Development of a reduction tool for complex fuels chemical kinetics

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Abstract:

The numerical prediction of pollutant emissions or bio-fuel flame structure in industrial combustors such as aeronautical engines, ground-based gas turbines or furnaces, requires an accurate description of combustion chemistry. Such precision may be achieved with detailed chemical kinetics mechanisms which have been developed in order to accurately capture all the details of the combustion process over a wide range of thermodynamic conditions. However, these mechanisms involve many species and reactions, making them too expensive for numerical simulation of 3D industrial cases. One solution to this problem is to reduce the complexity by targeting a specific operating range of temperature, pressure, and equivalence ratio, representative of the real case, as well as specific species that are of importance if one wants to account for NO_x or soot production for example.
Such reduced mechanisms have been successfully derived using the multi-stage reduction code YARC [1] with the following procedure. First, Direct Relation Graph with Error Propagation (DRGEP) [2] is applied on species and reactions with specified species as targets (typically fuel, oxidizer, and pollutants of interest), followed by chemical lumping, resulting in a skeletal mechanism accounting for the relevant species and reactions only. Finally, a timescale analysis along with DRGEP is used to identify species that can be set in Quasi-Steady State (QSS) in order to further speed up the calculation.
In collaboration with Pr. P. Pepiot, a new automatic reduction tool called ARCANE has been developed to make it more efficient, more flexible and easier to use. ARCANE relies on the Cantera chemistry solver [3] and is written in Python language. ARCANE tool has been benchmarked against YARC on canonical cases validating it.
This talk will first present the main features of ARCANE. Then, an example of reduction for methane-air combustion will be presented. Analytically Reduced Chemistries (ARC) are first compared to detailed mechanisms on 0D reactor and 1D flame configurations in the target operating range, and confirm that the error induced by the reduction is small enough to correctly capture important features such as intermediate species profiles, ignition delay time and laminar flame speed. Finally, several strategies to model complex fuels such as kerosene in the scope of Large Eddy Simulation (LES) will be presented: n-decane ($C_{10}H_{22}$) as a mono-component surrogate of kerosene, the HyChem mono-component model [4,5] but accounting for the full composition of kerosene, and finally the multi-component approach. This latter is necessary to study the impact of alternative fuel addition to Jet A1 on the operability of an aeronautical combustor, which is one main objective of the H2020 JETSCREEN European project.

[1] Pepiot-Desjardins, P. (2008). Automatic strategies to model transportation fuel surrogates. *Stanford University*, (June).
[2] Pepiot-Desjardins, P., & Pitsch, H. (2008). An efficient error-propagation-based reduction method for large chemical kinetic mechanisms. *Combustion and Flame*, *154*(1–2), 67–81.
[3] David G. Goodwin, Harry K. Moffat, and Raymond L. Speth. *Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes*. https://www.cantera.org, 2018. Version 2.4.0.
[4] Felden, A., Riber, E., Cuenot, B., Esclapez, L., & Wang, H. (2017). Including real fuel chemistry in LES of turbulent combustion. *Proceedings of the CTR summer program*.
[5] Xu, R., Chen, D., Wang, K., Tao, Y., Shao, J., Parise, T., … Wang, H. (2017). HyChem Model: Application to Petroleum- Derived Jet Fuels. *10th U.S. National Combustion Meeting*, (April).

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Development of an automatic tool for the reduction of complex fuels chemical kinetics

Quentin Cazères, 2nd year PhD

CERFACS

Advisors : Eléonore Riber, Bénédicte Cuenot

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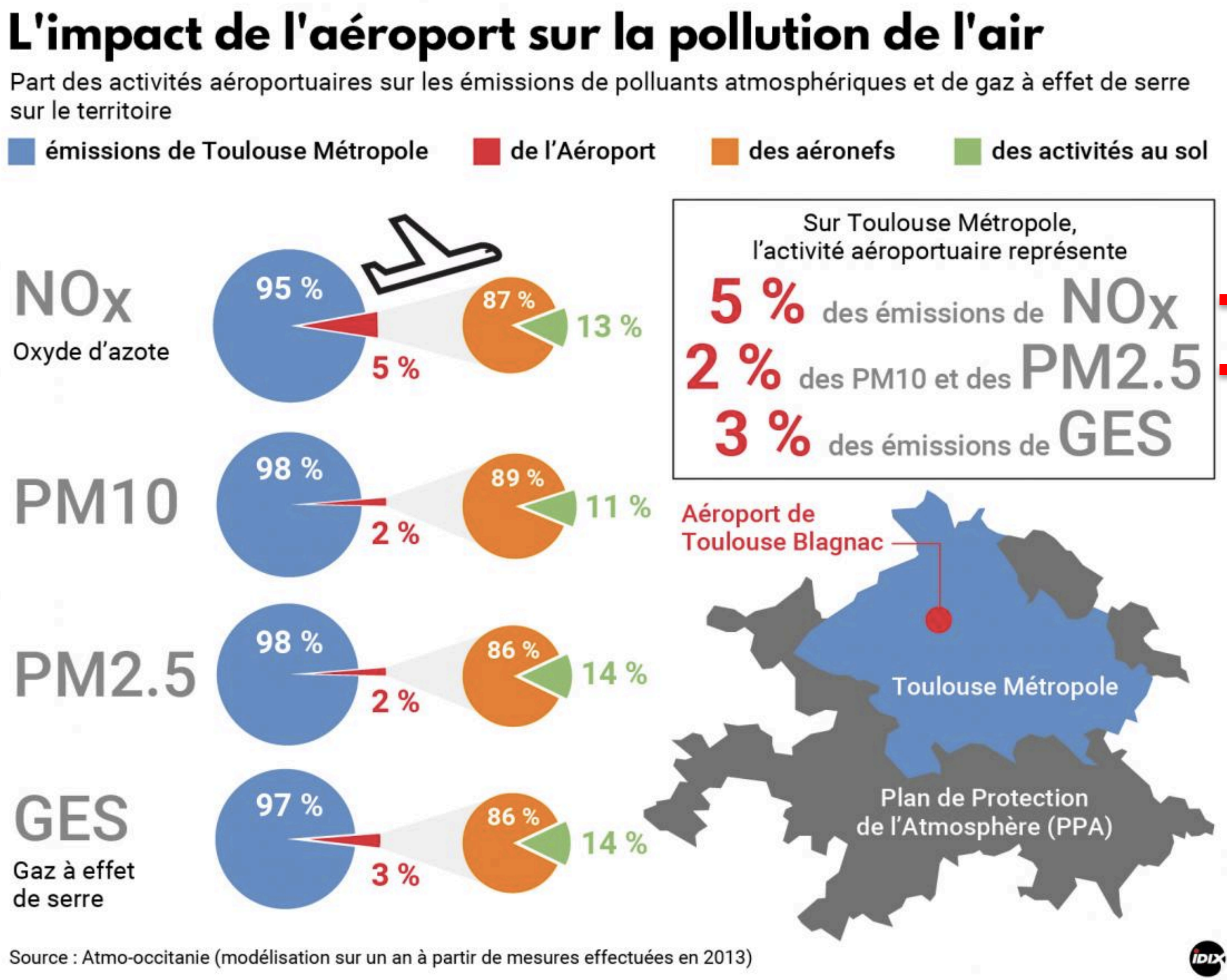
Why do we need complex chemistry ?



