Low NO_x Flameless Oxidation Combustor for High Efficiency Gas Turbines

Iyiola Awosope
Imperial College
London

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Work Package 2: Investigation of FLOX Fundamentals & Development of Engineering Prediction Tools

Supervisor: Prof. F. C. Lockwood

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1. Contents

- Objecvtives & aim of the project
- Introduction to Flameless Oxidation and High temperature Air Combustion concepts, benefits & motivation
- Principles of FLOX[1]
- Mathematical Modelling of FLOX
- Development of improved combustion model for FLOX
- Validation of combustion model against experimental data for FLOX, HITAC and new data from Technion FLOX device.
- Results & Discussions
- Recommendations & Conclusion

[1] Flameless Oxidation

2. Project aim

Investigation of the fundamentals of flameless oxidation fundamentals and development of a suitable engineering prediction tool.

3. Objectives of work package 2 (WP2)

- Devise improved model for the prediction of flameless oxidation combustion
- Develop and validate a NO_x prediction model in flameless oxidation combustion.
- Incorporate the improved combustion model in an existing three-dimensional computational fluid dynamics(CFD) prediction code.
- Validate mathematical models against existing and new laboratory data for flameless oxidation.
- To propose recommendations that would enhance mixing, combustion and emissions performance of gas turbine combustors.

3. Introduction

Preheated air increases combustion efficency & fuel savings

Preheat $\longrightarrow \Uparrow T_{air}$

High T_{air} + ambient air $\longrightarrow \Uparrow$T rise + $\Uparrow$NO$_x$ emissions

Since regulation on NO$_x$ emissions is getting tighter

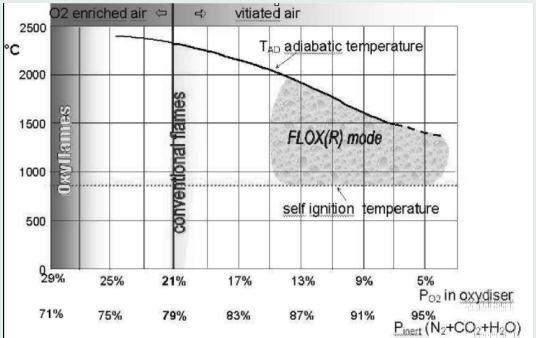
New Combustion technologies are emerging to tackle the problems

High T_{air} + diluted air $\longrightarrow \Downarrow$T$_{ad}$ + $\Downarrow$NO$_x$ emissions

e.g. HITAC[a] & FLOX[b]

[a] High Temperature Air Combustion

[b] Flameless Oxidation

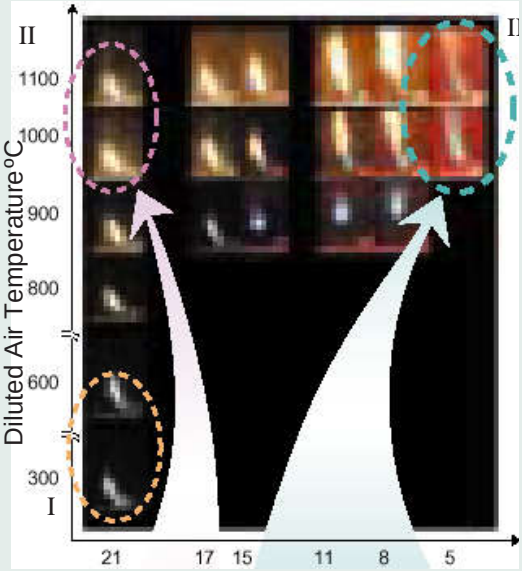


4. Introduction: High Temperature Air Combustion (HITAC)

Research started in Japan
by late Tanaka & Hasegawa (1994)

Technology applied to industrial furnaces equiped with Regenerative burners. e.g. NFK[a] furnace

High thermal efficiency 30% savings in energy, 30% reduction in CO_2
50% reduction in NO_x



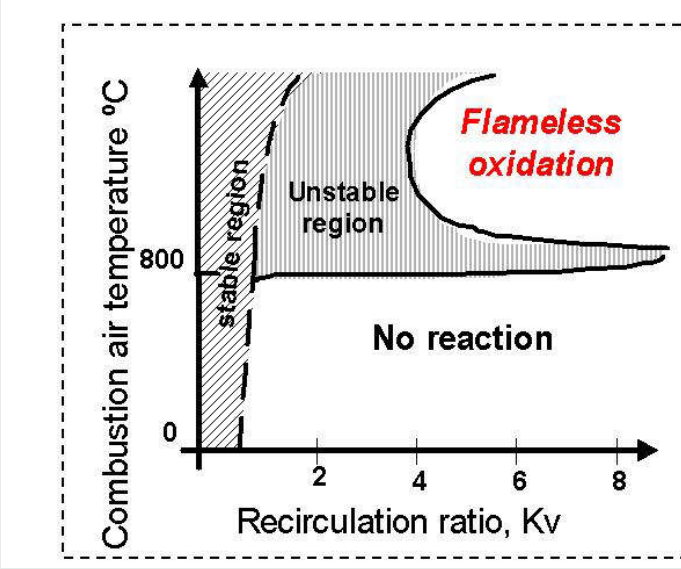
[a] Nippon Furnace Kogyo Kaisha Ltd (NFK)

5. Introduction: Flameless Oxidation Combustion (FLOX)

Research followed in other countries. 'FLOX' patented by J. Wunning (Germany, 1997), is commonly used in Europe.

