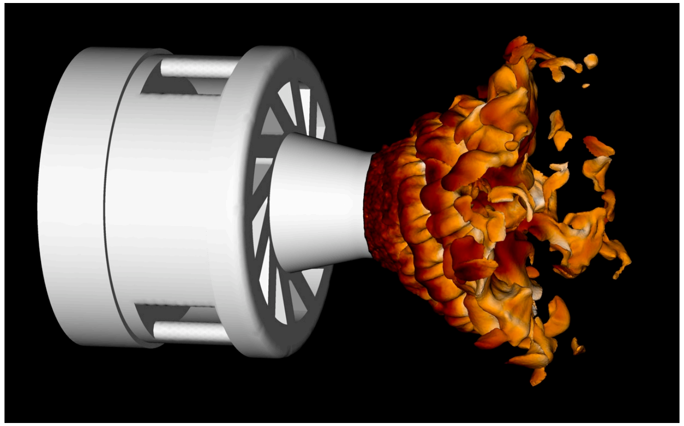
Biofuels: major issues in combustion



Nasser Darabiha

nasser.darabiha@em2c.ecp.fr

Ecole Centrale Paris, EM2C laboratory

Laboratoire d'Energétique Moléculaire et Macroscopique, Combustion

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Primary energy sources

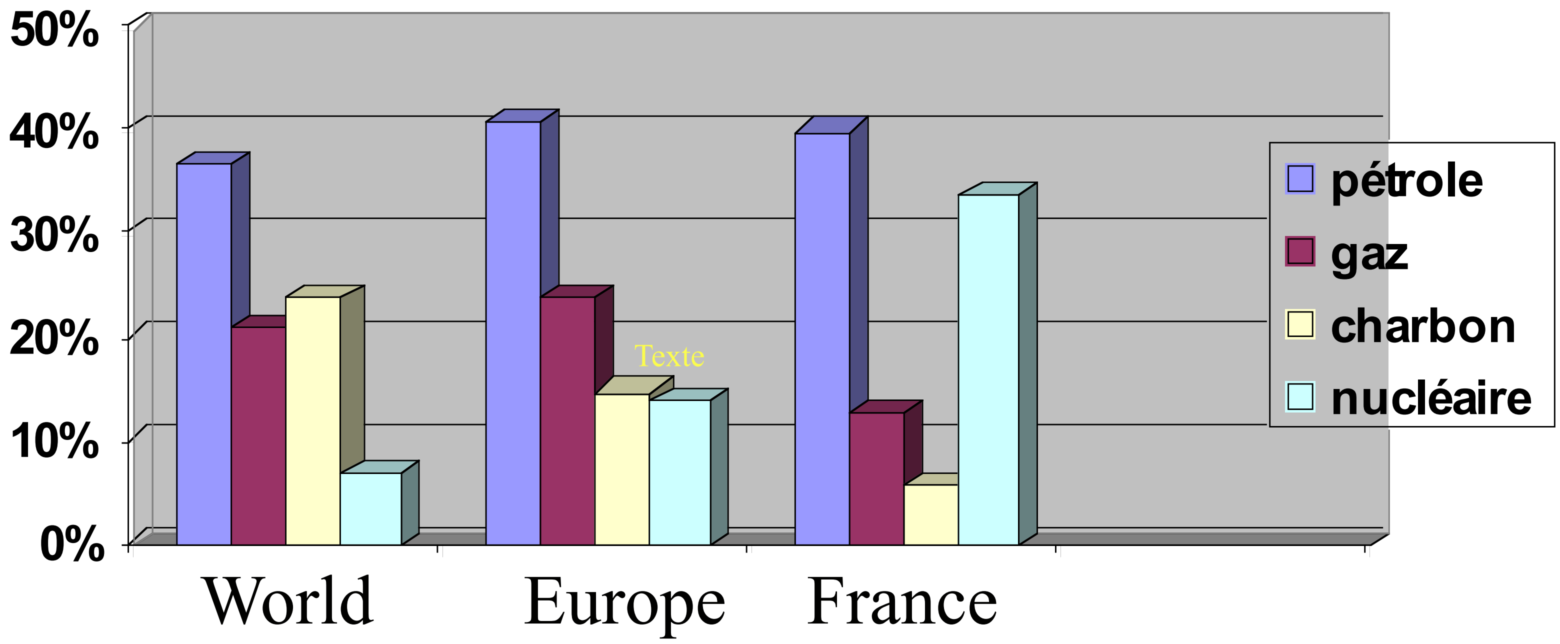


Figure 3 : Pourcentages de consommation d'énergie primaire issue du pétrole, gaz, charbon et uranium dans le monde, l'Union Européenne et la France.

Renewable energy sources<2%

(Source : rapport B. Tamain, MSTP)

Primary energy sources

source	**Pétrole**	**Gaz**	**Charbon**	**Nucléaire fission**	**Nucléaire fusion**	Total
Monde	37%	21%	24%	7%	0%	89%
Europe	41%	24%	15%	14%	0%	94%
France	39%	13%	6%	34%	0%	92%
Avantages	**Abondant** **coût** liquide	**Abondant** **coût** gazeux	**Abondant** **coût**	**Abondant** **coût**	**T. abondant** **coût**	
Inconvénients	**Réserves** **Effet serre** Pollution	**Réserves** **Effet serre**	**Réserves** **Effet serre** **Pollution**	**Réserves** **Déchets** Sûreté Rendement	Déchets **Non réussie**	
Réserves (en années de consommation actuelle)	*Prouvées* 40 ans *Ultimes* 135 ans	*Prouvées* 65 ans *Ultimes* 230 ans	*Prouvées* 220 ans *Ultimes* 1400 ans	*Prouvées* 70 (3000*) *Ultimes* 280 (12000*	**infinies**	

*ces chiffres ne tiennent compte que des réserves uranium terrestres. L'utilisation possible du thorium sera aussi possible ce qui multipliera ces chiffres par un facteur de l'ordre de 4: voir §4-c.

Tableau I : Importance relative des énerg ies fossiles dans la production globale d'énergie; avantages et inconvénients ; réserves prouvées et ultimes.

(Source : rapport B. Tamain, MSTP)

Let’s start with the power ...

Net calorific values

Fuel	net calorific value (MJ / kg)
methane (major compent of natural gas)	49
gasoline	42-45
diesel fuel	41-42
kerosene	43
H2	120

Hydrogen ?

➢ ***liquid fuel***

➢ ***Hydrogen***

500 km with a car

- *8 l / 100 km*
- *Heat power 45 000 kJ / kg*
- ρ *= 900 kg / m³*

Total energy
1600 MJoules

Liquid hydrocarbons
excellent energy/volume ratio

→ ***Bio-fuels!***

- *Heat power 120 000 kJ / kg*
- M_{H2} *= 2 g/mol*

For the same total enery:

- ***13.5 kg of hydrogène***
- ***150 m³ under 1 bar !!***
- ***200 litres under 750 bars !!!***

Problems :

- ***Production ?***
- ***Storage ?***
- ***Safety ?***

Environmental effects

- **Greenhouse effects**
  - *Carbon dioxide (CO_2 , H_2O ,CH_4)*
  - *Climate change*

Directly linked to hydrocarbon consumption

- *Reduce fuel consumption*
- *Burn fuels without carbon (H_2,…)*
- *CO_2 capture*

- **Pollution**
  - *Unburnt hydrocarbons (HC)*
  - *Carbon monoxide (CO)*
  - *Nitrogen oxides (NOx)*
  - *Sulfur oxides (SOx)*
  - *Particles…*

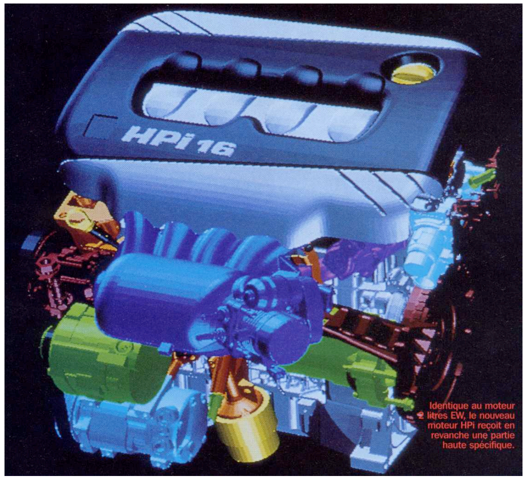
Dangerous in small quantities
(ppm to few hundreds of ppm)

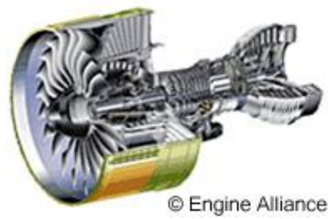
→ ***Combustion challenge***

- **Noise**

Applications

- Gas turbines
- Rocket engines
- Internal combustion engine
- Industrial furnaces
- Fire safety





New fuels ?

- ***Coal (only in power plants)***

- ***Bio-fuels***
  - *Cereals*
  - *Sugar beet, ...*
  - *Wood*

Problems :
- ***Efficiency ?***
- ***Available quantities ?***
- ***Pollution***

→ *Fuel dilution (15 % in 2015)*

- ***Hydrogen***
  - ***Production ?***
  - ***Storage ?***
  - ***Safety ?***

Spark ignition engines

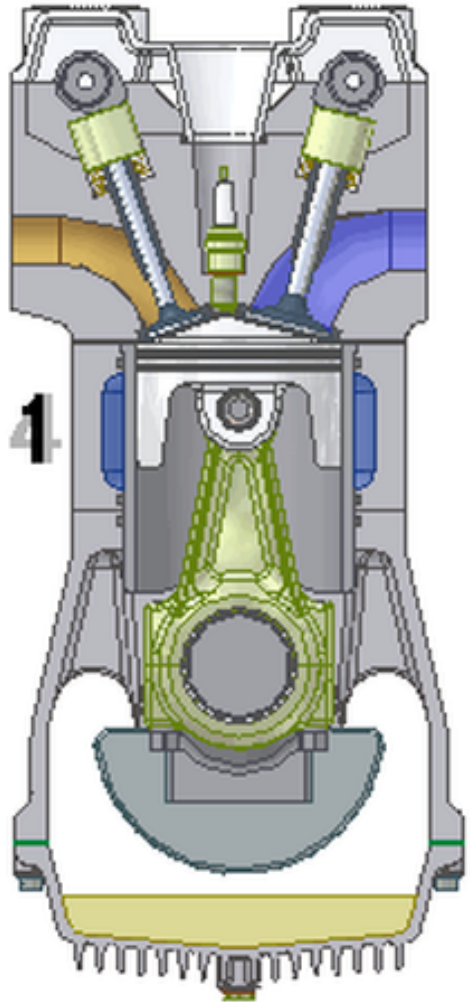
Technical challenges

- **Fuel and oxidizer premixing**
  - never perfectly premixed

- **Ignition stage control**
  - At the right time
  - Avoid auto-ignition phenomena

during the compression stage (pinking)

- **Combustion process**
  - full gas burning
  - Wall heat transfers
  - Pollutant formation



Diesel engines
Technical challenges

- **High pressure ratio**
  - increase efficiency (less CO_2 production)

- **Heterogeneous combustion (fuel and oxidizer are not premixed before combustion)**
  - High level of temperature (NO_x formation)
  - Combustion under rich conditions (soot, CO, un-burnt gases)

- **Auto-ignition**
  - no need of igniter
  - auto-ignition has to occur at the right time

Toward Diesel engines with homogeneous combustion regimes (Homogeneous Charge Combustion Engines)

- ***Homogeneous combustion***
  - ***Either direct injection earlier during the compression stage***
  - ***Or direct injection during the admission stage***