Can only be predicted if complex chemistry is accounted for in CFD solvers

Why do we reduce chemistry ?

Number of equations to solve = 5 + N_s Chemistry

Mass (ρ), Momentum ($\rho u, \rho v, \rho w$), Energy (ρE)

Simplest detailed mechanism: H2 + air → N_s = 12

H2 H O2 OH O H2O HO2 H2O2 N2

Intensively used mechanism GRI Mech 3.0: Methane + air → N_s = 53

H2 H O O2 OH H2O HO2 H2O2 C CH
CH2 CH2(S) CH3 CH4 CO CO2 HCO CH2O CH2OH CH3O
CH3OH C2H C2H2 C2H3 C2H4 C2H5 C2H6 HCCO CH2CO HCCOH
N NH NH2 NH3 NNH NO NO2 N2O HNO CN
HCN H2CN HCNN HCNO HOCN HNCO NCO N2 AR C3H7

Mechanism for biodiesel + air → N_s = 3299

Not going to show that !

Outline

- ARC methodology
- ARCANE : new reduction tool
  - Presentation
  - Examples
- ARC for kerosene modelling
- Conclusion and PhD continuation

Different levels of kinetics

Detailed mechanism

> 100 species, 1000 reactions

Does everything

-You can study species you never knew existed

- Too expensive for most people

ARC

~ 20 species, 200 reactions

Tailored for your needs

- Basic combustion features
- Pollutants (CO, NO_x, soot)
- Affordable

Global

6 species, 2 reactions

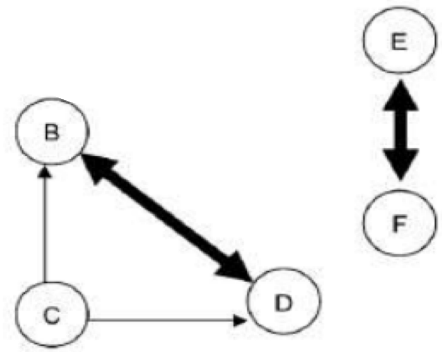
Does the job

- Laminar flame speed
- Adiabatic flame temperature
- Cheap

3 main reduction techniques :

Direct Relation Graph (DRG):

Contribution of A to the production of B



Chemical lumping:

$$[S_1] + [S_2] = [S_{lumped}]$$

$$[S_1] \xrightarrow{k_1} [S_3] \qquad [S_2] \xrightarrow{k_2} [S_4]$$

$$\Rightarrow \quad [S_{lumped}] \xrightarrow{\tilde{k}_1} [S_3] \qquad [S_{lumped}] \xrightarrow{\tilde{k}_2} [S_4]$$

Quasi-Steady State Assumption (QSSA):

$$\frac{d[S_{QSS}]}{dt} \approx 0$$

Set of linear equations to compute $[S_{QSS}]$
→ S_{QSS} is no longer transported
and its equation is no longer solved

ARCANE : new reduction tool

All reductions at CERFACS were performed with the YARC reduction tool (P. Pepiot's PhD thesis)

In Collaboration with Pr. Perrine Pepiot (Cornell University)
→ New reduction tool :

ARCANE

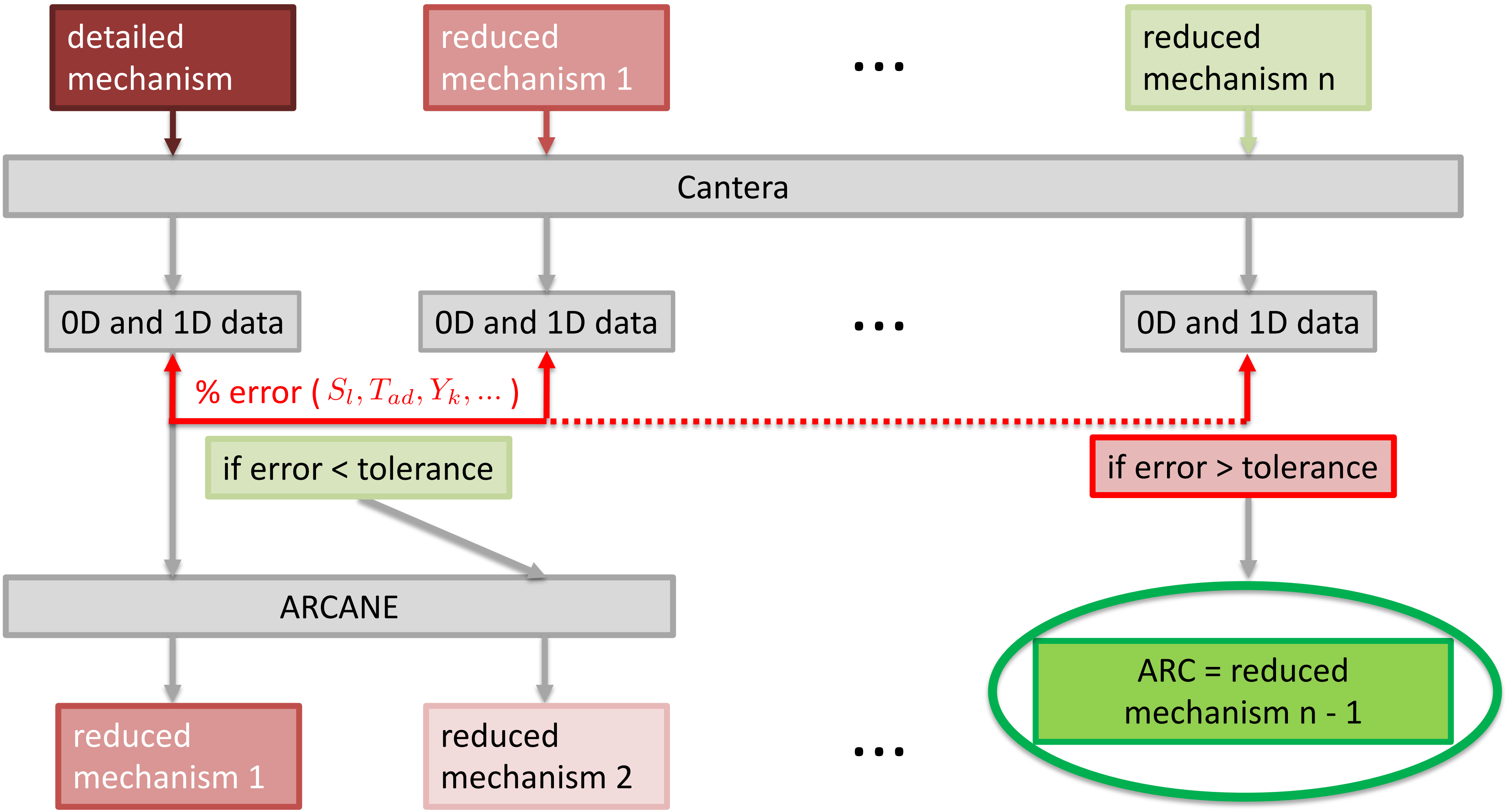
Analytically Reduced Chemistry: Automatic, Nice and Efficient

Relying on **Cantera chemistry solver** and written in **Python** :

- Compatible with CERFACS version of Cantera tailored for its needs

- User friendly language (python) for feature implementation

ARCANE structure



Advantages

Same reduction methods as YARC based on FlameMaster

+ Functions used for the reduction process can be used independently for deep kinetics insight