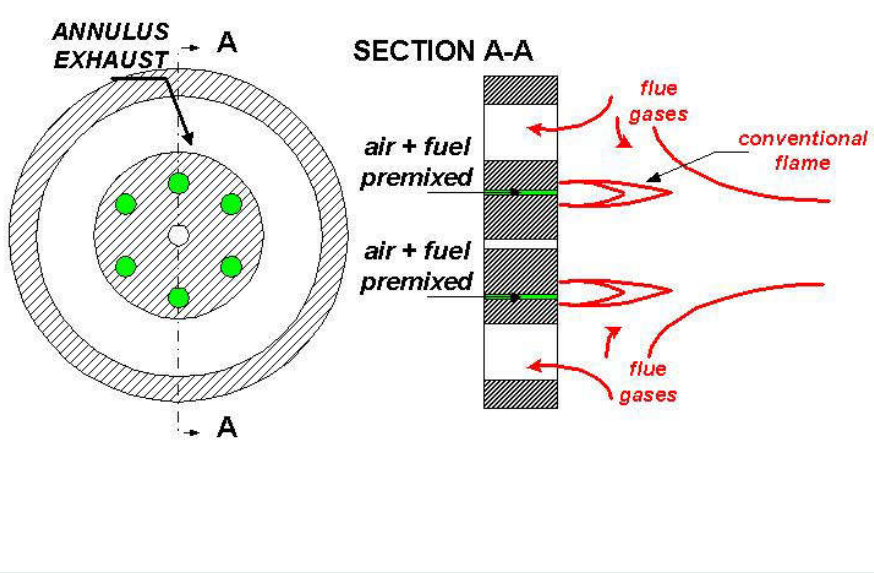
FLOX burner ensures segregation of air and fuel streams and strong dilution with flue gases, with recirculation ratio, K_v greater than 3.0

$$K_v = \frac{m_{rec}}{m_{air} + m_{fuel}}$$



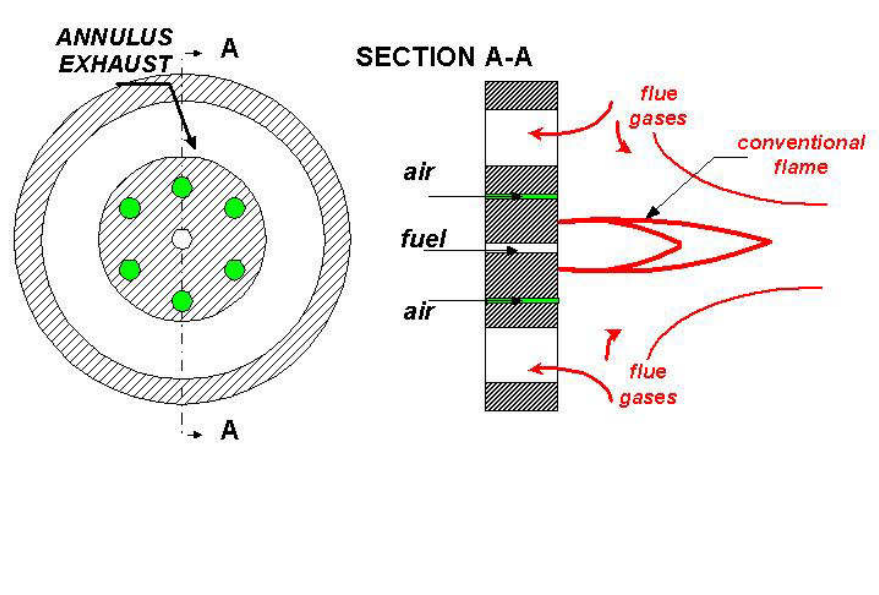
6. Principles of FLOX

Conventional flames: Premixed flame in FLOX burner



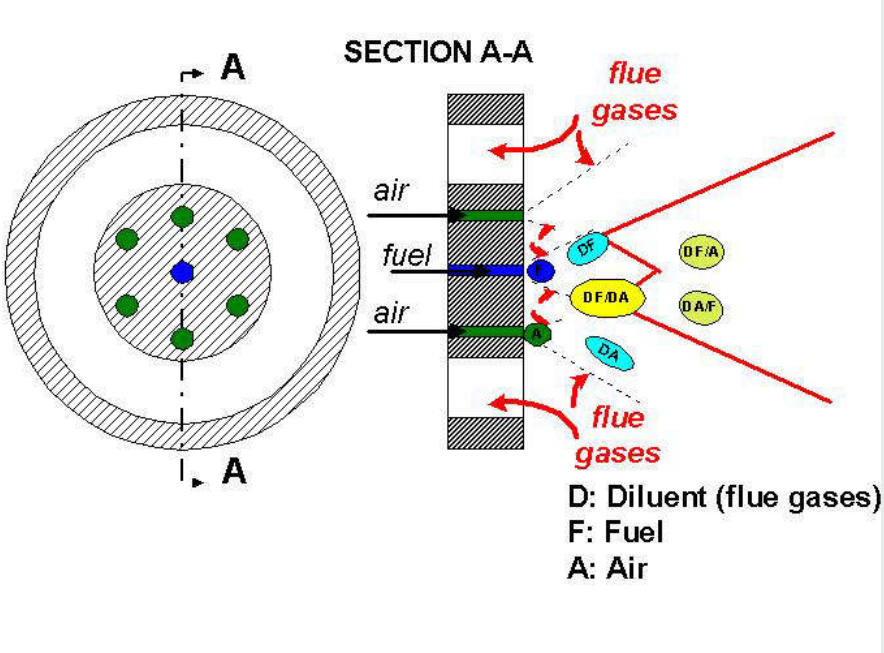
7. Principles of FLOX

Conventional flames: Diffusion flame in FLOX burner



8. Principles of FLOX

Flameless oxidation in FLOX burner



9. Mathematical Models

Mass Continuity

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \widetilde{\rho U_k}}{\partial x_k} = 0$$

