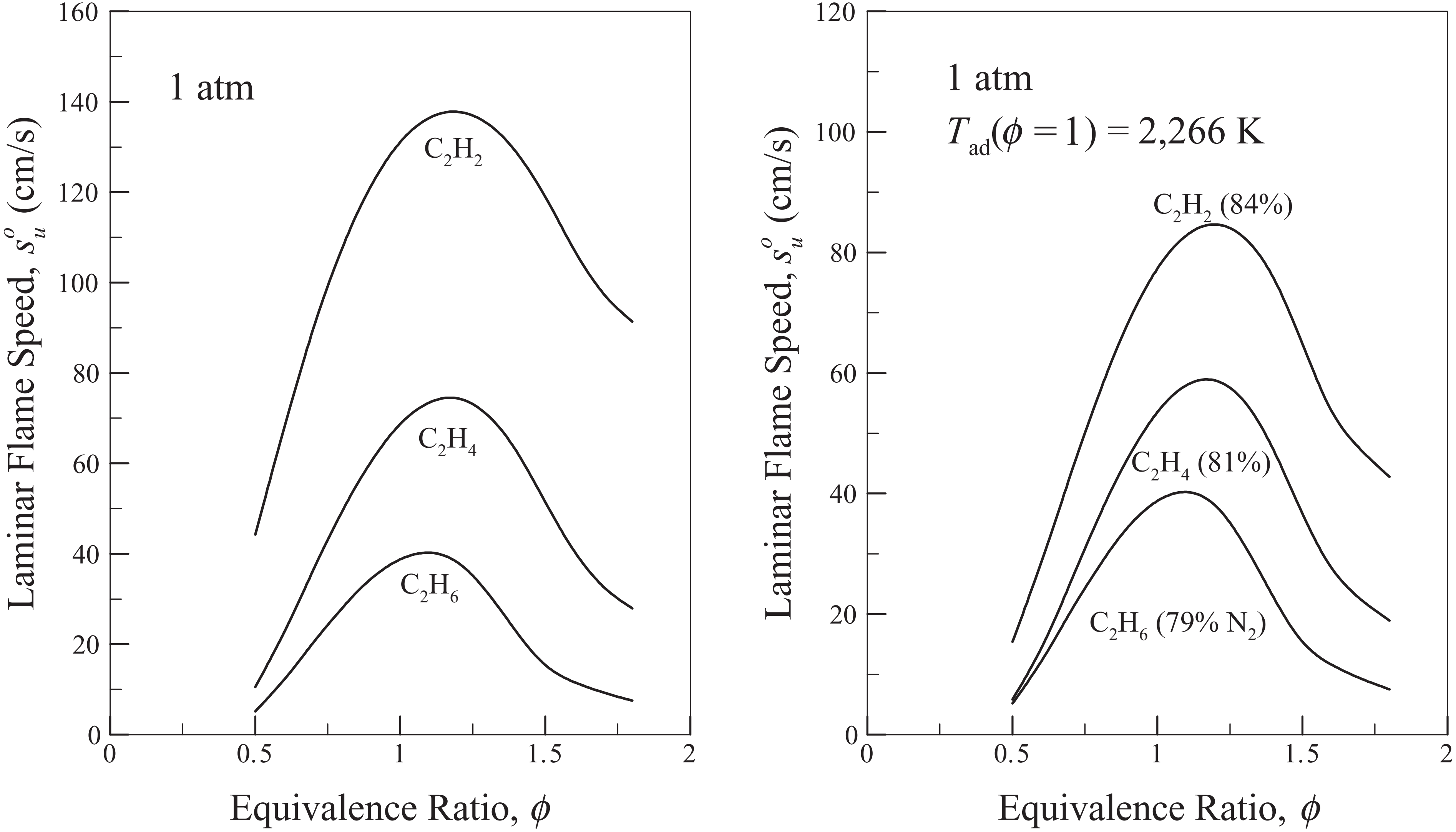
- **Numerical schemes: second-order finite difference, modified Newton method and adaptive mesh refinement**