+ Use through python allowing direct pre/post-processing

+ The full reduction process is made automatic

+ Reduction possible on every case that you can create on Cantera (complex reactor Network with valves and flow controllers)

+ Output f90 files for AVBP use

Methane-air combustion case

Target cases :
- 0D isochoric reactor T = 1000 K, P = 1 bar, phi = 1
- 1D premixed freely propagating flame T = 400 K, P = 1 bar, phi = 0.6, 1, 1.6

Reduction targets : $CH_4, CO_2, CO,$ Heat Release

Error evaluation : - ignition delay time for 0D case
- laminar flame speed for 1D cases

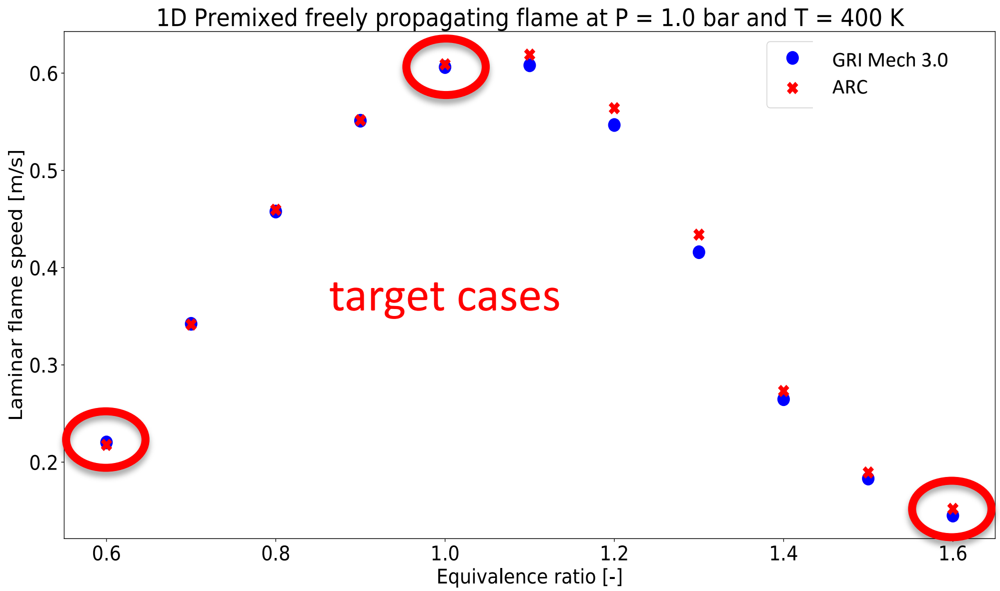
Initial mechanism : GRI Mech 3.0 : 53 species, 325 reactions

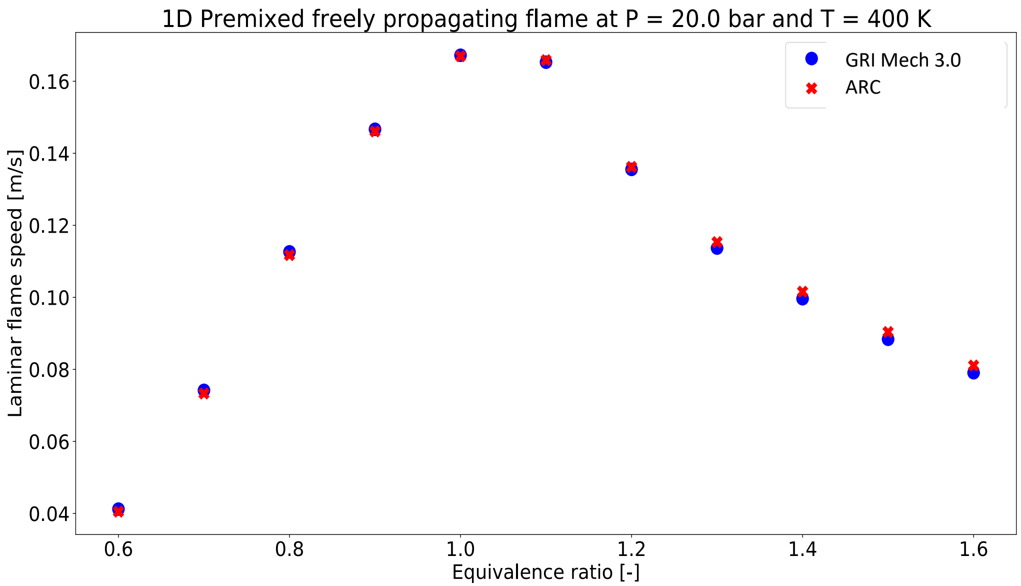
ARC : 22 transported species, 7 QSS species, 165 reactions