Momentum conservation equation

$$\frac{\partial(\overline{\rho}\widetilde{U}_i)}{\partial t} + \frac{\partial(\overline{\rho}\widetilde{U_k}\widetilde{U}_i)}{\partial x_k} = -\frac{\partial \widetilde{p}}{\partial x_i} + g_i + \frac{\partial \widetilde{\tau}_{ik}}{\partial x_k}$$

$$\tilde{\tau}_{ij} = \mu_{eff}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right) - \frac{2}{3}\mu\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}$$

Energy conservation equation

$$\frac{\partial \overline{\rho}\tilde{h}}{\partial t} + \frac{\partial(\overline{\rho}\tilde{U}_k\tilde{h})}{\partial x_k} = -\frac{\partial \tilde{p}}{\partial t} + \frac{\partial}{\partial x_k}\left(\Gamma_h \frac{\partial \tilde{h}}{\partial x_k}\right) + S_h$$

$$S_h = 4\sigma K_g\left[T_r^4 - T_g^4\right] \;;\quad \Gamma_{\psi,eff} = \frac{\mu}{\sigma_\psi} + \frac{\mu_t}{\sigma_{\psi,t}}$$

and

$$\mu_t = C_\mu \overline{\rho}\frac{\widetilde{k}^2}{\widetilde{\epsilon}} \qquad C_\mu = \text{constant}$$

Turbulence model: k-ϵ eddy viscosity model

Turbulence kinetic energy, k

$$\frac{\partial \overline{\rho}\tilde{k}}{\partial t} + \frac{\partial \overline{\rho}\tilde{U}_i\tilde{k}}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\Gamma_{k,t}\frac{\partial \tilde{k}}{\partial x_i}\right] + G - \overline{\rho}\tilde{\epsilon}$$

Turbulence kinetic energy dissipation rate, ϵ

$$\frac{\partial \overline{\rho}\tilde{\epsilon}}{\partial t} + \frac{\partial \rho U_i\tilde{\epsilon}}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\Gamma_{\epsilon,t}\frac{\partial \tilde{\epsilon}}{\partial x_i}\right] + \left(C_1 G - C_2\rho\tilde{\epsilon}\right)\frac{\tilde{\epsilon}}{\tilde{k}}$$

Radiation model: Non-equilibrium diffusion radiation model
Absorption modelled by Truelove correlations

Solution Algorithm: SIMPLE Algorithm

10. Combustion Models:

Simple Chemical Reacting Model

1kg of **Fuel** + skg of **Oxidant** $\Rightarrow$ (1 + s)kg of **Products**

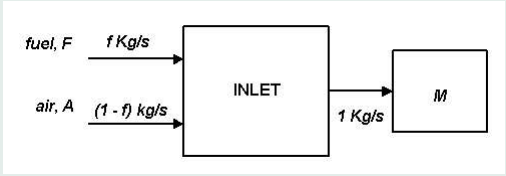
Infinitely fast chemical reactions $\Rightarrow$ conserved scalar approach is employed

A passive scalar variable, ψ such that $\psi = sm_{fu} - m_{ox}$

Mixture fraction $f = \frac{\psi - \psi_A}{\psi_F - \psi_A}$

$$f = \frac{\{sm_{fu} - m_{ox}\} - \{sm_{fu} - m_{ox}\}}{\{sm_{fu} - m_{ox}\}_F - \{sm_{fu} - m_{ox}\}_A}$$

$$f_{st} = \frac{m_{ox,A}}{sm_{fu,F} + m_{ox,A}}$$

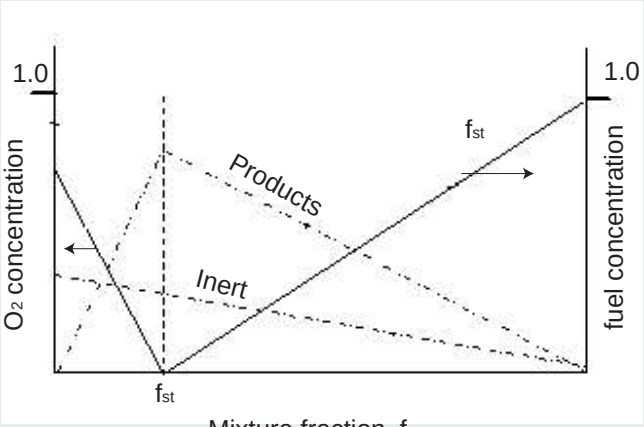


11. Combustion Models: (Contd)

Fast chemistry assumption implies

$$\text{if } 0 < f < f_{st} \quad m_{fu} = 0; \quad m_{ox} = \frac{f_{st} - f}{f_{st}} m_{ox,A}$$

$$\text{if } f_{st} < f < 1 \quad m_{ox} = 0; \quad m_{fu} = \frac{f - f_{st}}{1 - f_{st}} m_{fu,F}$$