Flame speed as a function of ϕ for different fuels





Flame speed as a function of ϕ for different fuels



ϕ is an important property of the premixture

Flame speed as a function of ϕ for various pressure

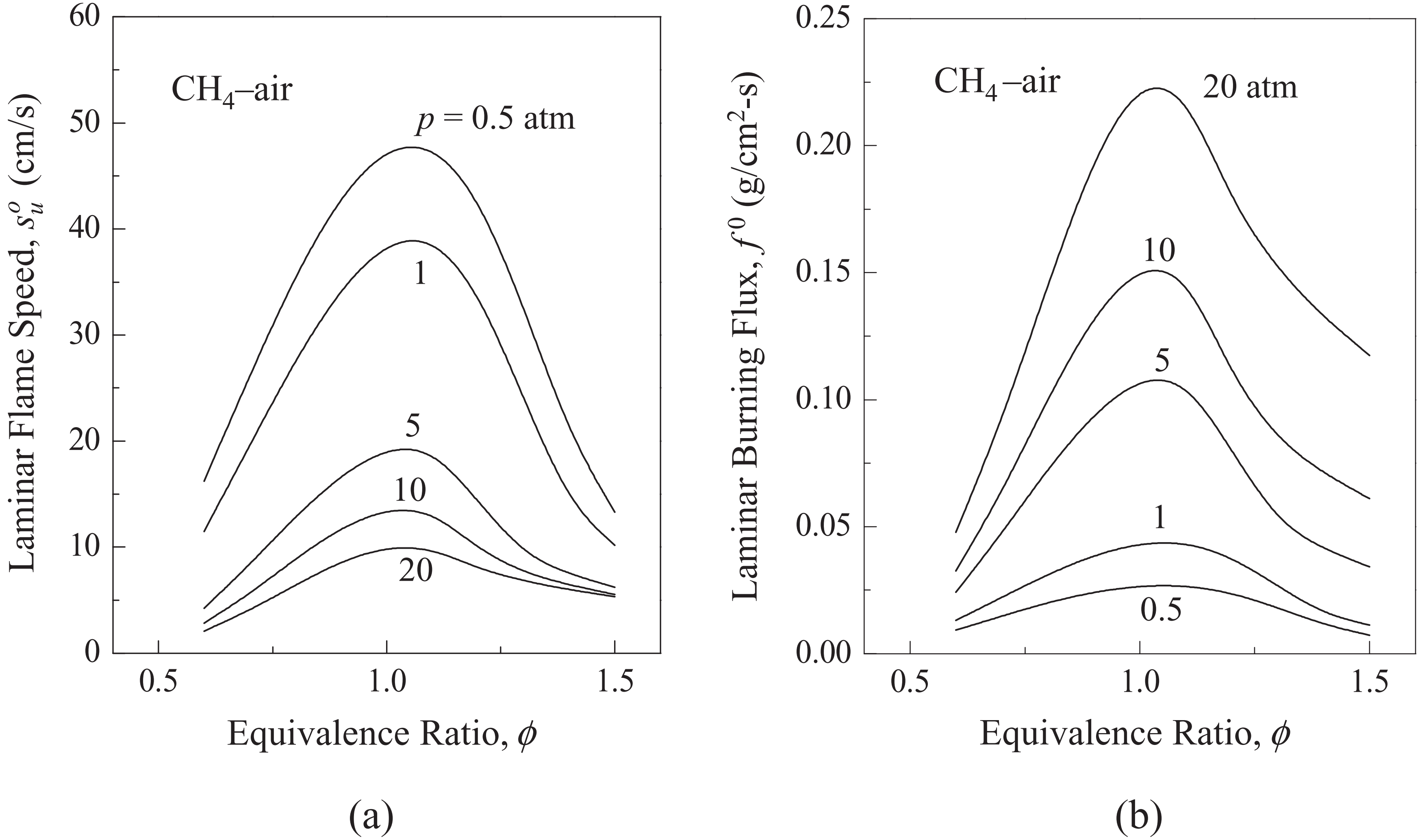
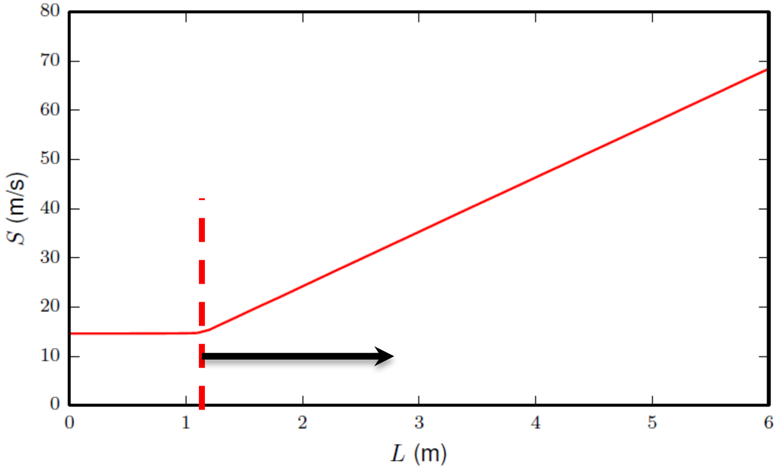