Methane-air combustion case

Derivation configuration
+ operational conditions of derivation

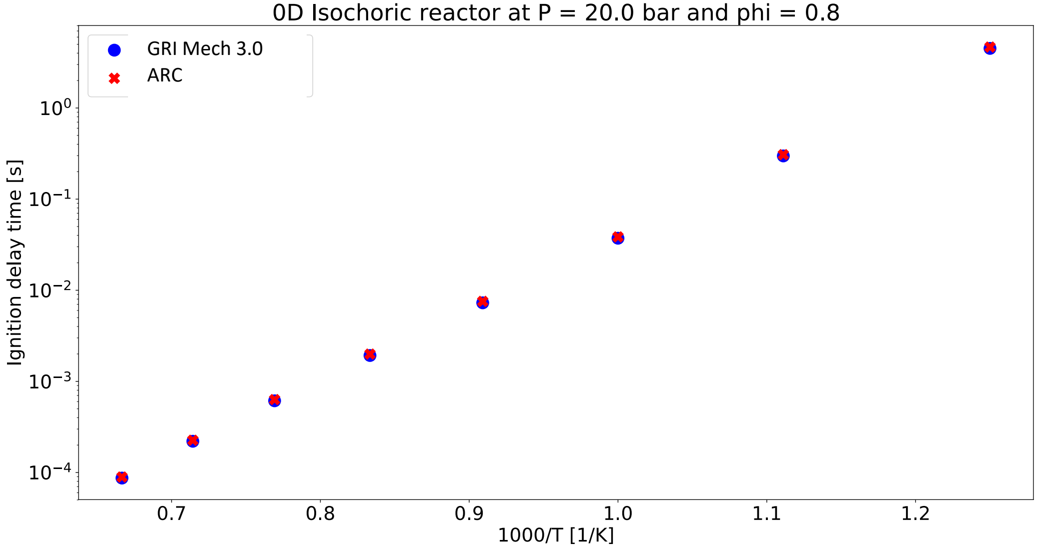
Same configuration BUT
High pressure



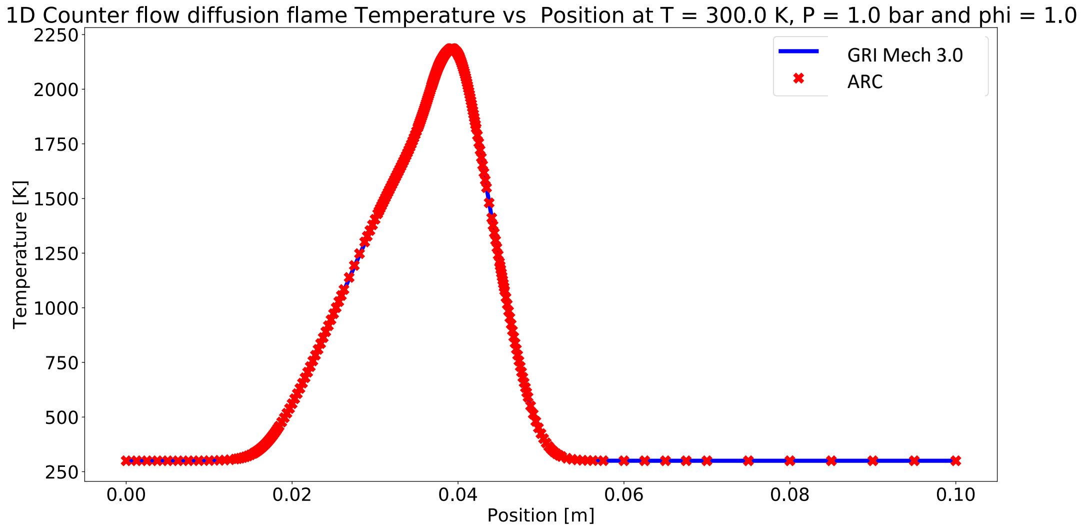


ARC chemistry is robust to operational conditions

Methane combustion case



ARC chemistry robust to configuration

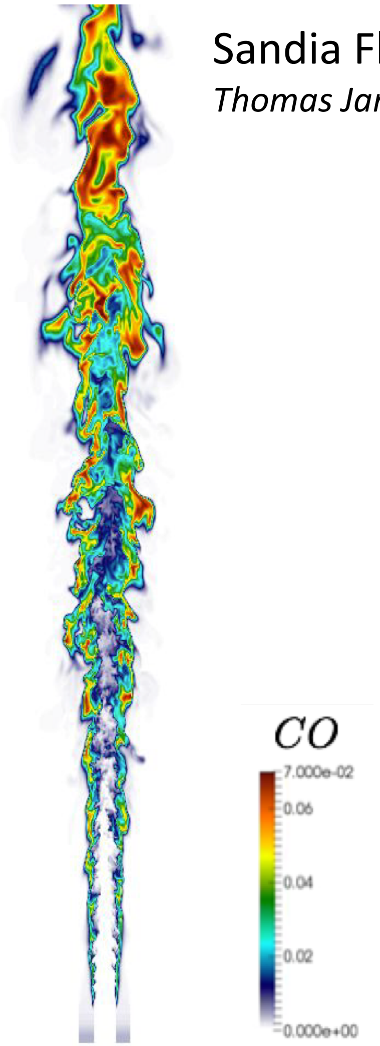


Input script :

```
"""Full reduction of GRI Mech 3.0"""

# Import statements

# ARCANE module
import reduction.cases as cases
import reduction.mechanisms as mechanisms
import reduction.automatic as automatic

# Cantera module
import cantera as ct

# User-specified: initial mechanism
cti = "gri30.cti"
ctmech = ct.Solution(cti)

cases.init_case_database(casedir='cases_GRI')

caselist = []
caselist.extend(cases.create_case(reactor="0DIsochor",
                                  ctmech=ctmech,
                                  fuel='X/CH4/1',
                                  oxidizer="X/O2/0.21/N2/0.79",
                                  pressure="1e5",
                                  temperature="1000",
                                  phi="1",
                                  targets=["CH4", "CO2", "CO", "HeatRelease"]))

caselist.extend(cases.create_case(reactor="1DPremixed",
                                  ctmech=ctmech,
                                  fuel="X/CH4/1",
                                  oxidizer="X/O2/0.21/N2/0.79",
                                  pressure="1e5",
                                  temperature="400",
                                  phi="0.6-1-1.6",
                                  targets=["CH4", "CO2", "CO", "HeatRelease"]))

# Create reference mechanism instance
root_mechanism = mechanisms.Mechanism(ctmech=ctmech)

# Setup automatic reduction
auto = automatic.Automatic(caselist, root_mechanism)
auto.set_super_root_mechanism(root_mechanism)
mech_list = auto.full_reduction(max_errors=[0.01, 0.01, 0.05])
```

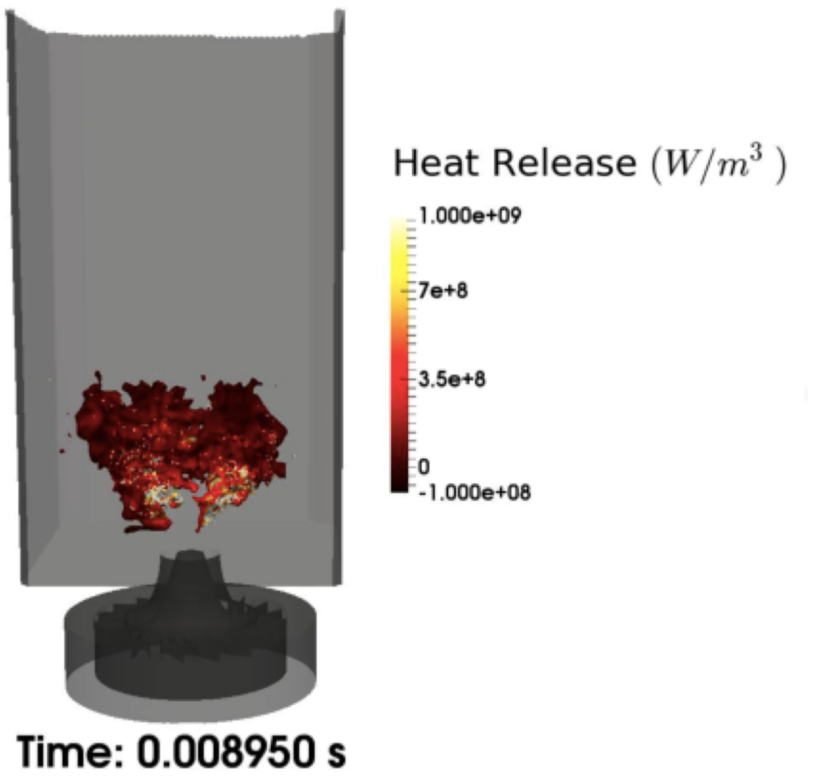
Time spent between pressing "enter" and results = 15 minutes

LES using ARCs



Sandia Flame D (methane + air)