12. Combustion Models: (Contd)

Mixture fraction with presumed β shape probability density function

$$\frac{\partial \overline{\rho}\tilde{f}}{\partial t} + \frac{\partial(\overline{\rho}U_k\tilde{f})}{\partial x_k} = \frac{\partial}{\partial x_k}\left[\Gamma_{f,t}\frac{\partial \tilde{f}}{\partial x_k}\right]$$

Mixture fraction variance transport equation

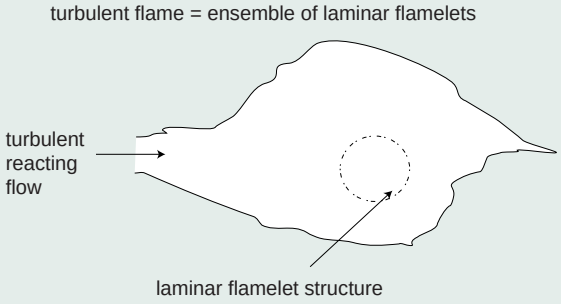
$$\frac{\partial \overline{\rho}\widetilde{f''^2}}{\partial t} + \frac{\partial(\overline{\rho}U_k\widetilde{f''^2})}{\partial x_k} = \frac{\partial}{\partial x_k}\left[\Gamma_{f,t}\frac{\partial \widetilde{f''^2}}{\partial x_k}\right] + C_g\mu_f\left(\frac{\partial \widetilde{f}}{\partial x_k}\right)^2 - C_d\overline{\rho}\frac{\epsilon}{k}\widetilde{f''^2}$$

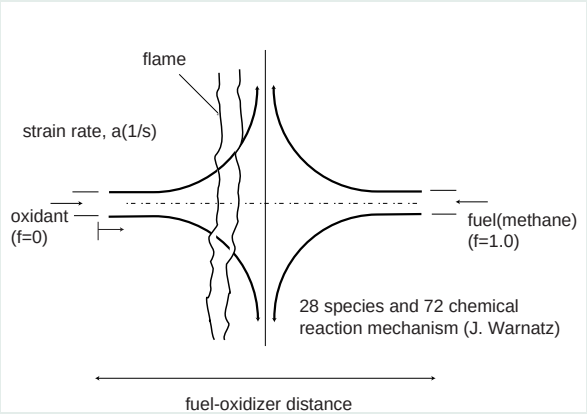
$$\tilde{\psi} = \int_0^1 \psi(\tilde{f})P(f)d\tilde{f}; \qquad P(f) = \frac{f^{a-1}(1-f)^{b-1}}{\int_0^1 f^{a-1}(1-f)^{b-1}df}$$

$$a = f\left[\frac{f(1-f)}{f''^2} - 1\right]; \qquad b = \frac{1-f}{f}a$$

13. Combustion Models

Flamelet theory





$$\rho \frac{\partial \psi_i}{\partial t} = \rho \frac{\mu}{\sigma_{SC}} \left(\frac{\partial f}{\partial x} \right)^2 \frac{\partial^2 \psi_i}{\partial f^2} + w_i$$

14. Combustion Models: (Contd)

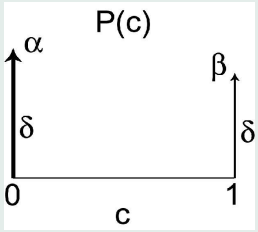
Premixed combustion flamelet model → reaction progress variable, c: (Bray-Moss-Libby model

Presumed double delta pdf for c:

$\tilde{P}(c) = \alpha\delta(c) + \beta\delta(1-c)$

$\widetilde{\psi} = \int_o^1 \psi(c)P(c)dc$

$\widetilde{\psi} = c\psi_b + (1-c)\psi_u$



$c = \frac{m_{f,u} - m_{fu,u}}{m_{fu,b} - m_{fu,u}}$ $c = 0$ (u, unburnt regions) $c = 1$ (b, burnt regions)

Reaction progress transport equation

$$\frac{\partial \overline{\rho}\tilde{c}}{\partial t} + \frac{\partial(\overline{\rho}U_k\tilde{c})}{\partial x_k} = \frac{\partial}{\partial x_k}\left[\Gamma_c \frac{\partial \tilde{c}}{\partial x_k}\right] + w_c$$

where the chemical source term w_c is modelled according to:

$$w_c = C_r\overline{\rho}_u \frac{S_L^0\epsilon}{U_k k}\tilde{c}(1-\tilde{c})$$

15. Combustion Models: (Contd)

Non-premixed combustion flamelet model → mixture fraction variable, f:

$$\frac{\partial \overline{\rho}\tilde{f}}{\partial t} + \frac{\partial(\overline{\rho}U_k\tilde{f})}{\partial x_k} = \frac{\partial}{\partial x_k}\left[\Gamma_f \frac{\partial \tilde{f}}{\partial x_k}\right]$$

Scalar dissipation rate accounts for flamelet stretching due to velocity field

$$\chi_{ref} = \left(\frac{\nu}{Sc}\right)_{ref}\left(\frac{\partial f}{\partial x_i}\right)^2_{ref}; \psi = \psi(f;\chi_{ref}) \rightarrow \text{library of flamelets}$$