- **Faster combustion**
  - **Better efficiency**

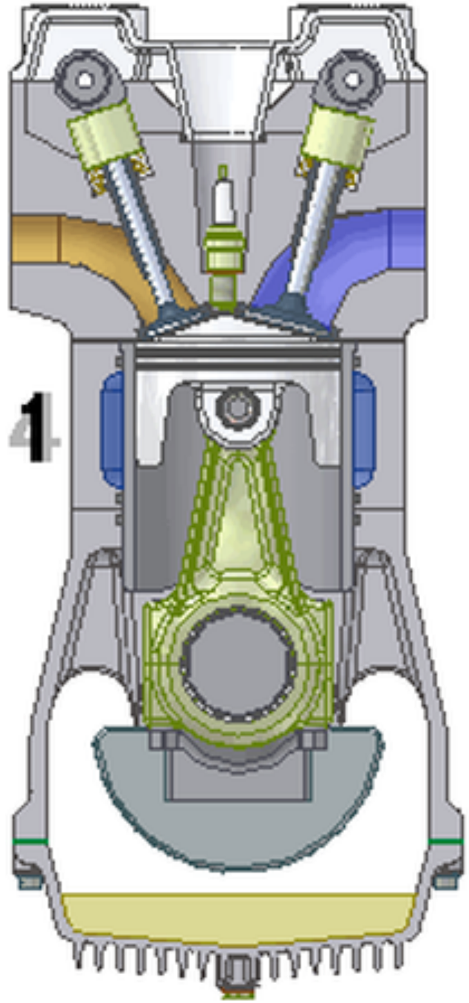
- **Lower burnt gases temperature**
  - **Less Nox formation**

…remains at the development stage

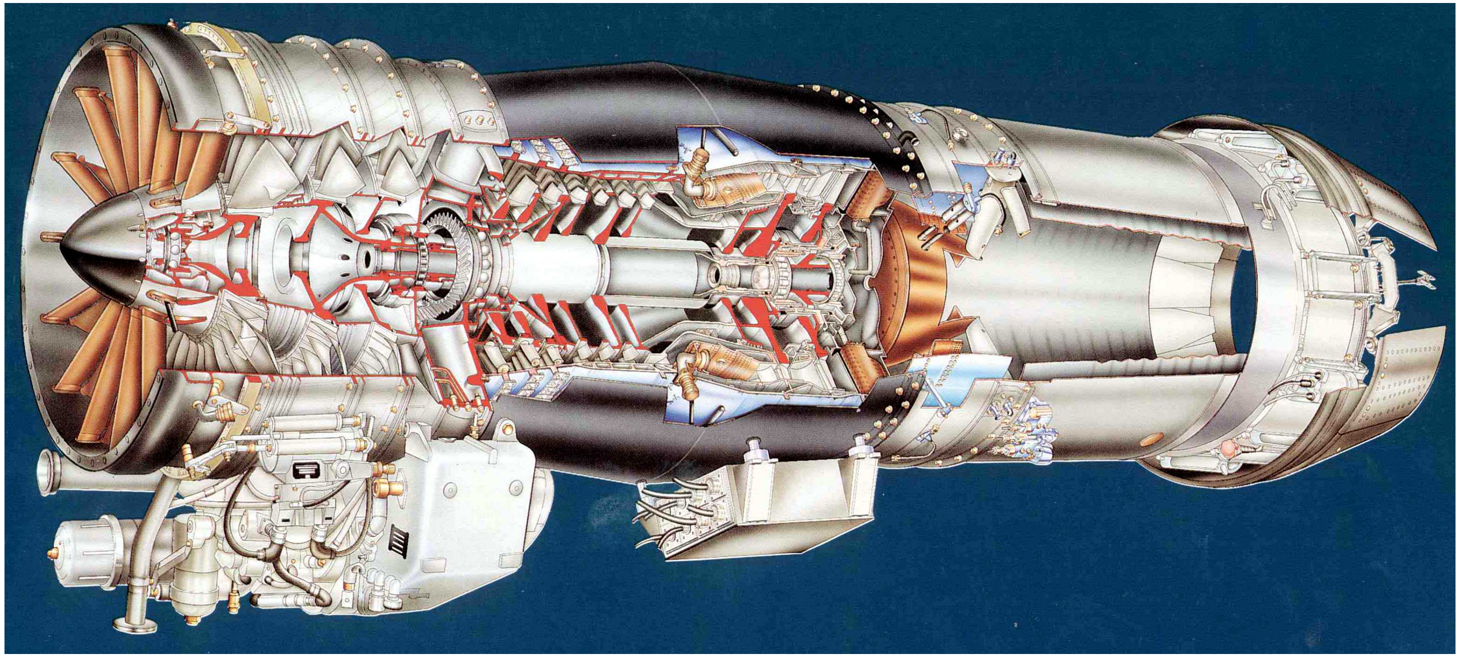
Applications

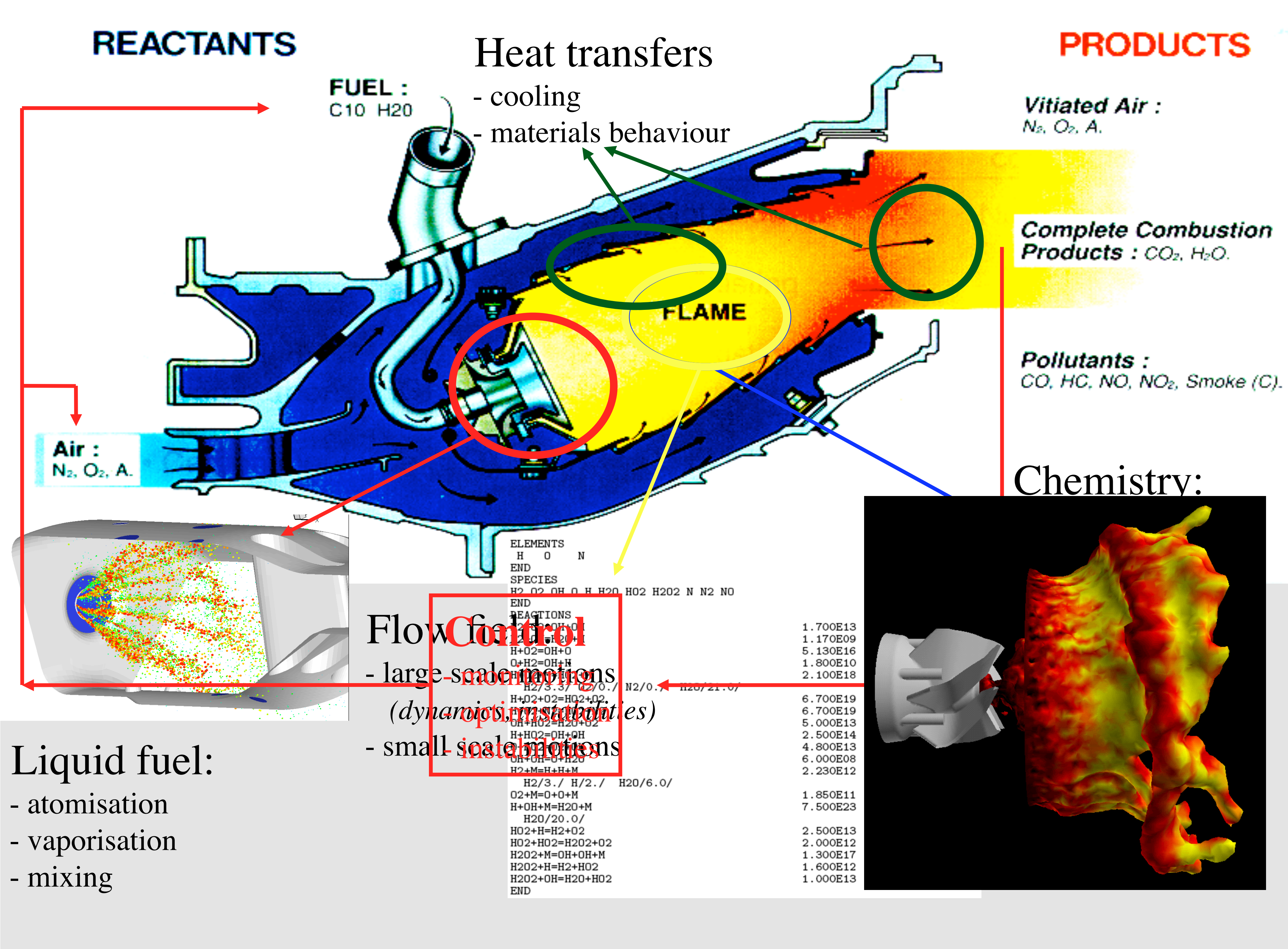
➢ ***Internal combustion engines using new fuels***

- *Consumption / Efficiency*
- *Reduced pollutant emissions*
  - *combustion*
  - *post-treatment*
- *Stability*
- *Ignition*
  - *auto-ignition (Diesel)*
  - *spark ignition*
- *Weight / Size*