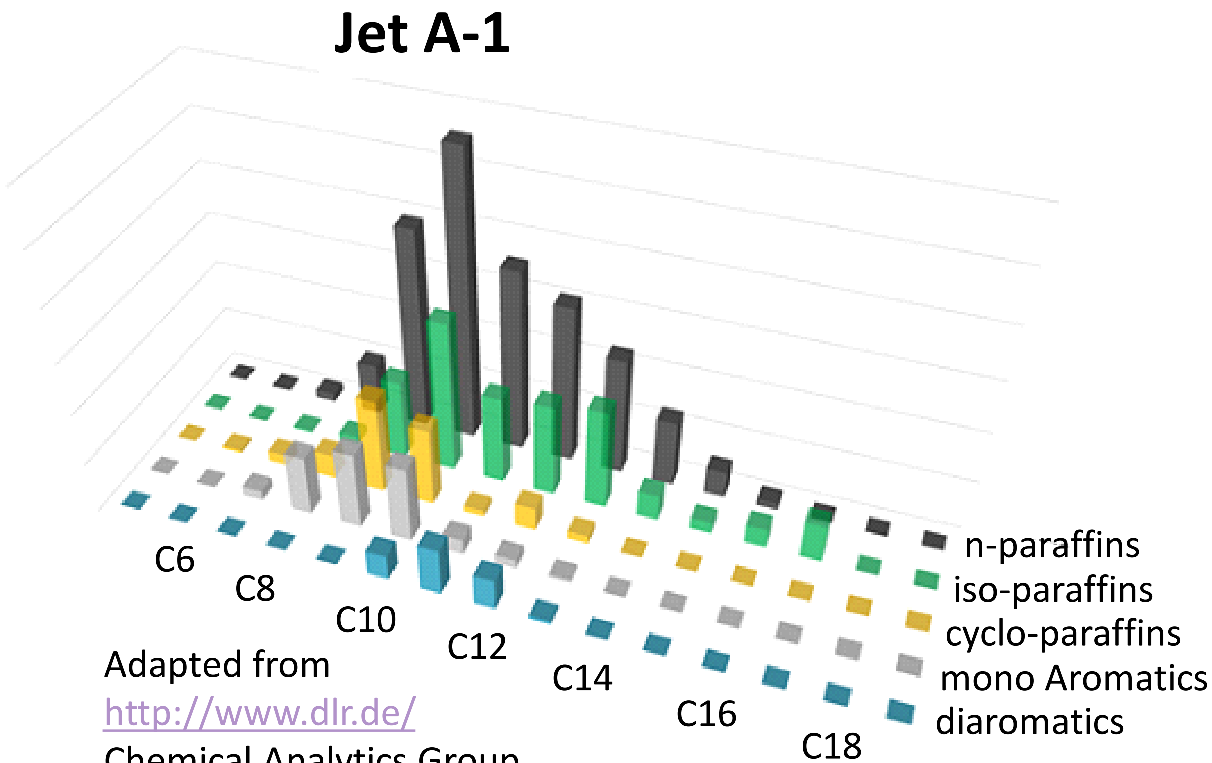
Thomas Jaravel's PhD thesis



KIAI burner ignition (n-heptane + air)

F. Collin-Bastiani et al., A joint experimental and numerical study of ignition in a spray burner, Proceedings of the Combustion Institute (2018)

Kerosene is a complex blend of many hydrocarbon species



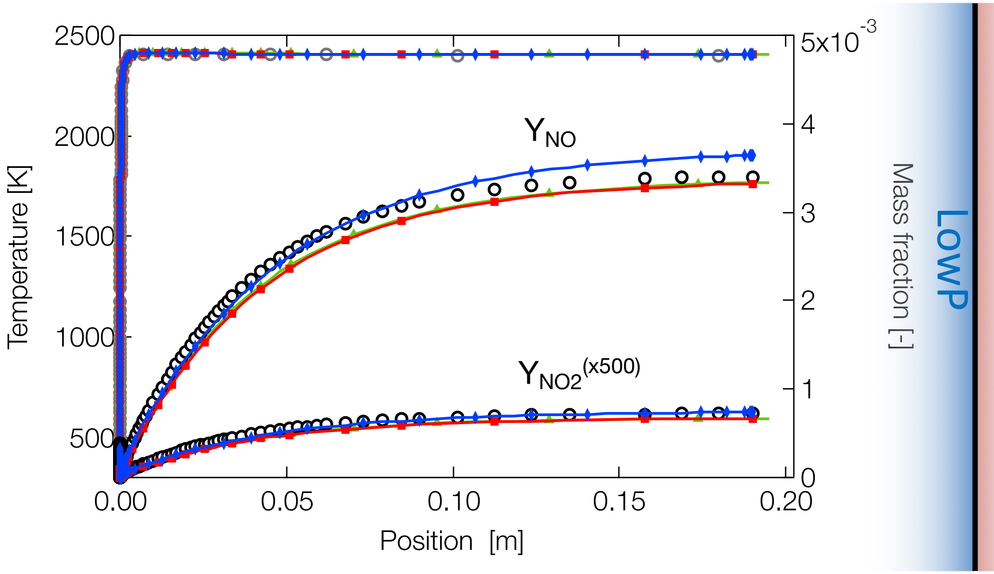
Adapted from
http://www.dlr.de/
Chemical Analytics Group

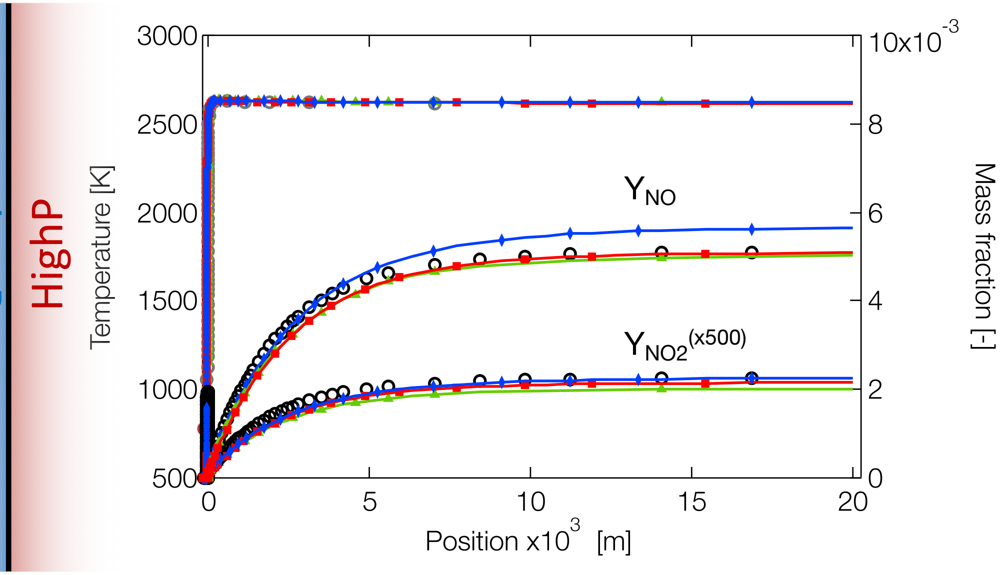
Pericles study (for SAFRAN)