Averaged property obtained from bivariate pdf $P(f,\chi)$

$$\tilde{\psi}_i = \int_0^\infty \int_0^1 \psi_i(f;\chi)P(f,\chi)df\,d\chi$$

$P(f,\chi_{ref}) \Rightarrow P(f)P(\chi_{ref})$ **(statistical independence)**

$$\tilde{\psi}_i = P_c \int_0^1 \psi_i(f,\chi)P(f)df + (1-P_c)\int_0^1 \psi_i(f,\chi)P(f)df$$

$P(\chi) = \frac{1}{\chi\sigma\sqrt{2\pi}}\exp\{-\frac{1}{2\sigma^2}(\log_e\chi-\mu)^2\}$ (log-normal pdf); $P(f) = \frac{f^{a-1}(1-f)^{b-1}}{\int_0^1 f^{a-1}(1-f)^{b-1}df}$ ($\beta-$ pdf)

$$P_c = \frac{1}{2}\{erf[\frac{1}{\sigma\sqrt{2}}(\log_e\chi_q-\mu)]+1\}$$

16. Combustion Models: Choice of Model

Model Formulation ⇒ Flamelet/Progress-variable model

Possible states include

$c = 1$ completely burnt zones, hence chemical species determined by
$\tilde{\psi_{i,b}} = \int_0^\infty \int_0^1 \psi_i(f;\chi) P(f,\chi) df\, d\chi$
where $\psi_i(f;\chi) \Rightarrow$ flamelet library setting dissipation of flamelet equal to local mean representative scalar dissipation rate, $\widetilde{\chi}$ defined as
$\widetilde{\chi} = C_x \frac{\epsilon}{k} \widetilde{f''^2}$

$c = 0$ The mass fractions are those of the fuel and air in an unburnt mixture at the local value of mixture fraction.

$0 < c < 1$ The double delta pdf of reaction progress variable in accordance with fast chemical kinetics allows interpolation between unburnt state and burnt state
$\psi_i = c\psi_{i,b} + (1-c)\psi_{i,u}$

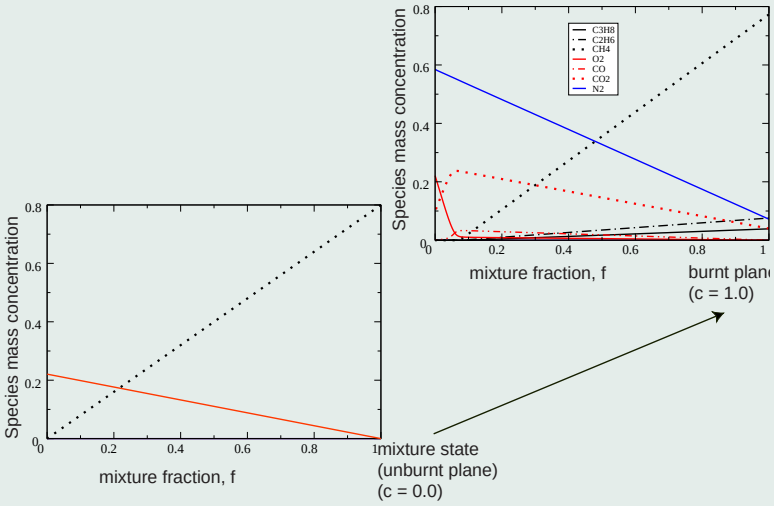
17. Combustion Models: Choice of Model

The mean temperature, $\tilde{T}$, is calculated from the local mean enthalpy $\tilde{h}$.

$$\tilde{T} = \frac{\tilde{h} - \sum_{i=1}^{N} \tilde{\psi}_i \Delta H_i}{C_p}$$

The density $\overline{\rho}$ is calculated from the mean temperature according to

$$\overline{\rho} = \frac{P}{R\tilde{T}} \sum_{k=1}^{N} \frac{\psi_k}{M_k}$$



18. Nitrogen Oxides (NO_x) emission model

Thermal NO_x[2]	**Prompt NO_x**	**Fuel NO_x**
$O + N_2 \leftrightarrow NO + N$	$CH + N_2 \leftrightarrow HCN + N$	negligible fuel-bound
$N + O_2 \leftrightarrow NO + O$	$CH_2 + N_2 \leftrightarrow HCN + NH$	nitrogen compounds
$N + OH \leftrightarrow NO + H$	$CH_2 + N_2 \leftrightarrow H_2CN + N$	
	$C + N_2 \leftrightarrow CN + N$	

Global Nitric Oxide scheme

R1: $N_2 + O_2 \rightarrow NO$ (simplification of Zeldovich mechanism)
R2: $N_2 + CH_i + O_2 \rightarrow NO$ (Prompt NO sequence)
R3: $NO + O_2 \rightarrow N_x$ (NO Oxidation)

$$\frac{\partial \rho m_i}{\partial t} + \frac{\partial \rho u_k m_i}{\partial x_k} = \frac{\partial}{\partial x_k}\left[\Gamma_{k,t}\frac{\partial m_i}{\partial x_k}\right] + S_i$$

$$S_{NO} = R_1 \chi_{O_2}\chi_{N_2} + R_2 \chi_O^b \chi_{N_2}\chi_{CH_i} + R_3 \chi_{O_2}^{-1/2}\chi_{NO}^2$$

$$S_{N_2} = -R_1 \chi_{O_2}\chi_{N_2} - R_2 \chi_O^b \chi_{N_2}\chi_{CH_i}$$

Reaction	**A_k (1/s)**	**E_k (Kcal/mole)**	α_k	β_k	**Source**
R1	1.0E+15.6	68.4	-1	-1/2	Sawyer (1981)
R1	1.2E+07.0	60.5	0	0	De Soete (1973)
R1	1.2E+10.0	72.0	0	0	Sawyer (1973)