Aircraft engines

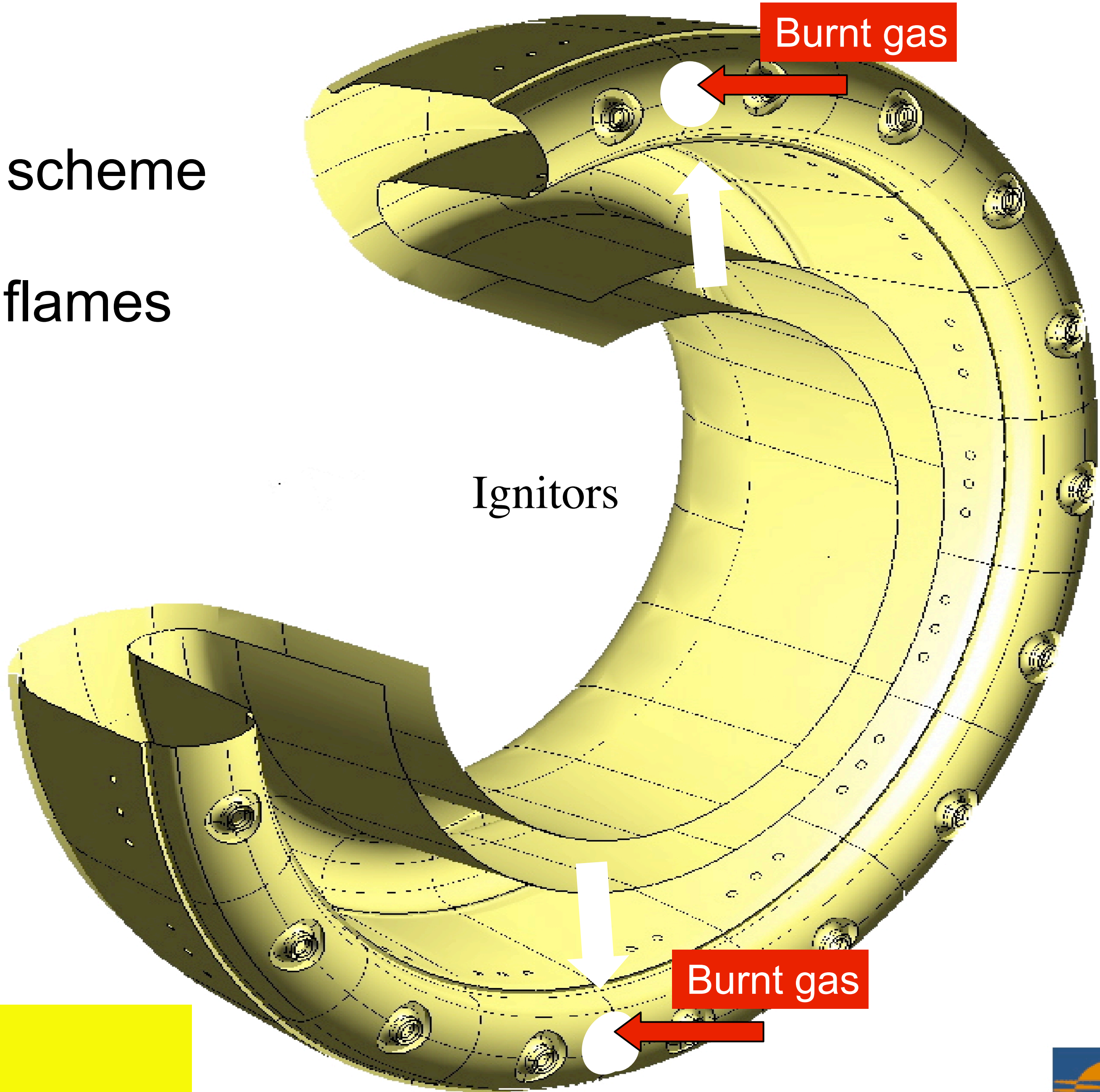




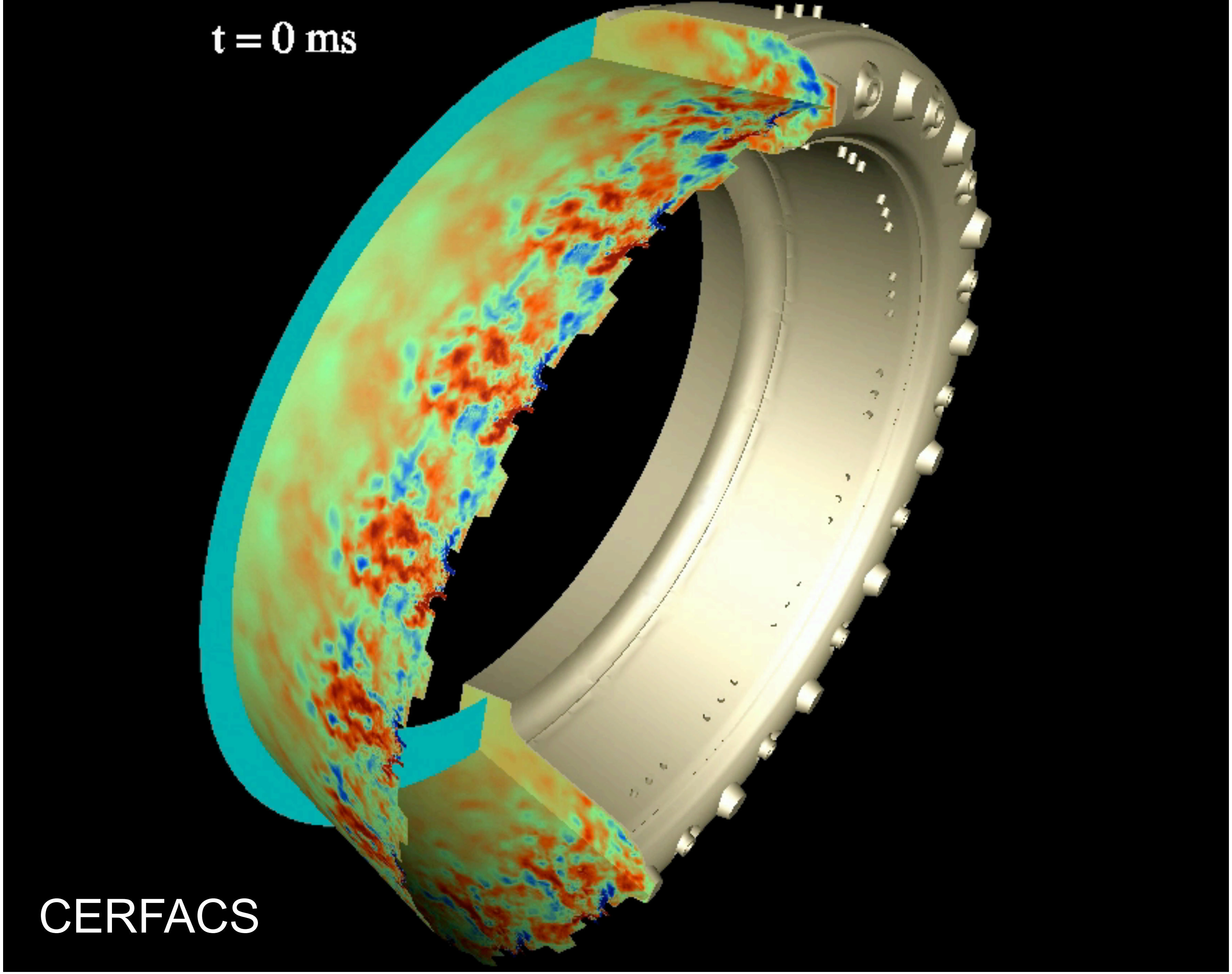
REACTANTS
Heat transfers
- cooling
- materials behaviour
PRODUCTS
FUEL :
C10 H20
Vitiated Air :
N2, O2, A.
Complete Combustion Products : CO2, H2O.
FLAME
Pollutants :
CO, HC, NO, NO2, Smoke (C).
Air :
N2, O2, A.
Chemistry:
ELEMENTS
H O N
END
SPECIES
H2 O2 OH O H H2O HO2 H2O2 N N2 NO
END
REACTIONS
H+O2=OH+O
O+H2=OH+H
H+O2+O2=HO2+O2
OH+HO2=H2O+O2
H+HO2=OH+OH
H2+M=H+H+M
H2/3./ H/2./ H2O/6.0/
O2+M=O+O+M
H+OH+M=H2O+M
H2O/20.0/
HO2+H=H2+O2
HO2+HO2=H2O2+O2
H2O2+M=OH+OH+M
H2O2+H=H2+HO2
H2O2+OH=H2O+HO2
END
1.700E13
1.170E09
5.130E16
1.800E10
2.100E18
6.700E19
6.700E19
5.000E13
2.500E14
4.800E13
6.000E08
2.230E12
1.850E11
7.500E23
2.500E13
2.000E12
1.300E17
1.600E12
1.000E13
Flow field:
- large scale motions
(dynamics, instabilities)
- small scale motions
Control
- monitoring
- optimisation
- instabilities
Liquid fuel:
- atomisation
- vaporisation
- mixing

<u>Ignition of an helicopter chamber</u> :

- 20 M cells
- 2000 BG procs
- kerosene/air 2 step scheme
- TFLES model
- ignition by two pilot flames



Collaboration between:
- CERFACS
- Argonne National Lab (Top 1 machine)
- Turbomeca



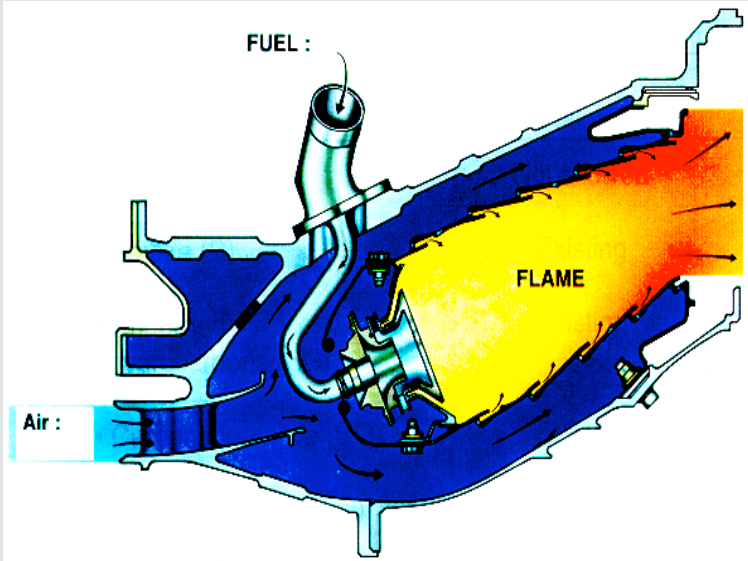
Axial velocity field + flame position (white line)

16

Applications

➢ ***Gas turbines using new fuels***

- o *Consumption / Efficiency*
- o *Reduced pollutant emission*
- o *Stability*
- o *Turbine inlet temperature profile*
- o *Ignition / re-ignition (aeronautics)*
  - *main combustion chamber*
  - *post-combustion*
- o *Versatility (ground turbines)*
- o *Weight / Size (aeronautics)*
- o *Life time*



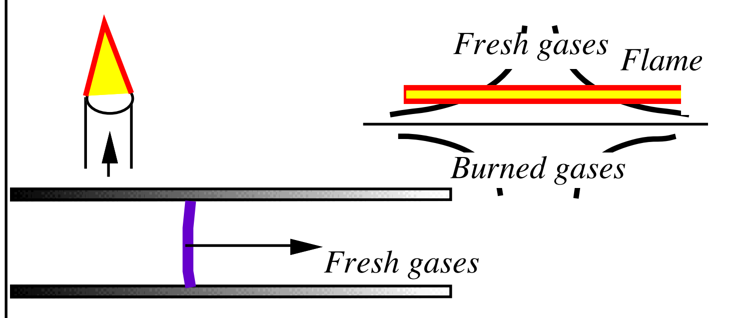
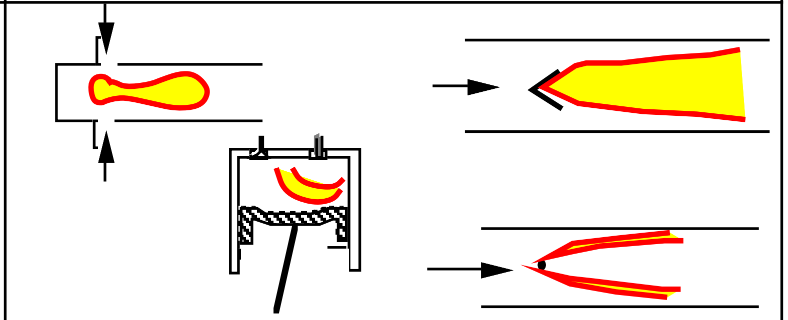
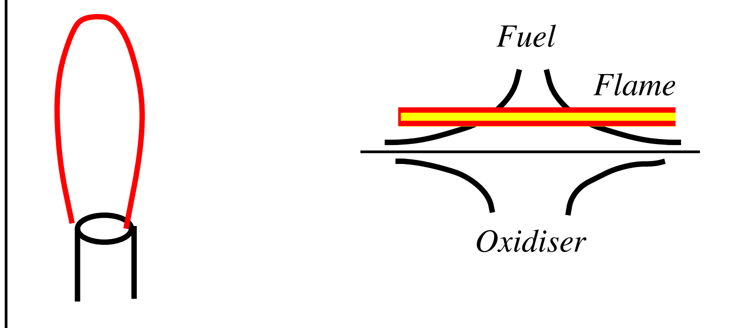
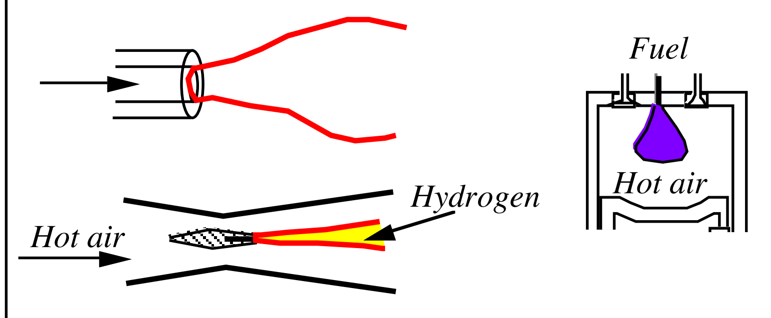
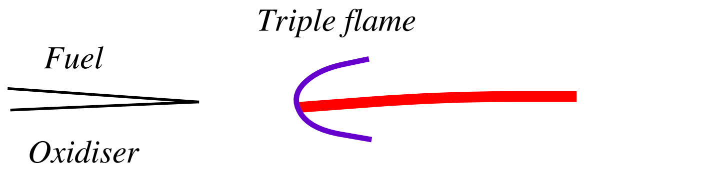
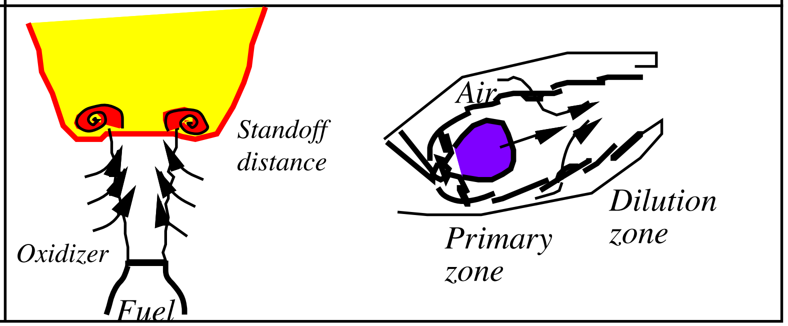
Main combustion chamber