Fuel : Decane (C10H22) as kerosene surrogate

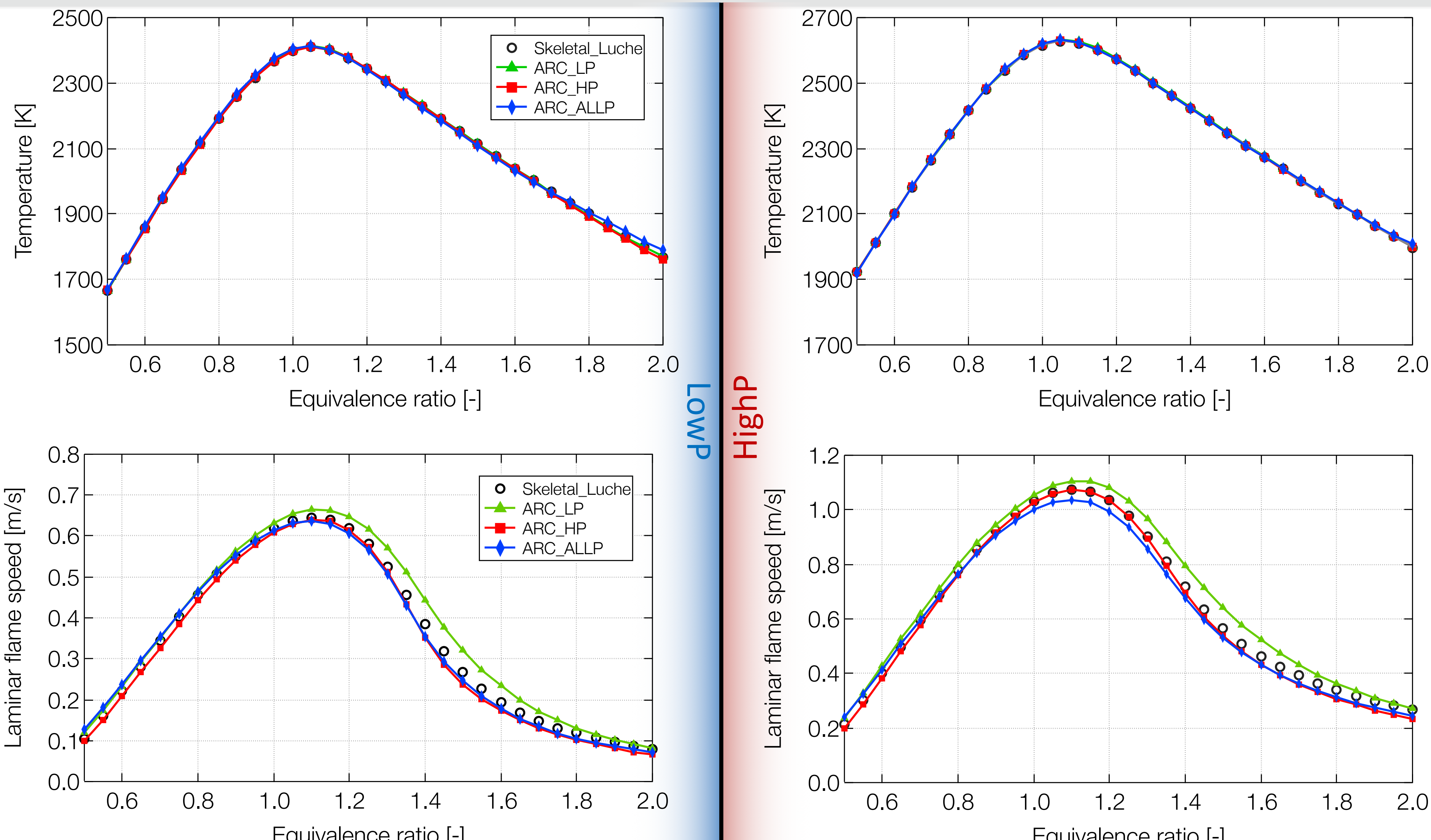
Designation	Pressure [Pa]	Temperature [K]
LowP	338 000	480
HighP	2 239 000	780

	Transported species	*Reac*	*QSS*
Luche	*89*	*680*	
ARC	*26*	*255*	*16*





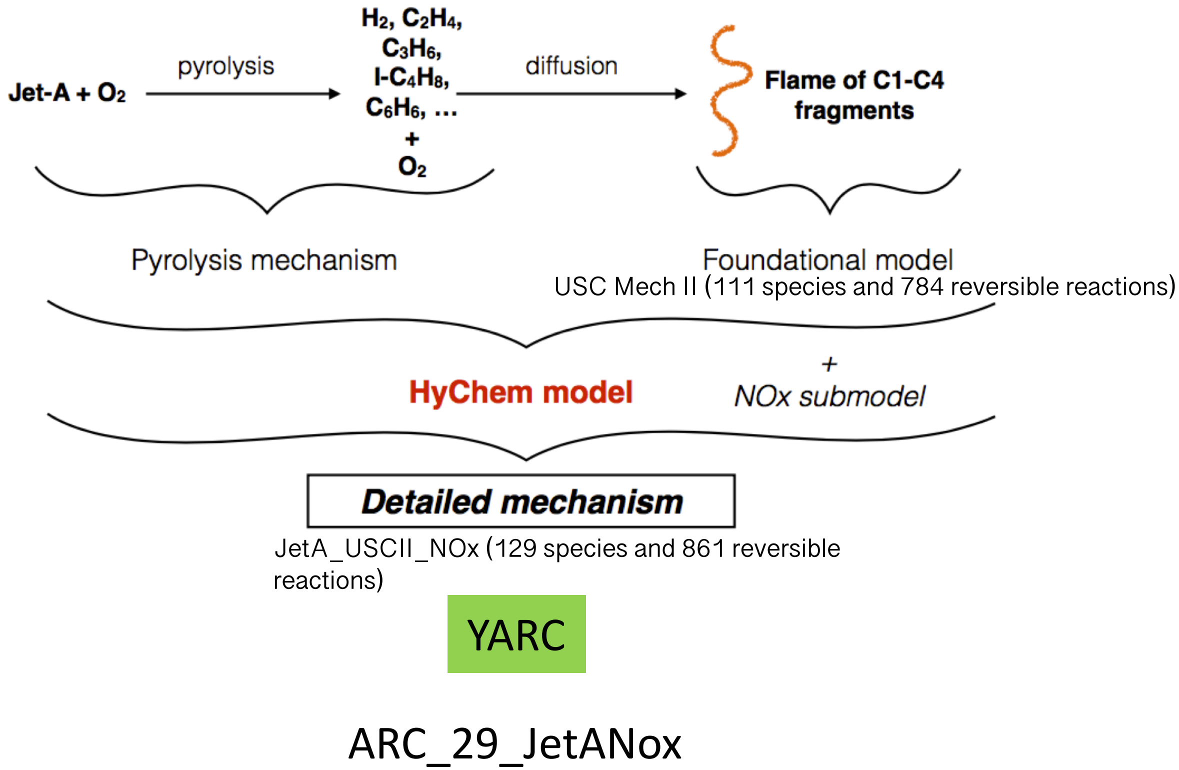
ARC for kerosene modelling
Single component fuel



ARC for kerosene modelling
HyChem model

HyChem model for Jet-A POSF10325 :

Assumption: Any fuel would first decompose into a handful of small molecules
→ Radical build-up and heat release rate ~ distribution of those pyrolysis products