Rate coeffficients of the global reaction sequence for NO computations

19. Reaction Mechanism for Methane Combustion 28 Species, 72 Reactions (J. Warnatz)

CH_4 Reaction mechanism

Number	Reaction	A	n	E
1f	$O_2 + H \rightarrow OH + O$	2.000E+14	0.00	70.3
2f	$H_2 + O \rightarrow OH + H$	5.060E+04	2.67	26.3
3f	$H_2 + OH \rightarrow H_2O + H$	1.000E+08	1.60	13.8
4f	$2OH \rightarrow H_2O + O$	1.500E+09	1.14	0.42
5f	$O_2 + H + M' \rightarrow HO_2 + M'$	2.300E+18	-0.80	0
6	$HO_2 + H \rightarrow 2OH$	1.500E+14	0.00	4.2
7	$HO_2 + H \rightarrow H_2 + O_2$	2.500E+13	0.00	2.9
8	$HO_2 + OH \rightarrow H_2O + O_2$	6.000E+13	0.00	0
9	$HO_2 + H \rightarrow H_2O + O$	3.000E+13	0.00	7.2
10	$HO_2 + O \rightarrow OH + O_2$	1.800E+13	0.00	-1.7
11	$2HO_2 \rightarrow H_2O_2 + O_2$	2.500E+11	0.00	-5.2
12f	$2OH + M' \rightarrow H_2O_2 + M'$	3.250E+22	-2.00	0
13	$H_2O_2 + H \rightarrow H_2O + OH$	1.000E+13	0.00	15
14f	$H_2O_2 + OH \rightarrow H_2O + HO_2$	5.400E+12	0.00	4.2
15	$2H + M' \rightarrow H_2 + M'$	1.800E+18	-1.00	0
16	$OH + H + M' \rightarrow H_2O + M'$	2.200E+22	-2.00	0

CH_4 Reaction mechanism

17	$2O + M' \rightarrow O_2 + M'$	2.900E+17	-1.00	0
18f	$CO + OH \rightarrow CO_2 + H$	4.400E+06	1.50	-3.1
19	$CH + O_2 \rightarrow CHO + O$	3.000E+13	0.00	0
20	$CO_2 + CH \rightarrow CHO + CO$	3.400E+12	0.00	2.9
21	$CHO + H \rightarrow CO + H_2$	2.000E+14	0.00	0
22	$CHO + OH \rightarrow CO + H_2O$	1.000E+14	0.00	0
23	$CHO + O_2 \rightarrow CO + HO_2$	3.000E+12	0.00	0
24f	$CHO + M' \rightarrow CO + H + M'$	7.100E+14	0.00	70.3
25f	$CH_2 + H \rightarrow CH + H_2$	8.400E+09	1.50	1.4
26	$CH_2 + O \rightarrow CO + 2H$	8.000E+13	0.00	0
27	$CH_2 + O_2 \rightarrow CO + OH + H$	6.500E+12	0.00	6.3
28	$CH_2 + O_2 \rightarrow CO_2 + 2H$	6.500E+12	0.00	6.3
29	$CH_2O + H \rightarrow CHO + H_2$	2.500E+13	0.00	16.7
30	$CH_2O + O \rightarrow CHO + OH$	3.500E+13	0.00	14.6
31	$CH_2O + OH \rightarrow CHO + H_2O$	3.000E+13	0.00	5
32	$CH_2O + M' \rightarrow CHO + H + M'$	1.400E+17	0.00	320
33f	$CH_3 + H \rightarrow CH_2 + H_2$	1.800E+14	0.00	63
34	$CH_3 + H \rightarrow CH_4$ k_0	6.257E+23	-1.80	0
	k_∞	2.108E+14	0.00	0
35	$CH_3 + O \rightarrow CH_2O + H$	7.000E+13	0.00	0
36f	$2CH_3 \rightarrow C_2H_6$ k_0	1.272E+41	-7.00	11.6