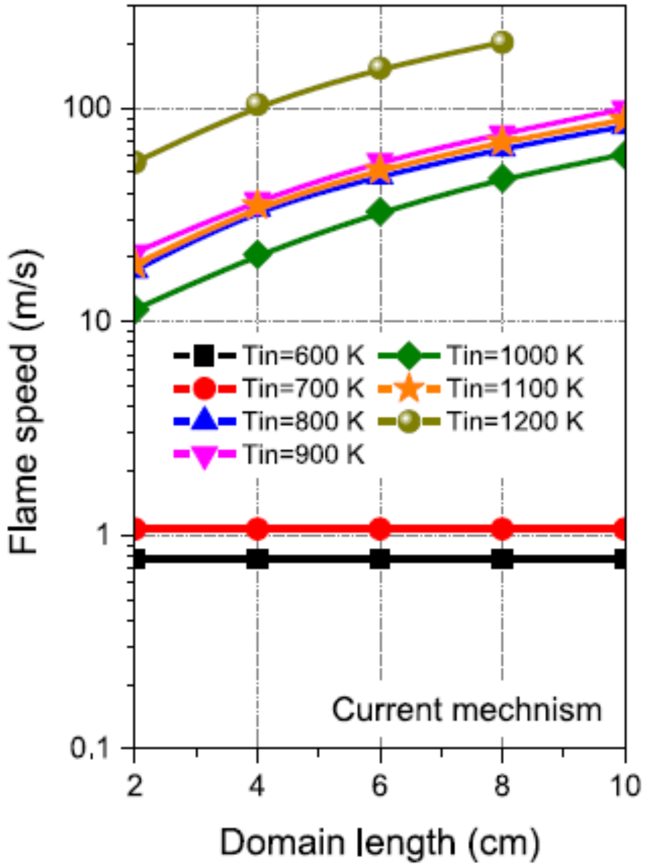
Figure 7.7.7. Computed (a) laminar flame speed, s_u^o, and (b) laminar burning flux, $f^o = \rho_u s_u^o$, for methane–air mixtures at various pressures, showing the trends of decreasing s_u^o but increasing f^o with increasing pressure.