Applications

➢ ***Industrial furnaces using new fuels***

- o *Consumption / Efficiency*
- o *Reduced pollutant emissions*
  - • *combustion*
  - • *post-treatment*
- o *Stability*
- o *Fuel versatility*
- o *Lifetime*
  - • *operating 24 h / 24*
  - • *limited maintenance*
- o *Co-generation*

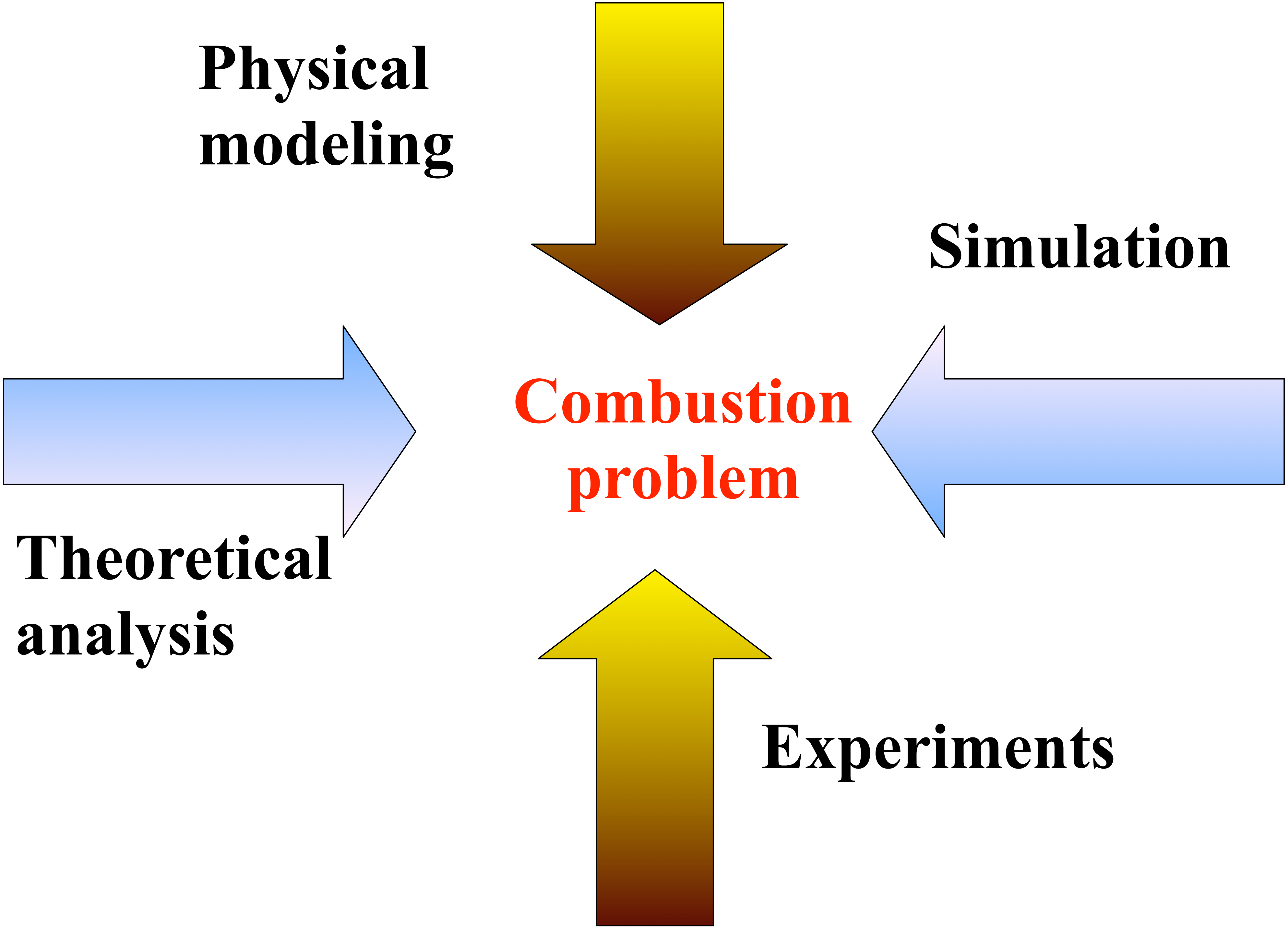
VARIOUS MODES OF COMBUSTION

	Laminar	Turbulent
Premixed combustion		
Non premixed combustion		
Partially premixed combustion		

Premixed / diffusion flames

	Diffusion flame	Premixed flame
Advantages	• No flame propagation • Easy to design / build	• Efficiency • Controled temperature
Drawbacks	• Efficiency (mixing) • Maximal temperature	• Safety (flame propagation) • Mixing • Flamability limits

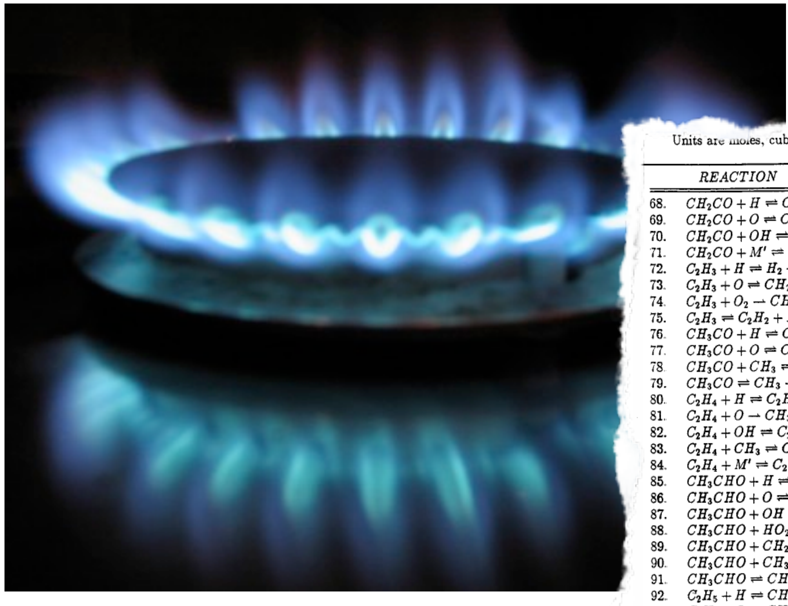
More and more devices use premixed combustion!


Physical modeling
Simulation
Combustion problem
Theoretical analysis
Experiments

Challenge: chemistry

~~$CH_4 + 2O_2 = CO_2 + 2\ H_2O$~~

Challenge: chemistry



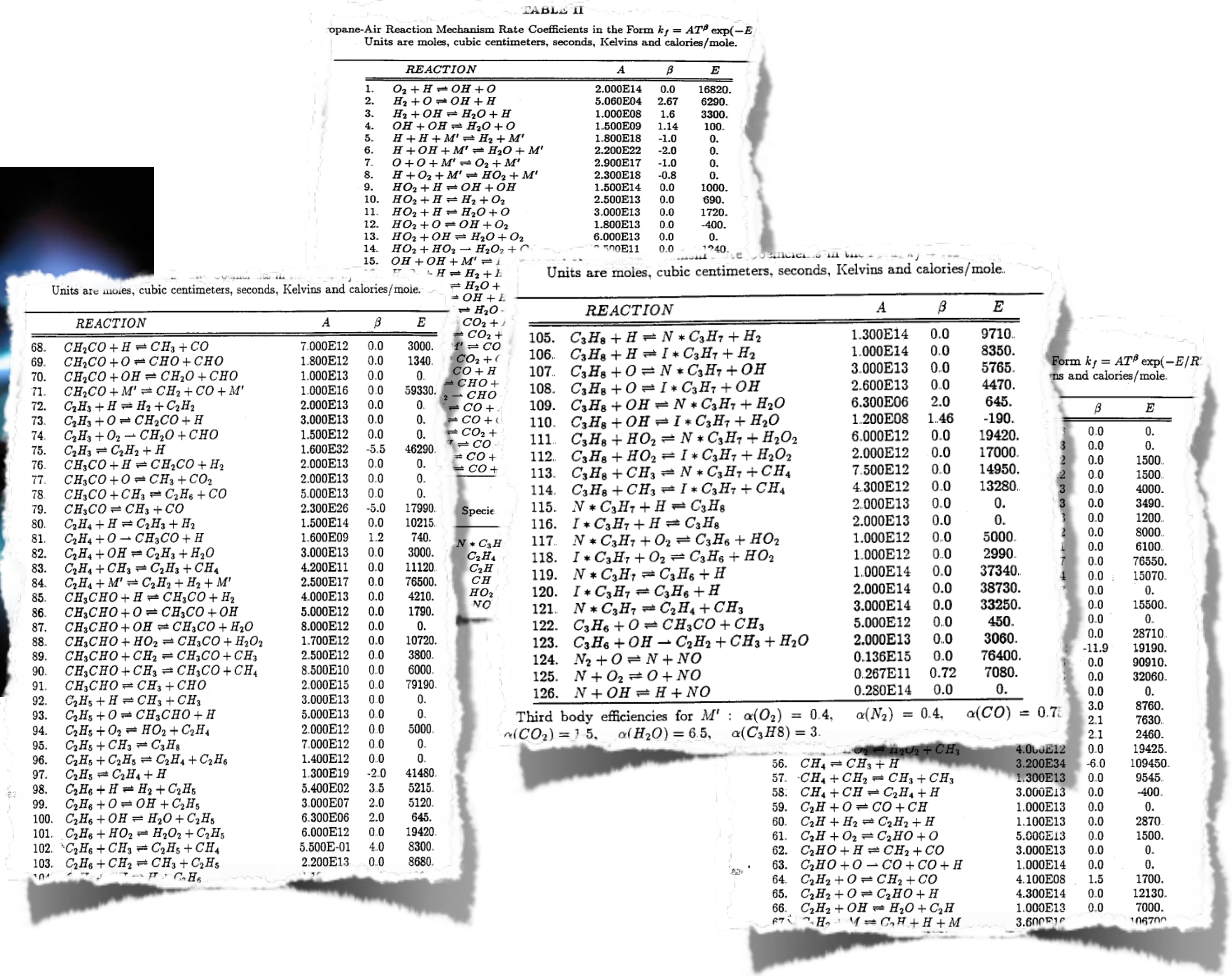


TABLE II

opane-Air Reaction Mechanism Rate Coefficients in the Form $k_f = AT^\beta \exp(-E$
Units are moles, cubic centimeters, seconds, Kelvins and calories/mole.