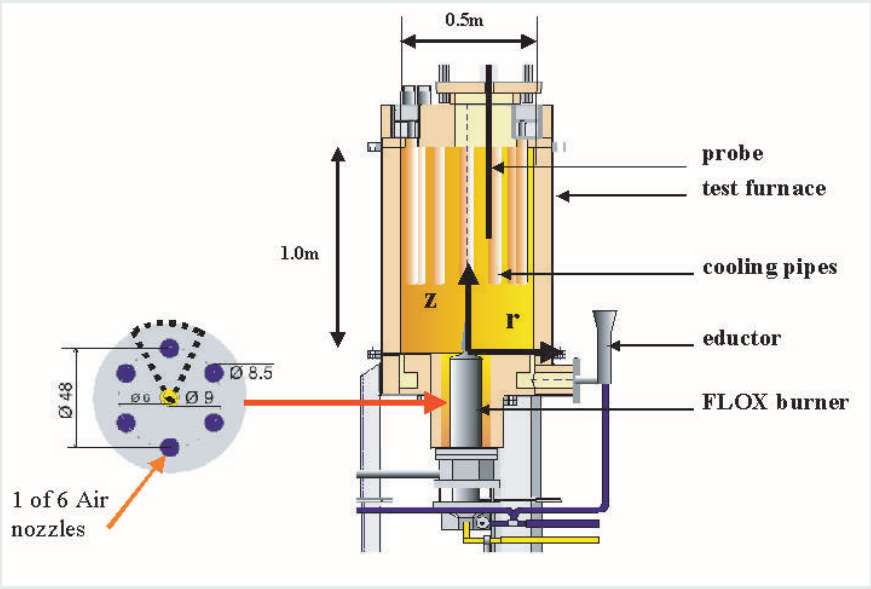
CH_4 Reaction mechanism

		k_∞	1.813E+13	0.00	0
37	$CH_3 + O_2 \rightarrow CH_2O + OH$		3.400E+11	0.00	37.4
38f	$CH_4 + H \rightarrow CH_3 + H_2$		2.200E+04	3.00	36.6
39	$CH_4 + O \rightarrow CH_3 + OH$		1.200E+07	2.10	31.9
40f	$CH_4 + OH \rightarrow CH_3 + H_2O$		1.600E+06	2.10	10.3
41f	$C_2H + H_2 \rightarrow C_2H_2 + H$		1.100E+13	0.00	12
42	$C_2H + O_2 \rightarrow CHCO + O$		5.000E+13	0.00	6.3
43f	$CHCO + H \rightarrow CH_2 + CO$		3.000E+13	0.00	0
44	$CHCO + O \rightarrow 2CO + H$		1.000E+14	0.00	0
45	$C_2H_2 + O \rightarrow CH_2 + CO$		4.100E+08	1.50	7.1
46	$C_2H_2 + O \rightarrow CHCO + H$		4.300E+14	0.00	50.7
47f	$C_2H_2 + OH \rightarrow C_2H + H_2O$		1.000E+13	0.00	29.3
48	$C_2H_2 + CH \rightarrow C_3H_3$		3.000E+13	0.00	0
49	$C_2H_3 + H \rightarrow C_2H_2 + H_2$		3.000E+13	0.00	0
50	$C_2H_3 + O_2 \rightarrow C_2H_2 + HO_2$		5.400E+11	0.00	0
51f	$C_2H_3 \rightarrow C_2H_2 + H$	k_0	1.187E+42	-7.50	190
		k_∞	2.000E+14	0.00	166
52f	$C_2H_4 + H \rightarrow C_2H_3 + H_2$		1.500E+14	0.00	42.7
53	$C_2H_4 + O \rightarrow CH_3 + CO + H$		1.600E+09	1.20	3.1
54f	$C_2H_4 + OH \rightarrow C_2H_3 + H_2O$		3.000E+13	0.00	12.6

CH_4 Reaction mechanism

55	$C_2H_4 + M' \rightarrow C_2H_2 + H_2 + M'$		2.500E+17	0.00	320
56f	$C_2H_5 + H \rightarrow 2CH_3$		3.000E+13	0.00	0
57	$C_2H_5 + O_2 \rightarrow C_2H_4 + HO_2$		2.000E+12	0.00	20.9
58f	$C_2H_5 \rightarrow C_2H_4 + H$	k_0	1.000E+16	0.00	126
		k_∞	1.300E+13	0.00	167
59	$C_2H_6 + H \rightarrow C_2H_5 + H_2$		5.400E+02	3.50	21.8
60	$C_2H_6 + O \rightarrow C_2H_5 + OH$		3.000E+07	2.00	21.4
61	$C_2H_6 + OH \rightarrow C_2H_5 + H_2O$		6.300E+06	2.00	2.7
62	$C_3H_3 + O_2 \rightarrow CHCO + CH_2O$		6.000E+12	0.00	0
63	$C_3H_3 + O \rightarrow C_2H_3 + CO$		3.800E+13	0.00	0
64f	$C_3H_4 \rightarrow C_3H_3 + H$		5.000E+14	0.00	370
65	$C_3H_4 + O \rightarrow C_2H_2 + CH_2O$		1.000E+12	0.00	0
66	$C_3H_4 + O \rightarrow C_2H_3 + CHO$		1.000E+12	0.00	0
67	$C_3H_4 + OH \rightarrow C_2H_3 + CH_2O$		1.000E+12	0.00	0
68	$C_3H_4 + OH \rightarrow C_2H_4 + CHO$		1.000E+12	0.00	0
69f	$C_3H_5 \rightarrow C_3H_4 + H$		3.980E+13	0.00	293
70	$C_3H_5 + H \rightarrow C_3H_4 + H_2$		1.000E+13	0.00	0
71f	$C_3H_6 \rightarrow C_2H_3 + CH_3$		3.150E+15	0.00	359
72	$C_3H_6 + H \rightarrow C_3H_5 + H_2$		5.000E+12	0.00	6.3