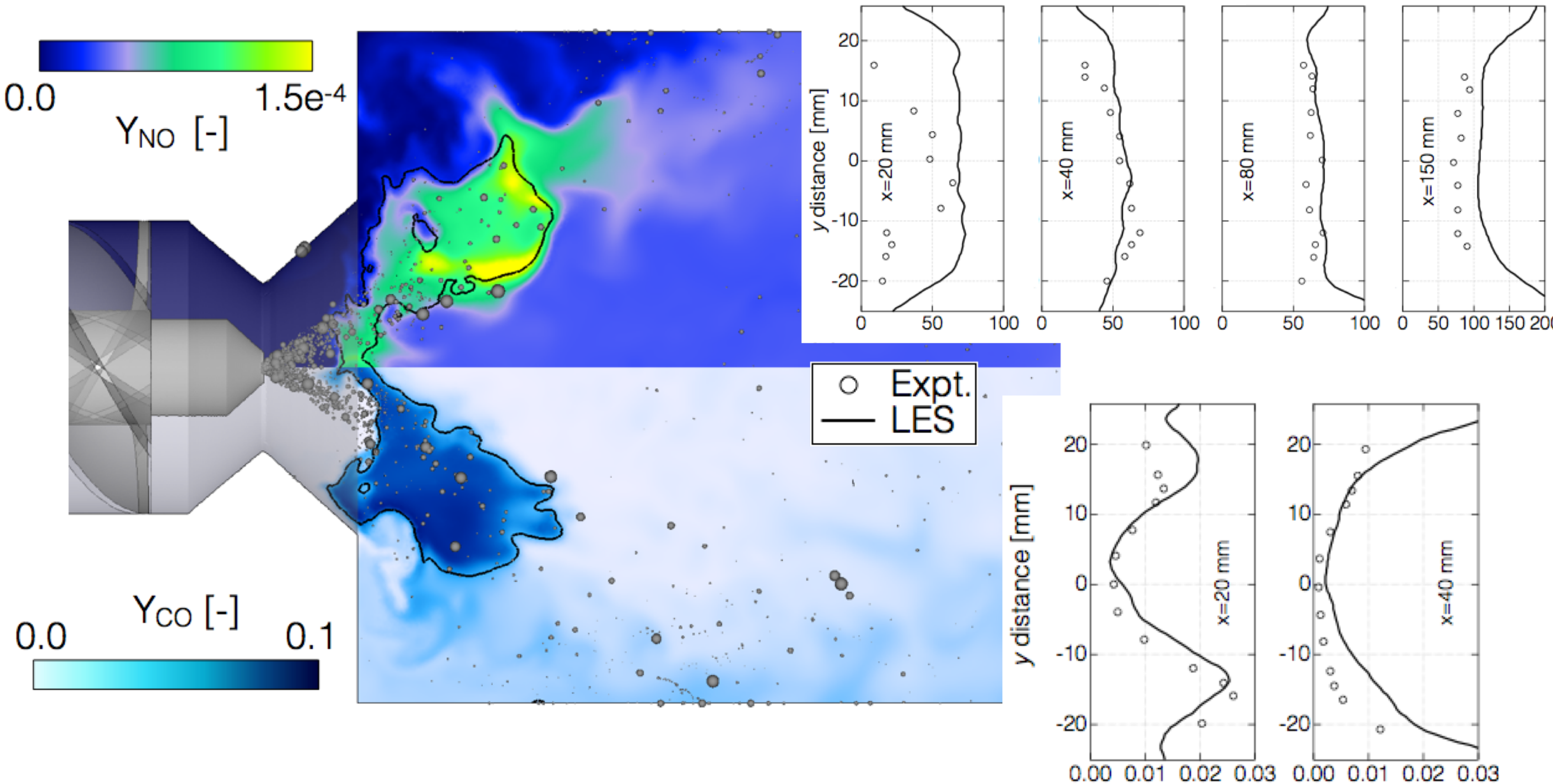
Transported species:

POSF10325 H H2 O OH O2 H2O H2O2 HO2 CO CH2O C2H2 CH3 CO2 CH4 C2H4 C2H6 CH2CO C3H6 I-C4H8 C5H6 C6H6 C7H8 C6H5O C6H4O2 NO HCN NO2

QSS species:

CH HCO CH2 CH2* CH3O C2H5 C2H3 HCCO A-C3H5 CH2CHO C6H5 N NCO H2CN CN NH HNO

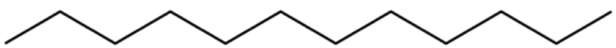
ARC for kerosene modelling
HyChem model



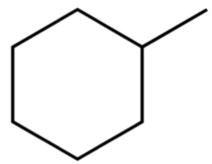
* from Anne Felden's PhD thesis

ARC for kerosene modelling
Multi-component fuel

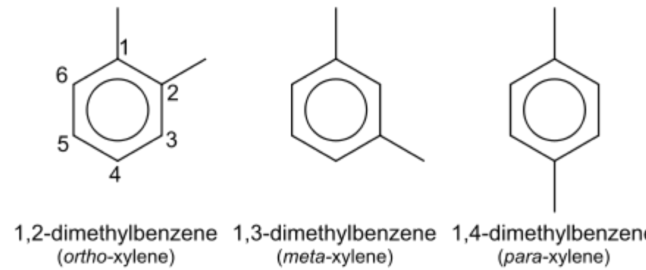
In literature, Jet A best represented by a three component surrogate [1]