	REACTION	A	β	E
1.	$O_2 + H \rightleftharpoons OH + O$	2.000E14	0.0	16820.
2.	$H_2 + O \rightleftharpoons OH + H$	5.060E04	2.67	6290.
3.	$H_2 + OH \rightleftharpoons H_2O + H$	1.000E08	1.6	3300.
4.	$OH + OH \rightleftharpoons H_2O + O$	1.500E09	1.14	100.
5.	$H + H + M' \rightleftharpoons H_2 + M'$	1.800E18	-1.0	0.
6.	$H + OH + M' \rightleftharpoons H_2O + M'$	2.200E22	-2.0	0.
7.	$O + O + M' \rightleftharpoons O_2 + M'$	2.900E17	-1.0	0.
8.	$H + O_2 + M' \rightleftharpoons HO_2 + M'$	2.300E18	-0.8	0.
9.	$HO_2 + H \rightleftharpoons OH + OH$	1.500E14	0.0	1000.
10.	$HO_2 + H \rightleftharpoons H_2 + O_2$	2.500E13	0.0	690.
11.	$HO_2 + H \rightleftharpoons H_2O + O$	3.000E13	0.0	1720.
12.	$HO_2 + O \rightleftharpoons OH + O_2$	1.800E13	0.0	-400.
13.	$HO_2 + OH \rightleftharpoons H_2O + O_2$	6.000E13	0.0	0.

Units are moles, cubic centimeters, seconds, Kelvins and calories/mole.

	REACTION	A	β	E
68.	$CH_2CO + H \rightleftharpoons CH_3 + CO$	7.000E12	0.0	3000.
69.	$CH_2CO + O \rightleftharpoons CHO + CHO$	1.800E12	0.0	1340.
70.	$CH_2CO + OH \rightleftharpoons CH_2O + CHO$	1.000E13	0.0	0.
71.	$CH_2CO + M' \rightleftharpoons CH_2 + CO + M'$	1.000E16	0.0	59330.
72.	$C_2H_3 + H \rightleftharpoons H_2 + C_2H_2$	2.000E13	0.0	0.
73.	$C_2H_3 + O \rightleftharpoons CH_2CO + H$	3.000E13	0.0	0.
74.	$C_2H_3 + O_2 \rightarrow CH_2O + CHO$	1.500E12	0.0	0.
75.	$C_2H_3 \rightleftharpoons C_2H_2 + H$	1.600E32	-5.5	46290.
76.	$CH_3CO + H \rightleftharpoons CH_2CO + H_2$	2.000E13	0.0	0.
77.	$CH_3CO + O \rightleftharpoons CH_3 + CO_2$	2.000E13	0.0	0.
78.	$CH_3CO + CH_3 \rightleftharpoons C_2H_6 + CO$	5.000E13	0.0	0.
79.	$CH_3CO \rightleftharpoons CH_3 + CO$	2.300E26	-5.0	17990.
80.	$C_2H_4 + H \rightleftharpoons C_2H_3 + H_2$	1.500E14	0.0	10215.
81.	$C_2H_4 + O \rightarrow CH_3CO + H$	1.600E09	1.2	740.
82.	$C_2H_4 + OH \rightleftharpoons C_2H_3 + H_2O$	3.000E13	0.0	3000.
83.	$C_2H_4 + CH_3 \rightleftharpoons C_2H_3 + CH_4$	4.200E11	0.0	11120.
84.	$C_2H_4 + M' \rightleftharpoons C_2H_2 + H_2 + M'$	2.500E17	0.0	76500.
85.	$CH_3CHO + H \rightleftharpoons CH_3CO + H_2$	4.000E13	0.0	4210.
86.	$CH_3CHO + O \rightleftharpoons CH_3CO + OH$	5.000E12	0.0	1790.
87.	$CH_3CHO + OH \rightleftharpoons CH_3CO + H_2O$	8.000E12	0.0	0.
88.	$CH_3CHO + HO_2 \rightleftharpoons CH_3CO + H_2O_2$	1.700E12	0.0	10720.
89.	$CH_3CHO + CH_2 \rightleftharpoons CH_3CO + CH_3$	2.500E12	0.0	3800.
90.	$CH_3CHO + CH_3 \rightleftharpoons CH_3CO + CH_4$	8.500E10	0.0	6000.
91.	$CH_3CHO \rightleftharpoons CH_3 + CHO$	2.000E15	0.0	79190.
92.	$C_2H_5 + H \rightleftharpoons CH_3 + CH_3$	3.000E13	0.0	0.
93.	$C_2H_5 + O \rightleftharpoons CH_3CHO + H$	5.000E13	0.0	0.
94.	$C_2H_5 + O_2 \rightleftharpoons HO_2 + C_2H_4$	2.000E12	0.0	5000.
95.	$C_2H_5 + CH_3 \rightleftharpoons C_3H_8$	7.000E12	0.0	0.
96.	$C_2H_5 + C_2H_5 \rightleftharpoons C_2H_4 + C_2H_6$	1.400E12	0.0	0.
97.	$C_2H_5 \rightleftharpoons C_2H_4 + H$	1.300E19	-2.0	41480.
98.	$C_2H_6 + H \rightleftharpoons H_2 + C_2H_5$	5.400E02	3.5	5215.
99.	$C_2H_6 + O \rightleftharpoons OH + C_2H_5$	3.000E07	2.0	5120.
100.	$C_2H_6 + OH \rightleftharpoons H_2O + C_2H_5$	6.300E06	2.0	645.
101.	$C_2H_6 + HO_2 \rightleftharpoons H_2O_2 + C_2H_5$	6.000E12	0.0	19420.
102.	$C_2H_6 + CH_3 \rightleftharpoons C_2H_5 + CH_4$	5.500E-01	4.0	8300.
103.	$C_2H_6 + CH_2 \rightleftharpoons CH_3 + C_2H_5$	2.200E13	0.0	8680.

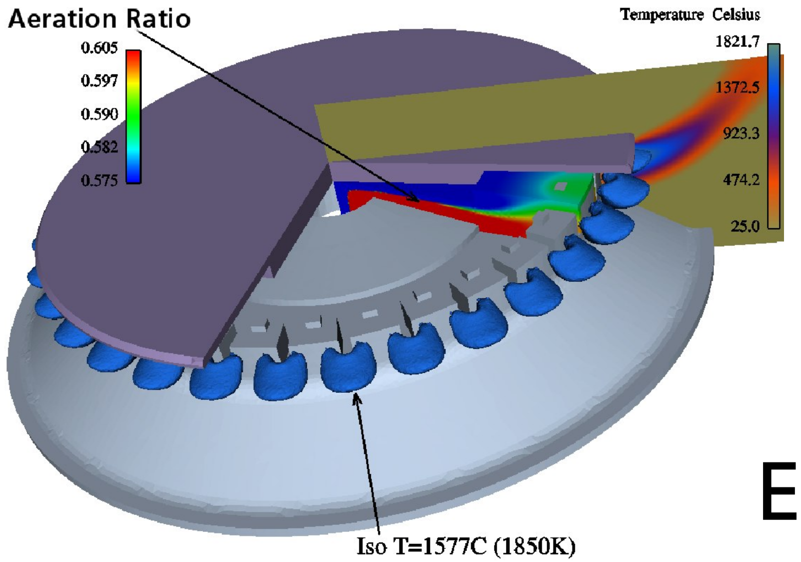
Units are moles, cubic centimeters, seconds, Kelvins and calories/mole.

	REACTION	A	β	E
105.	$C_3H_8 + H \rightleftharpoons N*C_3H_7 + H_2$	1.300E14	0.0	9710.
106.	$C_3H_8 + H \rightleftharpoons I*C_3H_7 + H_2$	1.000E14	0.0	8350.
107.	$C_3H_8 + O \rightleftharpoons N*C_3H_7 + OH$	3.000E13	0.0	5765.
108.	$C_3H_8 + O \rightleftharpoons I*C_3H_7 + OH$	2.600E13	0.0	4470.
109.	$C_3H_8 + OH \rightleftharpoons N*C_3H_7 + H_2O$	6.300E06	2.0	645.
110.	$C_3H_8 + OH \rightleftharpoons I*C_3H_7 + H_2O$	1.200E08	1.46	-190.
111.	$C_3H_8 + HO_2 \rightleftharpoons N*C_3H_7 + H_2O_2$	6.000E12	0.0	19420.
112.	$C_3H_8 + HO_2 \rightleftharpoons I*C_3H_7 + H_2O_2$	2.000E12	0.0	17000.
113.	$C_3H_8 + CH_3 \rightleftharpoons N*C_3H_7 + CH_4$	7.500E12	0.0	14950.
114.	$C_3H_8 + CH_3 \rightleftharpoons I*C_3H_7 + CH_4$	4.300E12	0.0	13280.
115.	$N*C_3H_7 + H \rightleftharpoons C_3H_8$	2.000E13	0.0	0.
116.	$I*C_3H_7 + H \rightleftharpoons C_3H_8$	2.000E13	0.0	0.
117.	$N*C_3H_7 + O_2 \rightleftharpoons C_3H_6 + HO_2$	1.000E12	0.0	5000.
118.	$I*C_3H_7 + O_2 \rightleftharpoons C_3H_6 + HO_2$	1.000E12	0.0	2990.
119.	$N*C_3H_7 \rightleftharpoons C_3H_6 + H$	1.000E14	0.0	37340.
120.	$I*C_3H_7 \rightleftharpoons C_3H_6 + H$	2.000E14	0.0	38730.
121.	$N*C_3H_7 \rightleftharpoons C_2H_4 + CH_3$	3.000E14	0.0	33250.
122.	$C_3H_6 + O \rightleftharpoons CH_3CO + CH_3$	5.000E12	0.0	450.
123.	$C_3H_6 + OH \rightarrow C_2H_2 + CH_3 + H_2O$	2.000E13	0.0	3060.
124.	$N_2 + O \rightleftharpoons N + NO$	0.136E15	0.0	76400.
125.	$N + O_2 \rightleftharpoons O + NO$	0.267E11	0.72	7080.
126.	$N + OH \rightleftharpoons H + NO$	0.280E14	0.0	0.

Third body efficiencies for M' : $\alpha(O_2) = 0.4$, $\alpha(N_2) = 0.4$, $\alpha(CO) = 0.7$
$\alpha(CO_2) = 1.5$, $\alpha(H_2O) = 6.5$, $\alpha(C_3H8) = 3.$

	REACTION	A	β	E
56.	$CH_4 \rightleftharpoons CH_3 + H$	3.200E34	-6.0	109450.
57.	$CH_4 + CH_2 \rightleftharpoons CH_3 + CH_3$	1.300E13	0.0	9545.
58.	$CH_4 + CH \rightleftharpoons C_2H_4 + H$	3.000E13	0.0	-400.
59.	$C_2H + O \rightleftharpoons CO + CH$	1.000E13	0.0	0.
60.	$C_2H + H_2 \rightleftharpoons C_2H_2 + H$	1.100E13	0.0	2870.
61.	$C_2H + O_2 \rightleftharpoons C_2HO + O$	5.000E13	0.0	1500.
62.	$C_2HO + H \rightleftharpoons CH_2 + CO$	3.000E13	0.0	0.
63.	$C_2HO + O \rightarrow CO + CO + H$	1.000E14	0.0	0.
64.	$C_2H_2 + O \rightleftharpoons CH_2 + CO$	4.100E08	1.5	1700.
65.	$C_2H_2 + O \rightleftharpoons C_2HO + H$	4.300E14	0.0	12130.
66.	$C_2H_2 + OH \rightleftharpoons H_2O + C_2H$	1.000E13	0.0	7000.