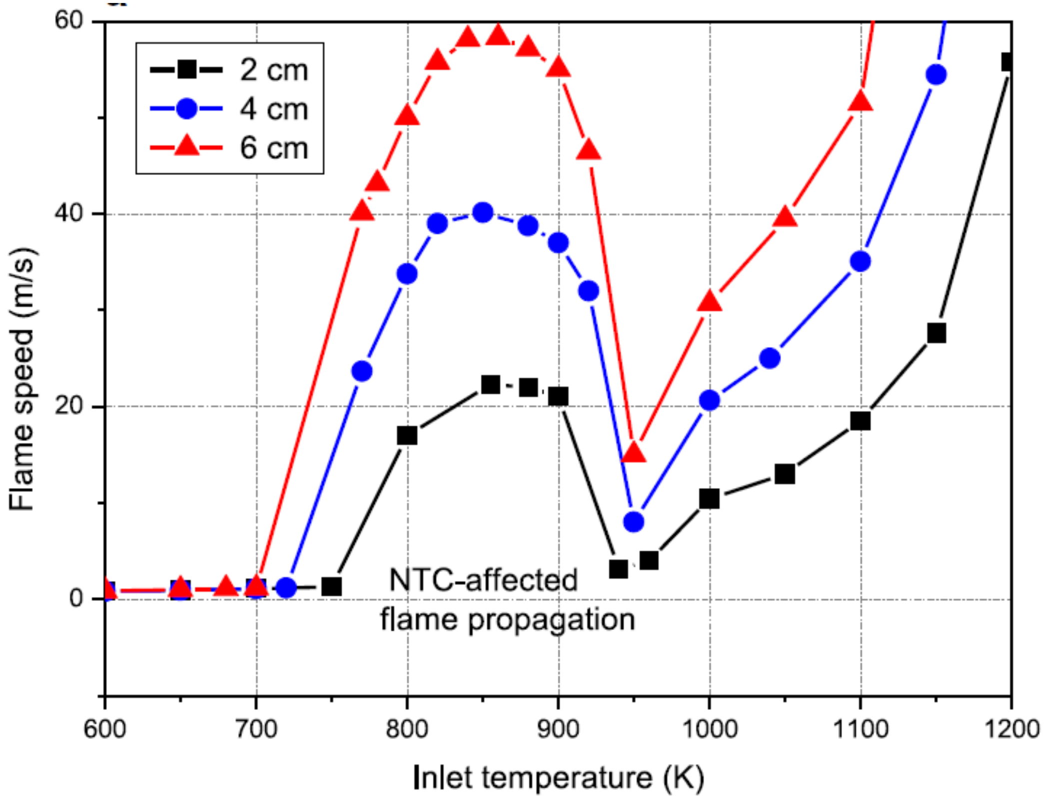
Characteristics of autoignitive premixed flame speed

Variation of the propagation velocity of the combustion front, S, as a function of the length of the induction zone.



Domain length





NTC-affected flame speed as a function of inlet temperature with domain size of 2, 4 and 6 cm.

[1] R. Sankaran, 9th U.S. National Combustion Meeting (2015) Paper 114LF-0349
[2] J. Pan, H. Wei, G. Shu, Z. Chen, P. Zhao, Combust. Flame 174 (2016) 179–193

Hands-on

From the command line of the terminal, type

- Load Cantera

```
source /opt/cantera-2.4/bin/setup_cantera
```

- List the examples provided by Cantera

```
ls /opt/cantera-2.4/lib/python3.5/site-packages/cantera/examples/
```

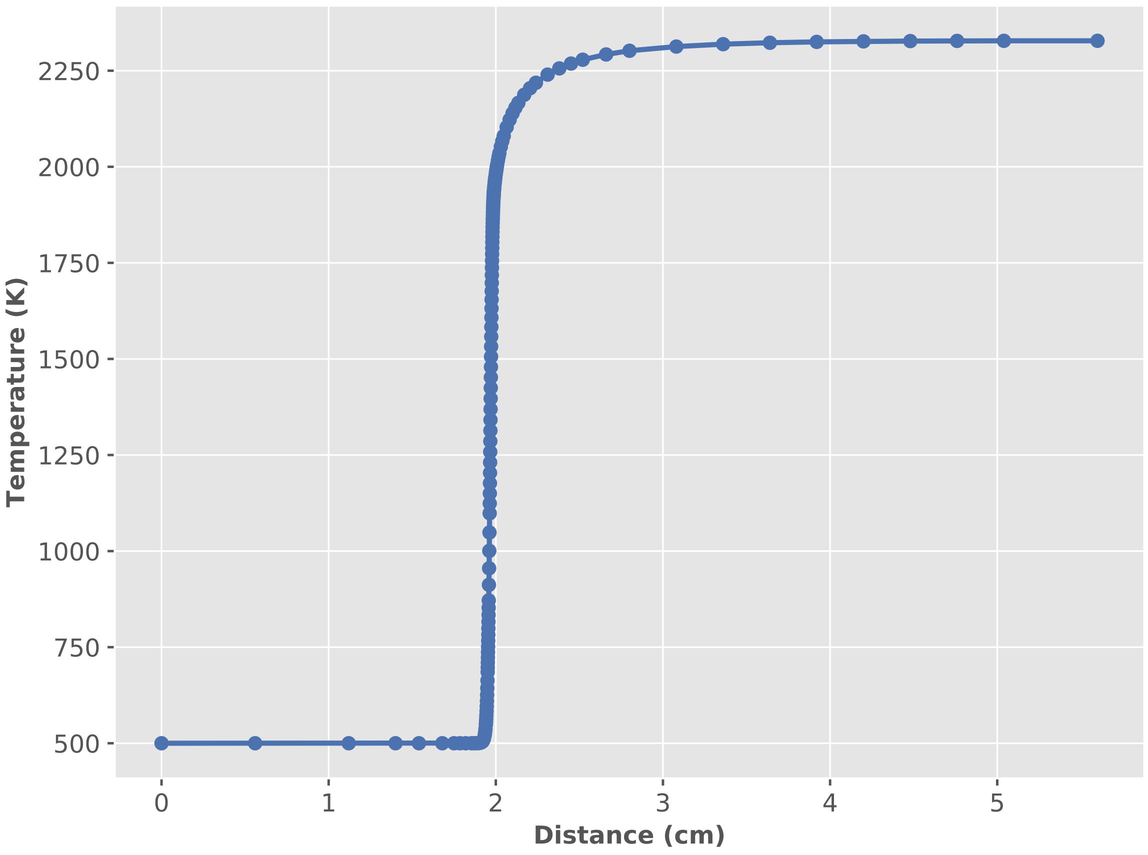
>> kinetics/ multiphase/ onedim/ reactors/ surface_chemistry/ thermo/ transport/