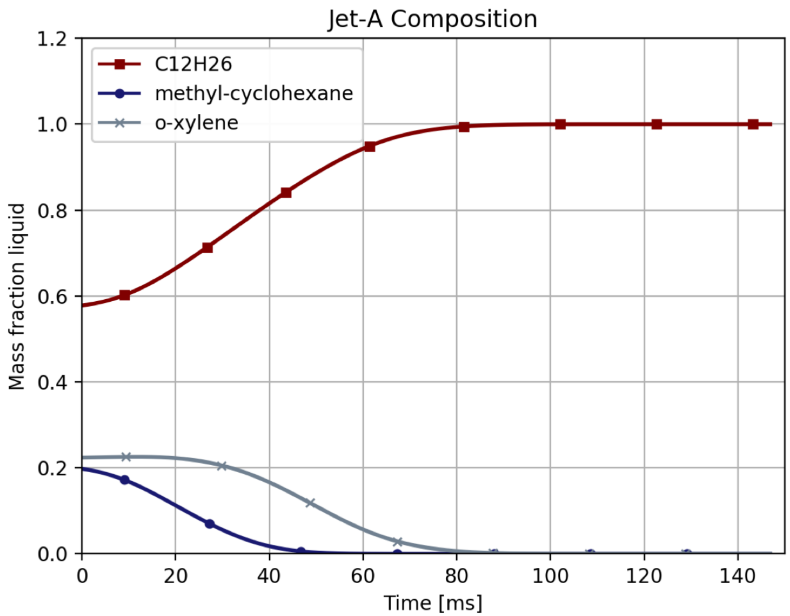
n-dodecane

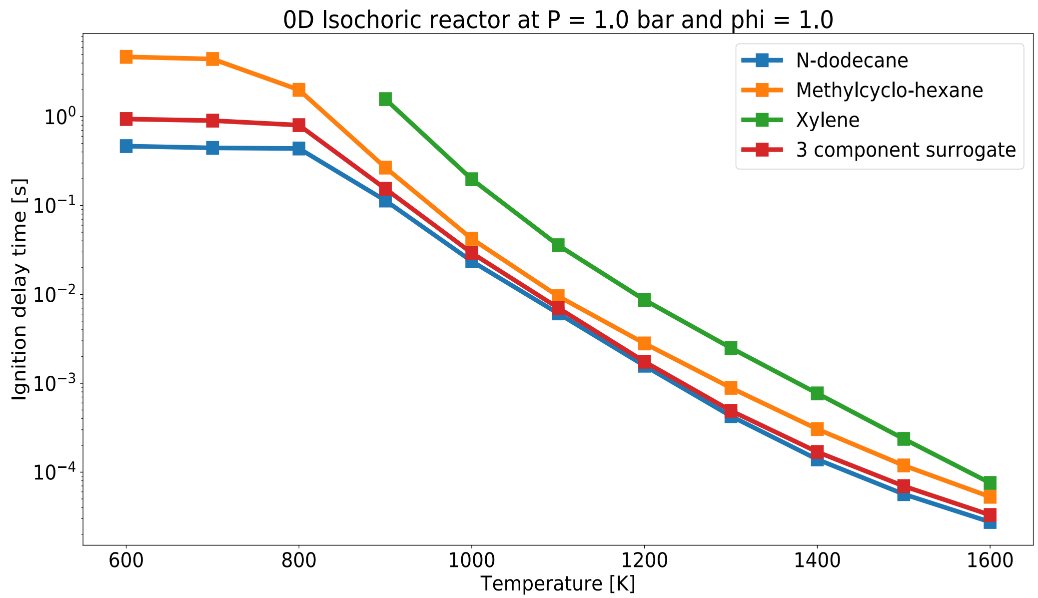


Methylcyclohexane



Xylene





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[1] K. Narayanaswamy, H. Pitsch, P. Pepiot, A component library framework for deriving kinetic mechanisms for multi-component fuel surrogates: Application for jet fuel surrogates, Combust. Flame 165 (2016) 288{ 309.

JETSCREEN

Multi-component fuel

- The HyChem model requires pyrolysis data and cannot account for multi-components evaporation.

- This model was used because YARC was not able to reduce enough the multi-component fuel to a “LES-friendly” size (< 60 species in the skeletal mechanism)

→ Better results expected with ARCANE because its flexibility will allow more complex reductions

- easier analysis of kinetics data
- new reduction algorithms can be implemented (PCA, CSP, ...)
- more accurate error assessment

My PhD :

PhD financed by the JETSCREEN European project (CERFACS, DLR, Safran AE, Safran Tech, ...)

This project aims at creating a platform comparing alternative jet fuels at classical ones on many aspects (Ignition, Lean Blow Out and Thermo-acoustic instabilities).

Alternative fuels addition:

Jet A1 + $C_xH_yO_z$ → more difficult because pyrolysis step will no be similar

Multi-component approach will be needed as no single component surrogate is possible

Conclusions and PhD continuation

Improved reduction tool, ARCANE

- No need for advanced chemical kinetics knowledge for reducing simple fuels
- Easier reduction of complex multi-component fuels
- Better control of the error metric
- More insight on the reduction process
- Reduction on non-classical cases (Complex reactor networks)

Multi-component ARC is the next step in complex chemistry modelling

Conclusions and PhD continuation

<u>In the following of my PhD:</u>

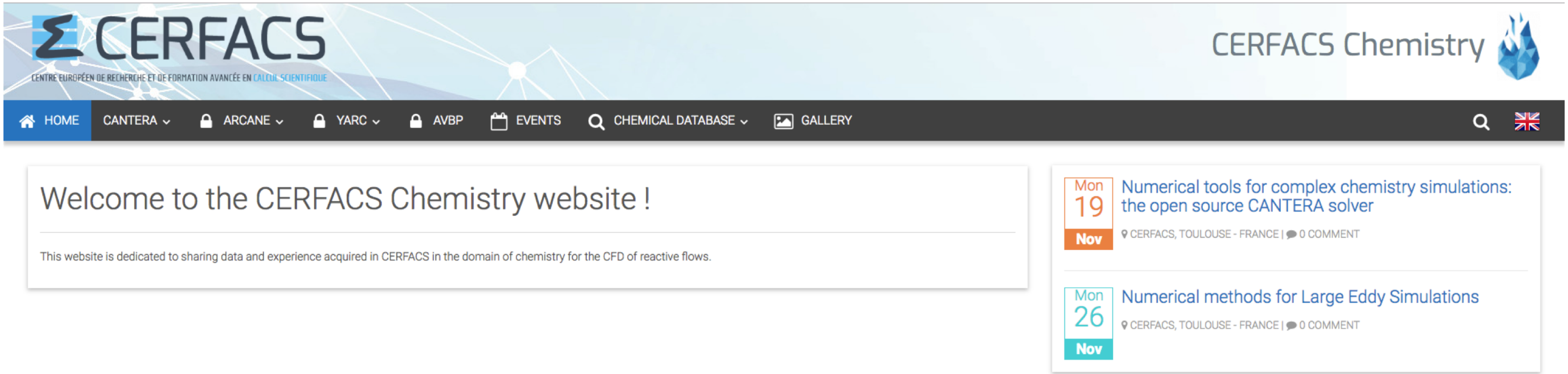
Study of chemistry modelling effects on two-phase flames (1D cases) with AVBP

Study of ignition in the MERCATO configuration (ONERA) with ARC chemistry of alternative fuels

CERFACS Chemistry website

Sharing our experience

CERFACS Chemistry website https://chemistry.cerfacs.fr/en/



Will replace the old website : http://www.cerfacs.fr/cantera/description.php

Chemical kinetics mechanisms database available

Still work in progress for the tutorials and scripts sharing

CERFACS Chemistry website
Chemical database

HOME | CANTERA | ARCANE | YARC | AVBP | EVENTS | CHEM

/ CHEMICAL DATABASE / Data table

Data table

Combustion

Fuel	Oxidizer	========	=======	=====	======
hydrogen (H2)	air	Detailed	Skeletal		
methane (CH4)	air	Detailed		ARC	Global
	oxygen		Skeletal		
ethylene (C2H4)	air	Detailed	Skeletal	ARC	Global
propane (C3H8)	air	Detailed	Skeletal	ARC	Global
iso-octane (C8H18)	air	Detailed		ARC	Global
kerosene	air	Detailed	Skeletal	ARC	Global

Combustion sub-mechanisms (must be added to a base mechanism)

Nitrogen sub-mechanisms

Cracking

Fuel	Oxidizer	=======
ethane (C2H6)	water	Skeletal

Pyrolysis

Fuel	======
methane (CH4)	Global

HOME | CANTERA | ARCANE | YARC | AVBP | EVENTS | CHEMICAL DATABASE | GALLERY

Mechanisms list

Here is a list of every mechanism available on this website

Detailed mechanisms :

GRI-Mech 3.0 (53 species and 325 reactions)

GRI-Mech 2.11 (49 species and 279 reactions)

San Diego (57 species in 268 reactions)

USC II (111 species and 784 reactions)

Wang (75 species and 529 reactions)

Curran (1034 species and 8453 reactions)

Anderlhor(536 species and 3000 reactions)

Jerzembeck (203 species and 1001 reactions)

Dagaut (225 species and 1800 reactions)

JetSurf (348 species and 2163 reactions)

Narayanaswamy (362 species and 1861 reactions)

Skeletal mechanisms :

Boivin (9 species and 12 reactions)

Frassoldati (10 species and 6 reactions)

Lu methane (30 species, 184 reactions)

Sankaran (17 species, 73 reactions)

Lu ethylene (32 species and 206 reactions)

Peters propane (31 species and 107 reactions)

C3H8_34_173_FC (34 transported species, 173 reactions)

Thank you,

Do you have any questions ?

Acknowledgements :

Jonathan Wirtz, Lucas Esclapez for the Pericles configuration