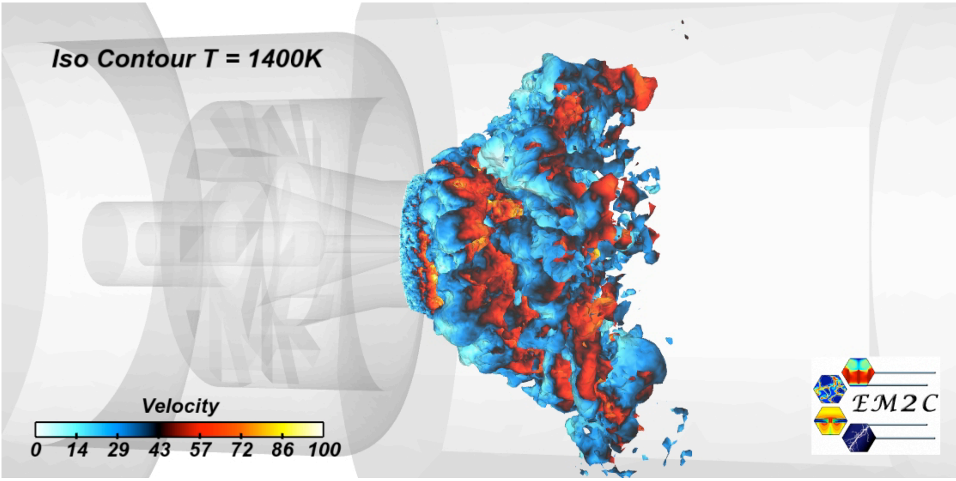
Challenge: chemistry

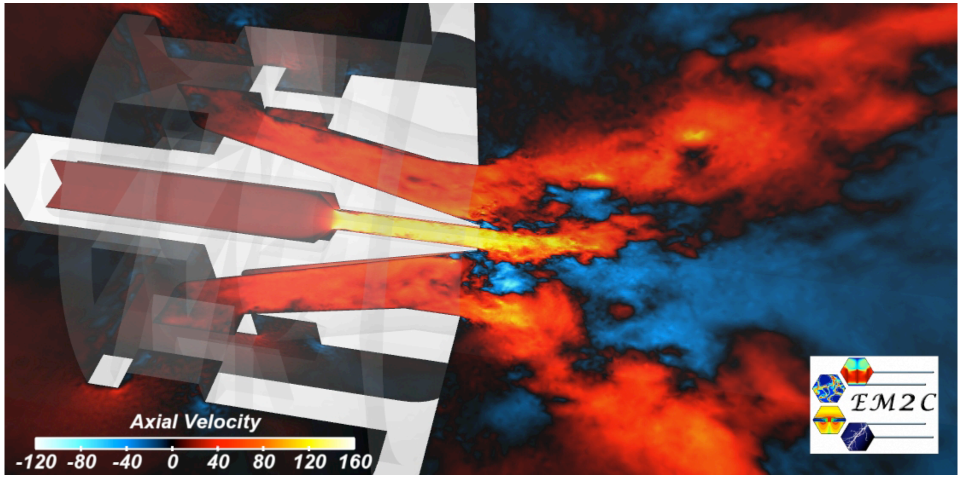


EM2C

models required to reduce the chemistry

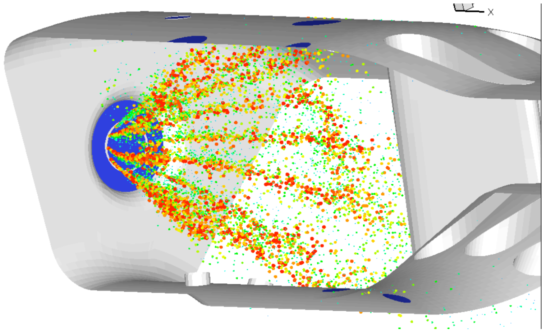
Challenge: flame stability





EM2C

Challenge: two-phase flow

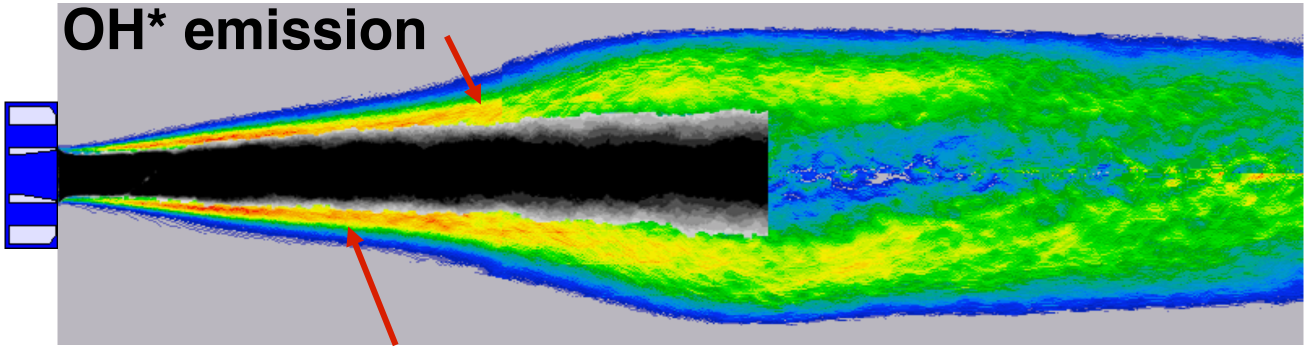


Cerfacs

Liquid fuel

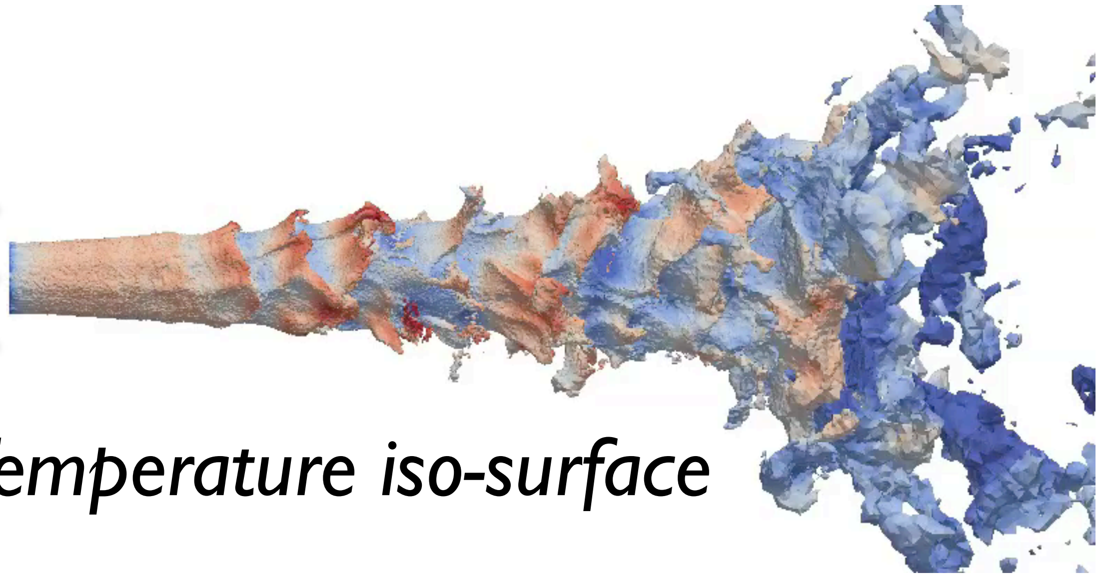
- atomisation
- vaporisation
- mixing

Challenge: supercritical conditions



Experiment

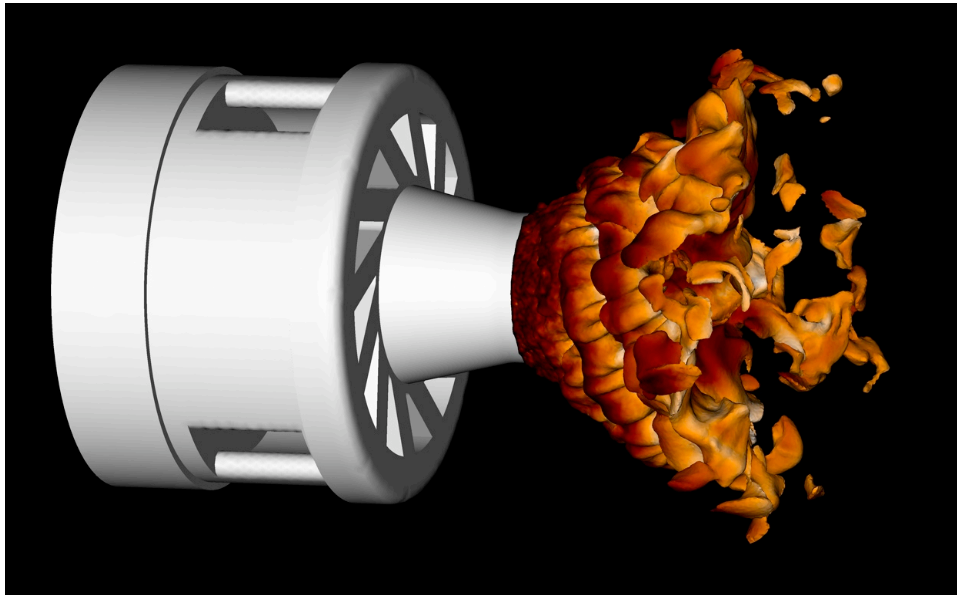
Structure of cryogenic transcritical flames



Temperature iso-surface

EM2C

Challenge: turbulence



EM2C

Models required

Mass:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\, \tilde{u}_i}{\partial x_i} = 0$$

Momentum:

$$\frac{\partial}{\partial t}\overline{\rho}\tilde{u}_i + \frac{\partial}{\partial x_j}\left(\overline{\rho}\tilde{u}_i\tilde{u}_j + \overline{\rho}\widetilde{u_i''u_j''}\right) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial \overline{\tau}_{ij}}{\partial x_j} + \sum_{k=1}^{N} \overline{\rho Y_k f_{k,i}}$$