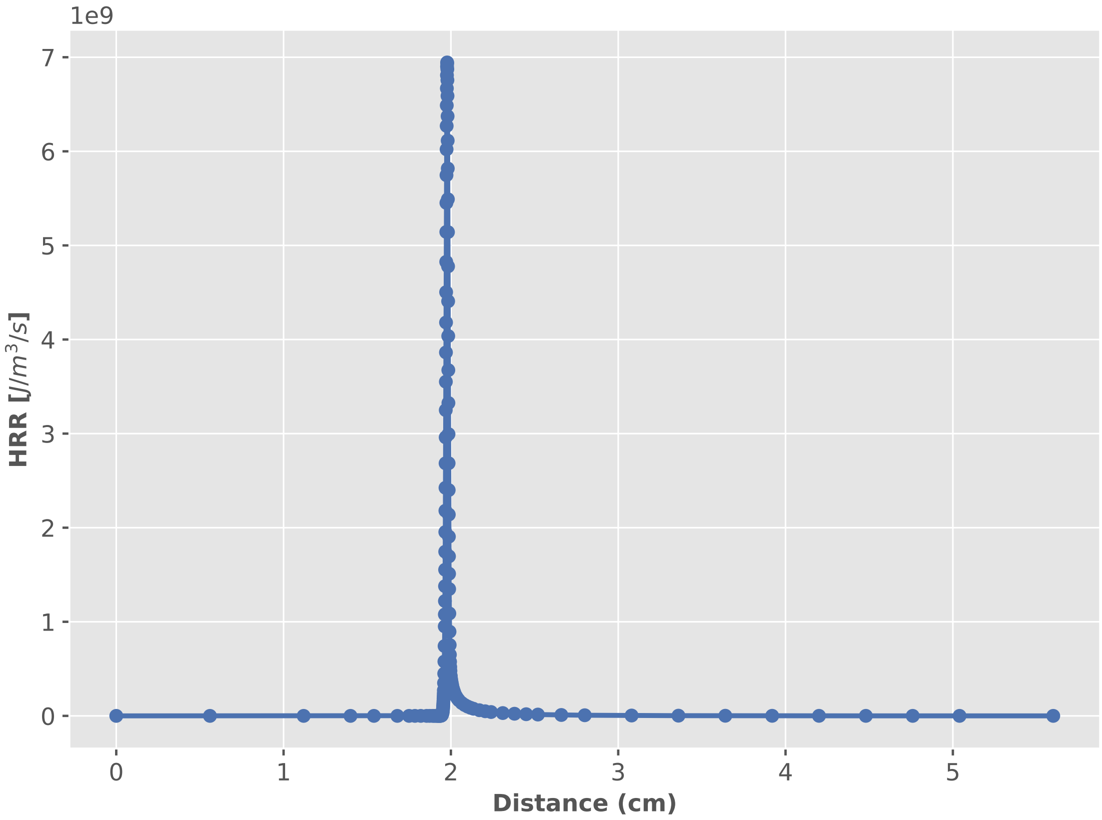
- **Run an example test**

```
cd $HOME/cantera_tutorial_CCRC_winterSchool
git pull
source /opt/cantera-2.4/bin/setup_cantera
python3 flame_speed_with_sensitivity_analysis_rev.py
python3 1dPremixedFlame.py
```