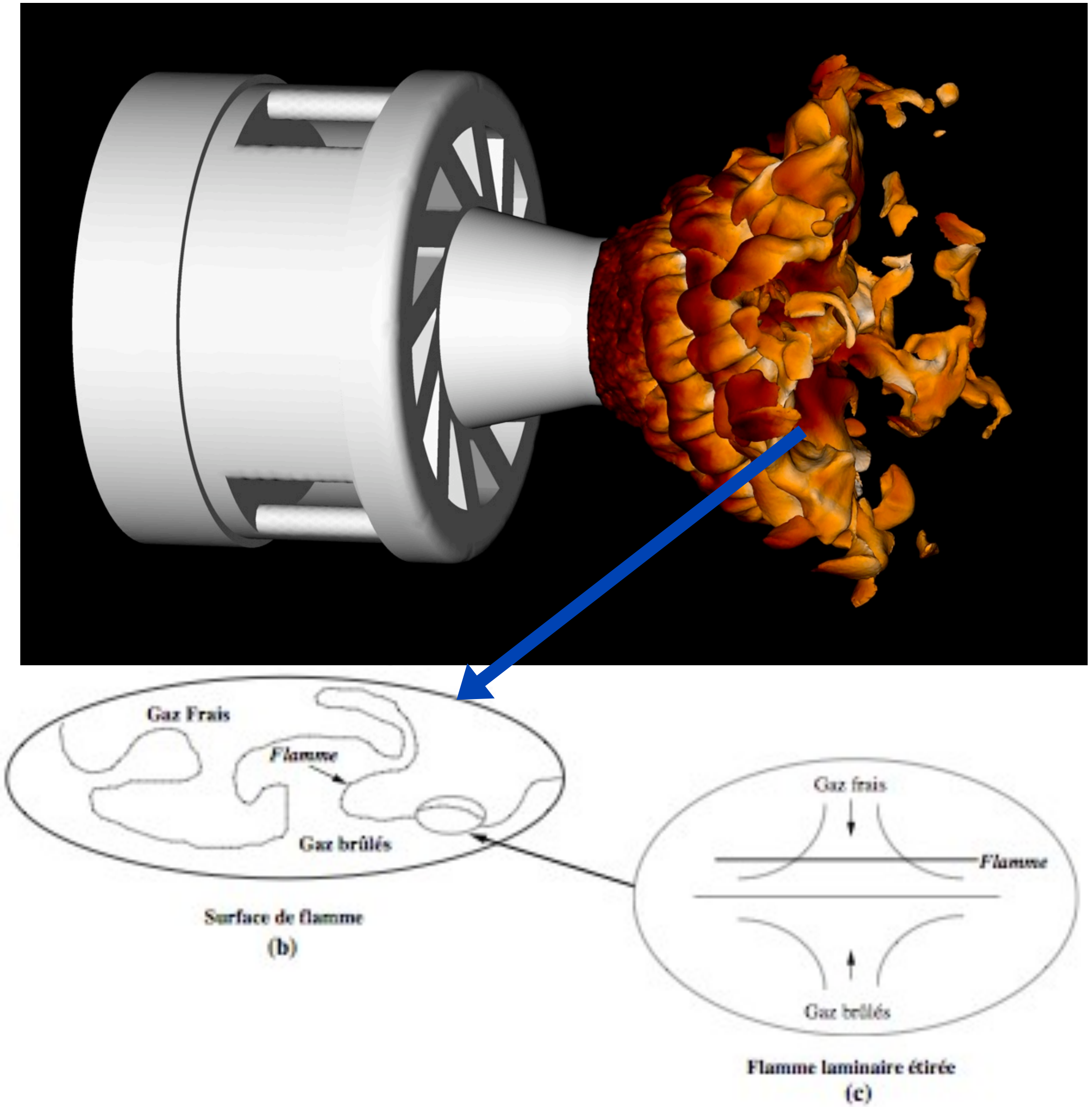
Unknow

Species mass fractions:

$$\frac{\partial \overline{\rho}\widetilde{Y}_k}{\partial t} + \frac{\partial}{\partial x_i}\left(\overline{\rho}\tilde{u}_i\widetilde{Y}_k + \overline{\rho}\widetilde{u_i''Y_k''}\right) + \frac{\partial}{\partial x_i}\overline{\rho V_{k,i} Y_k} = \overline{\dot{\omega}}_k$$

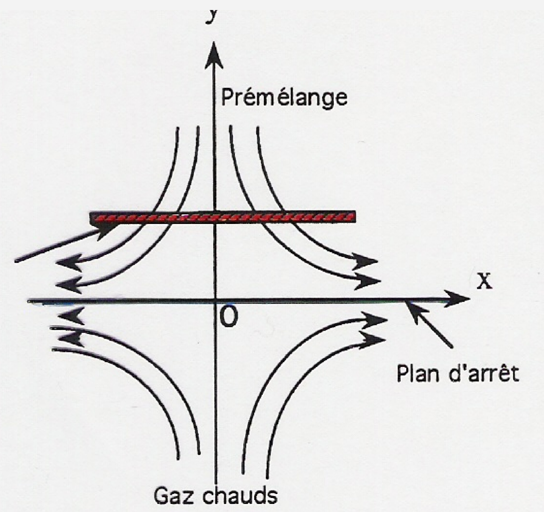
Formally identical to classical Reynolds averaged equations

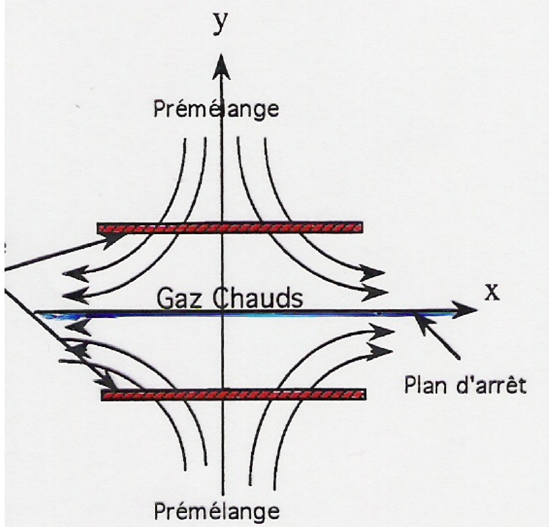
Counterflow flames



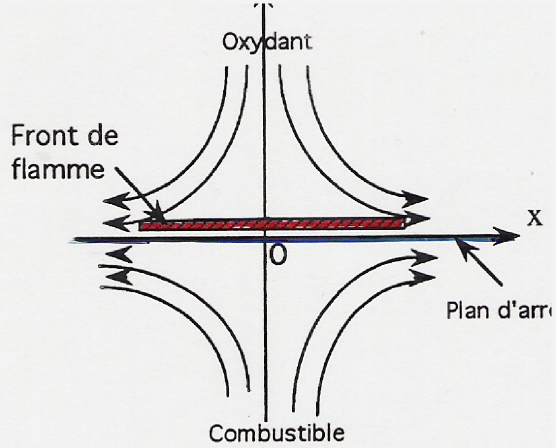
Counterflow flames

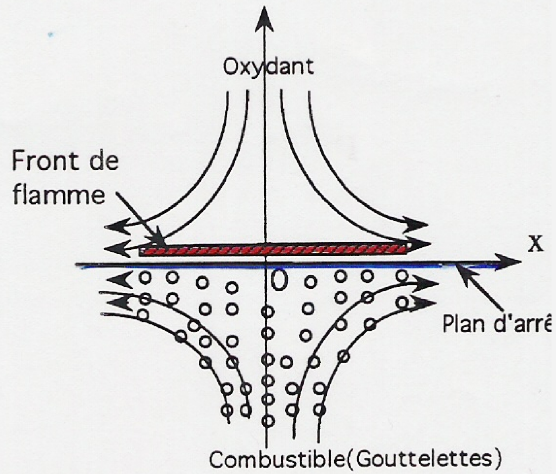
Premixed flames





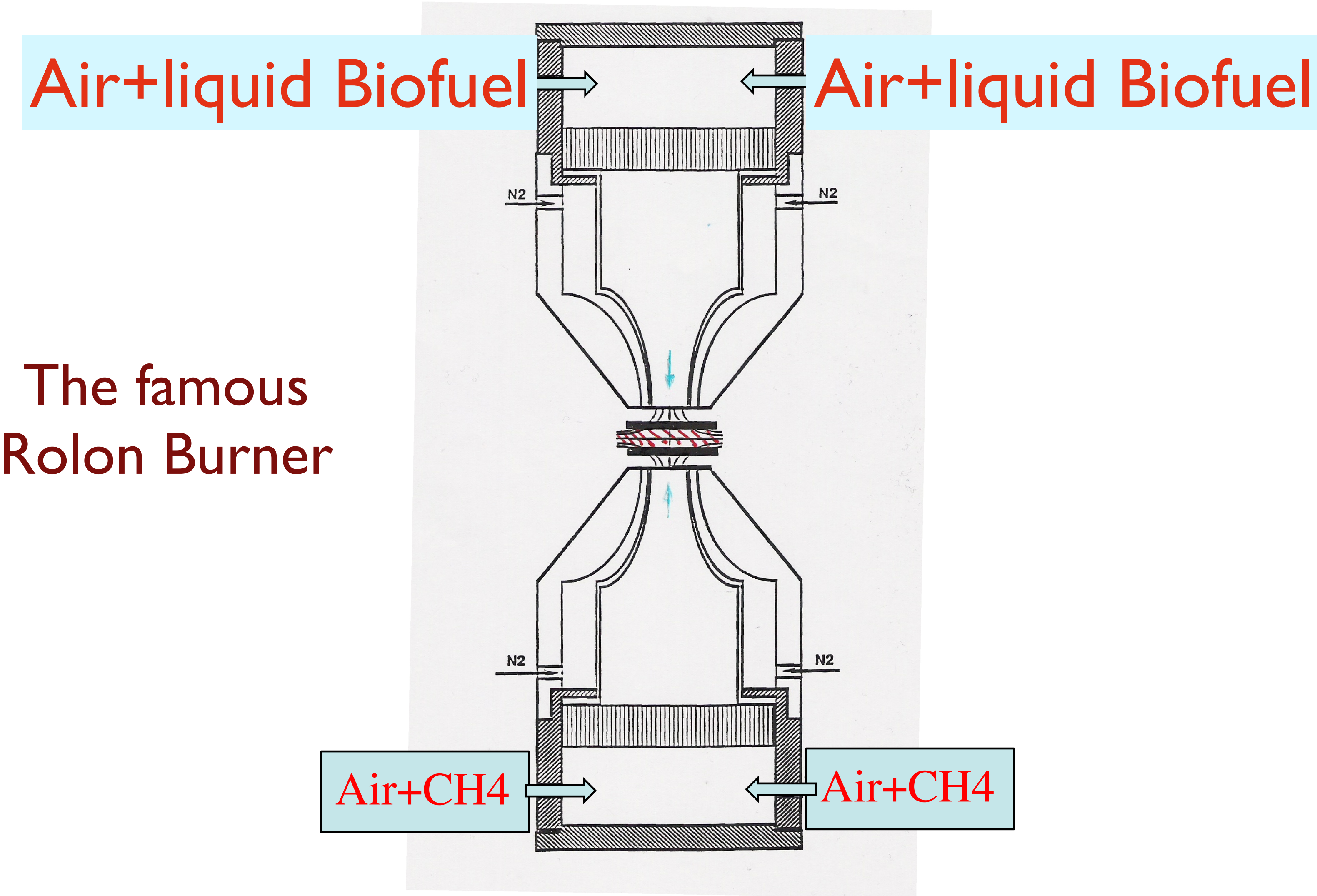
Non-premixed flames



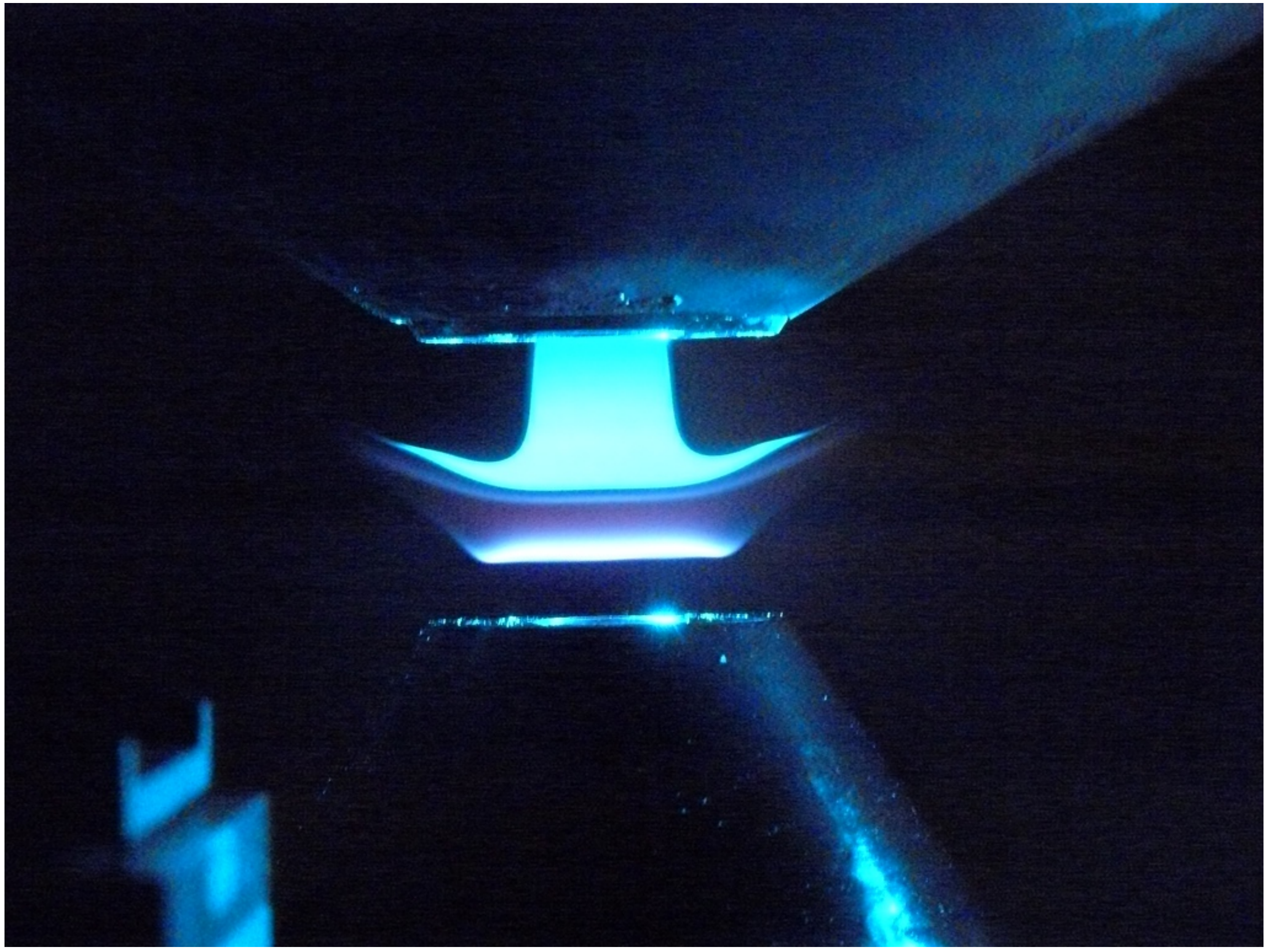


Counterflow flame at FIUNA (PhD Dario Alviso, ITAIPU scholarship)

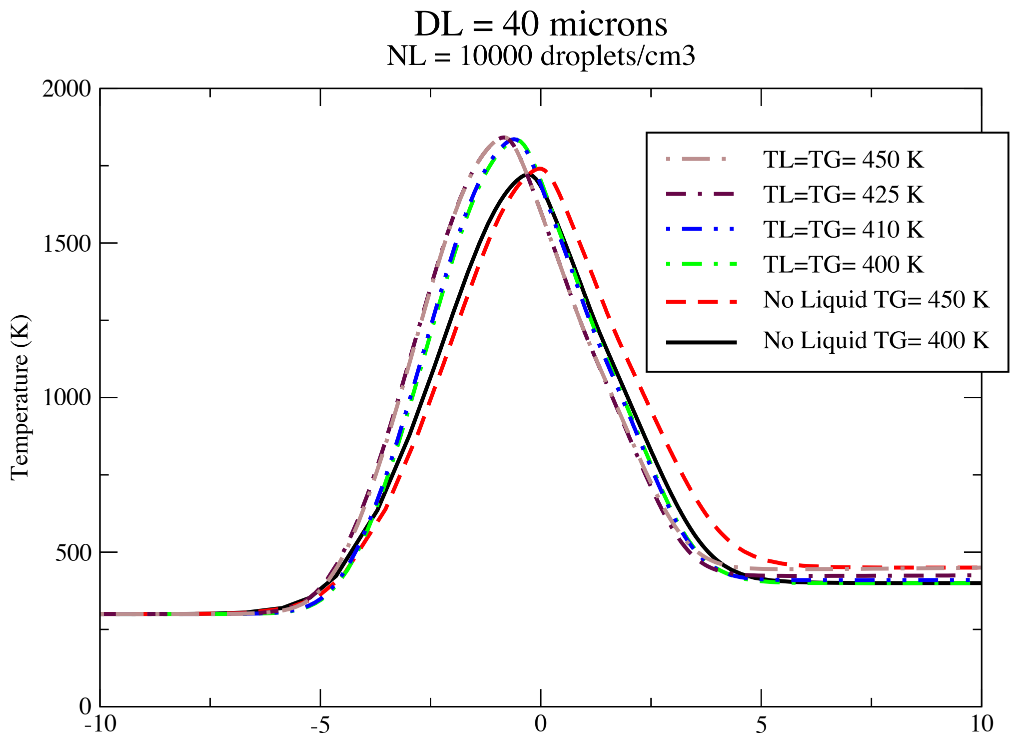
The famous Rolon Burner

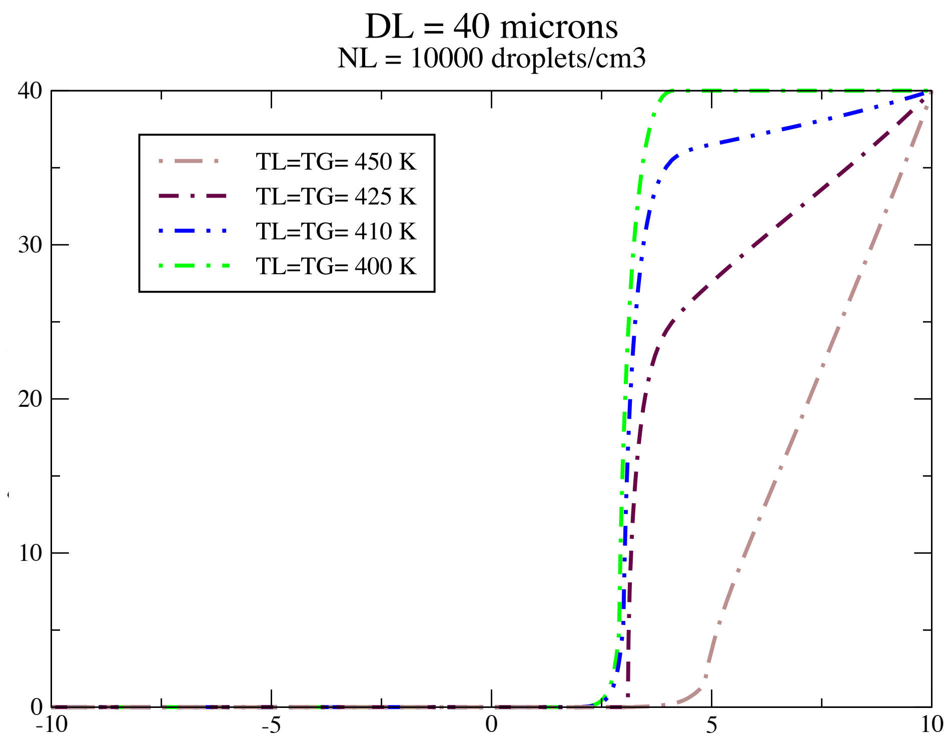


Counterflow flame at FIUNA

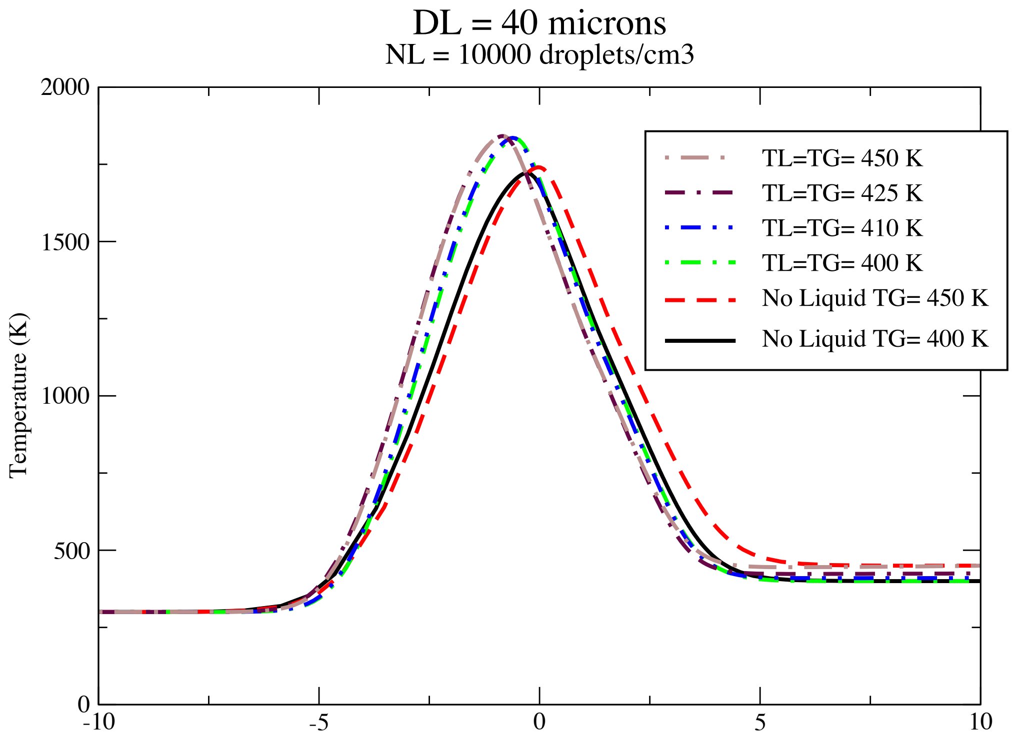


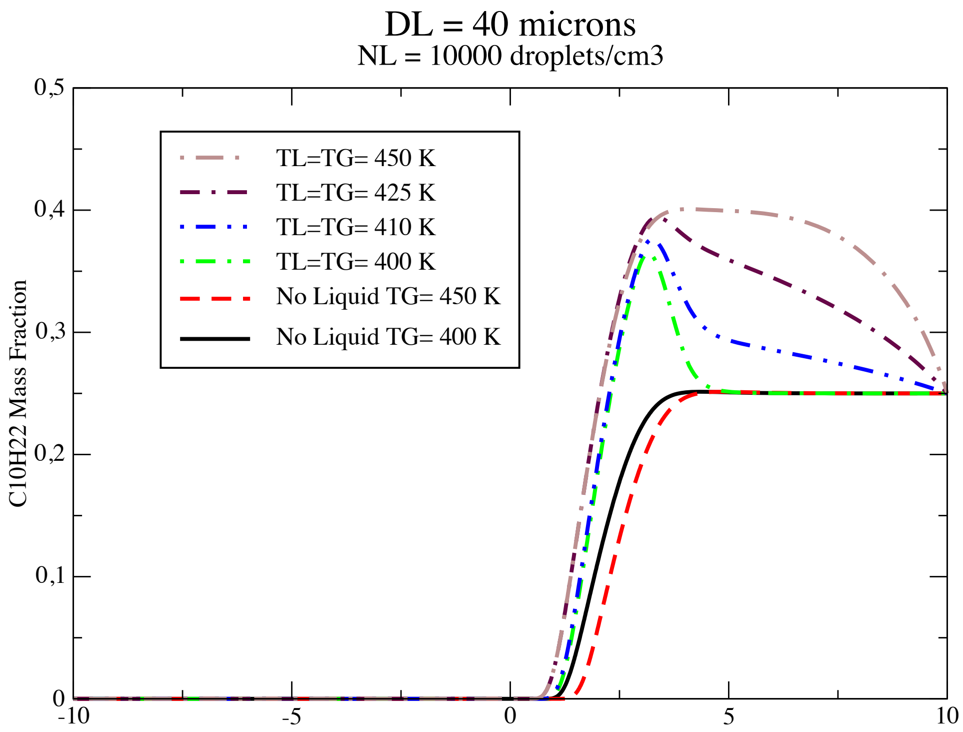
Typical expected results





Typical expected results





Perspectives for Biofuel studies

- Study the Chemical composition and schemes of bio-fuels
- Analyze gaseous counterflow flame structure experimentally and numerically
- Analyze spray counterflow flame structure experimentally and numerically
- Analyze pollutant emission mechanisms

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Thank you

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