https://github.com/minhbau/cantera_tutorial_CCRC_winterSchool.git

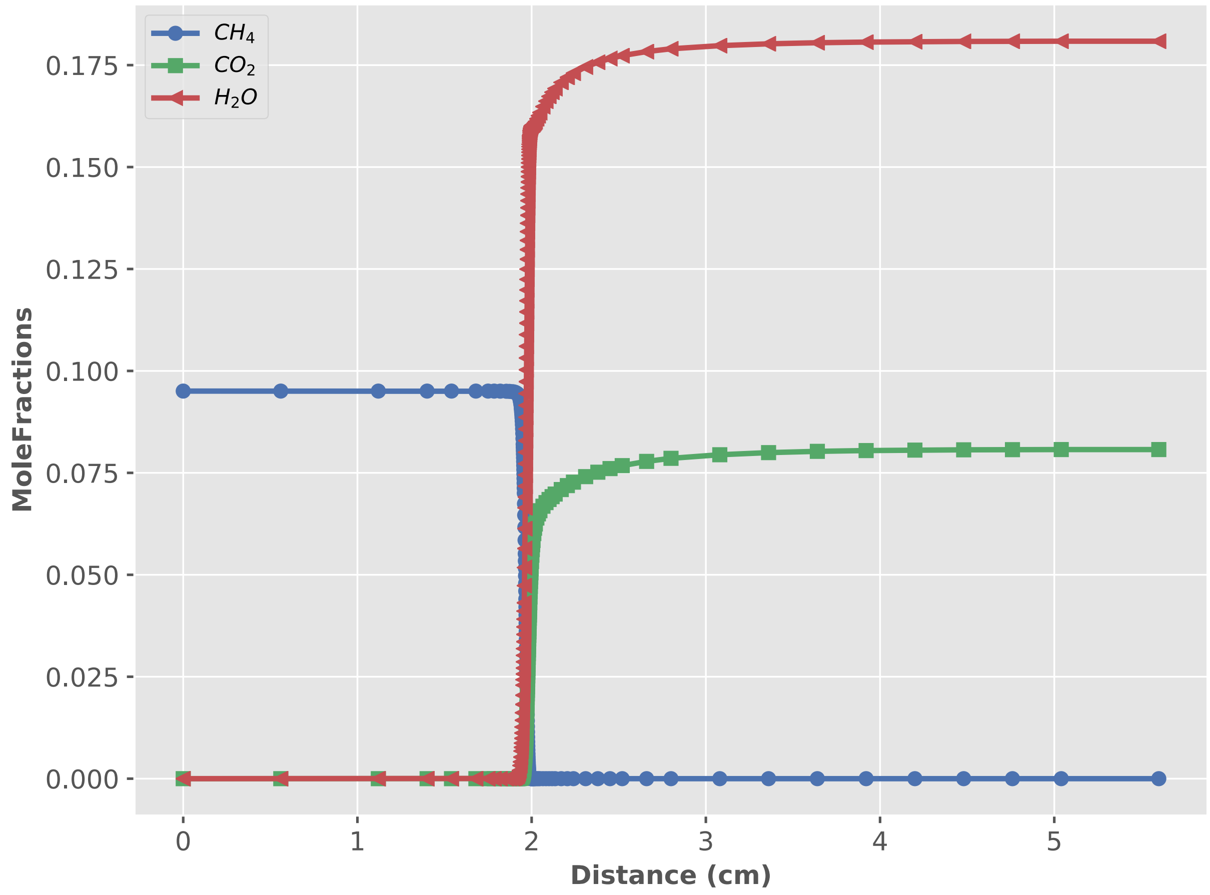
1-D Flame Example

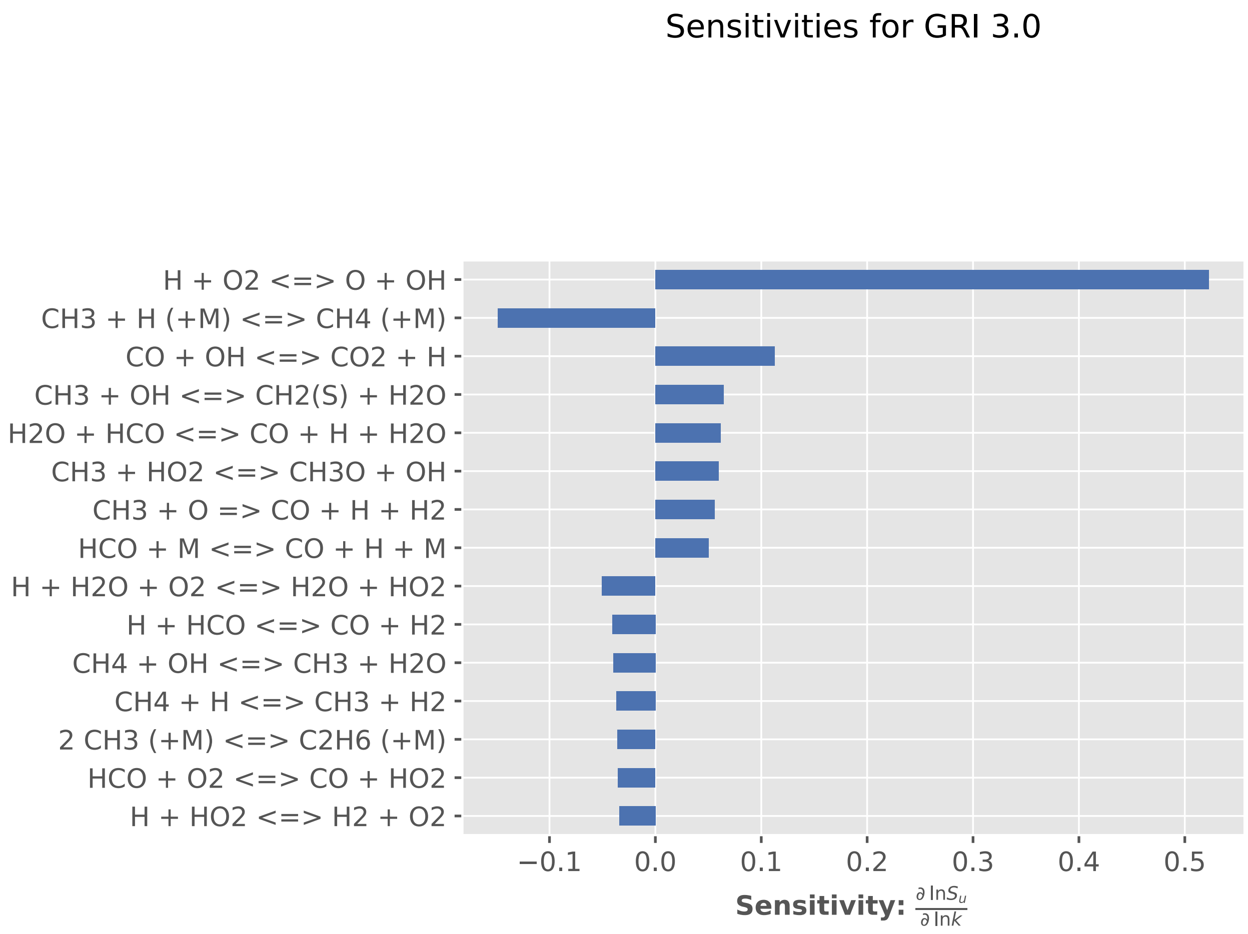





```
python3 flame_speed_with_sensitivity_analysis_rev.py
```

1-D Flame Example






```
python3 flame_speed_with_sensitivity_analysis_rev.py
```

Thank you for your attention !!!

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