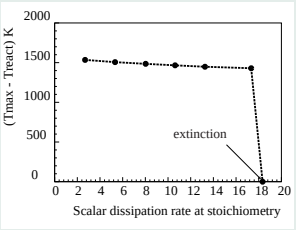
20. FLOX experiment by Wunning



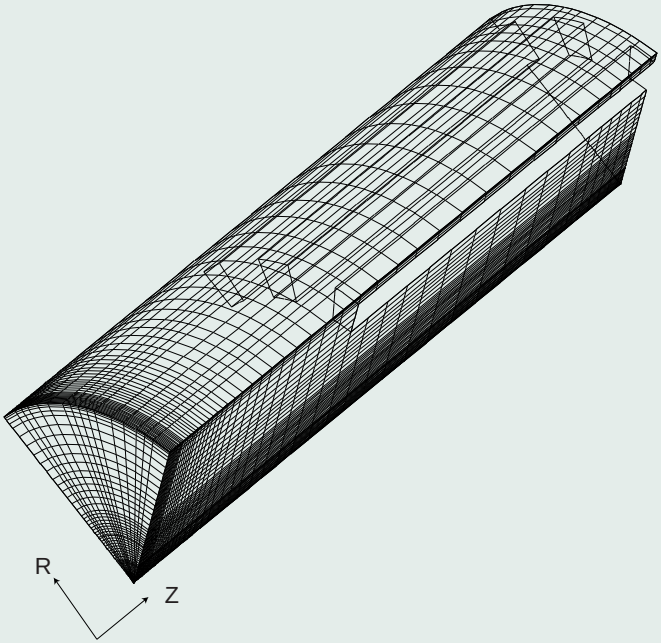
21. Discretised Mesh & Specifications: Wunning expt

Operating conditions
Fuel volume flow rate $= 2.5m^3/hr$
Fuel type $=$ methane
Excess air $= 15\%$
Air preheat temperature $= 650°C$
Air jet velocity $= 100m/s$

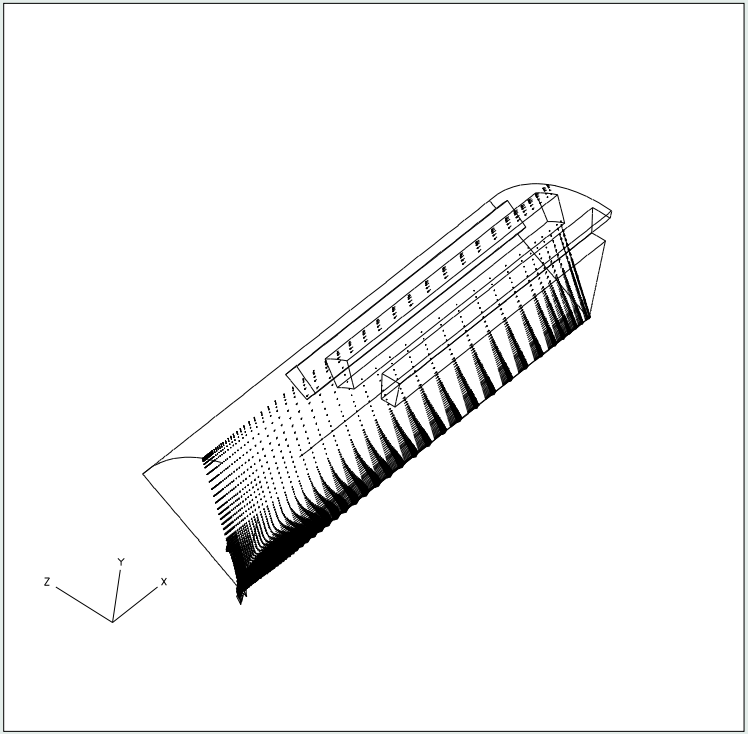
Computational details
Mesh size: 57x56x17 ($60°$ sector)
Combustion model
1. Fast chemistry model
2. Flamelet model
CH_4 Reaction mechanism:
28 Species, 72 reaction (Warnatz J.)



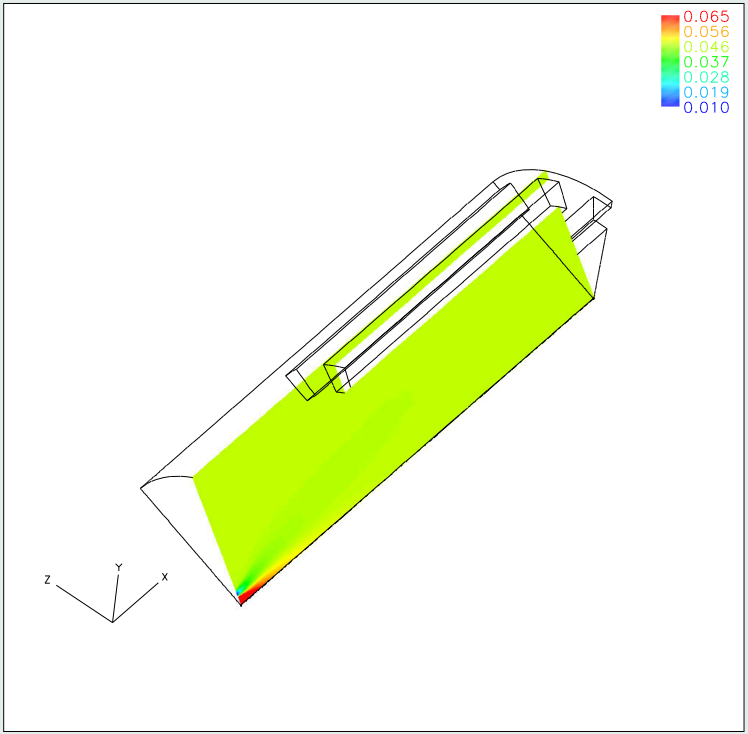
Extinction limit, $\chi_{st} \approx 18.4s^{-1}$



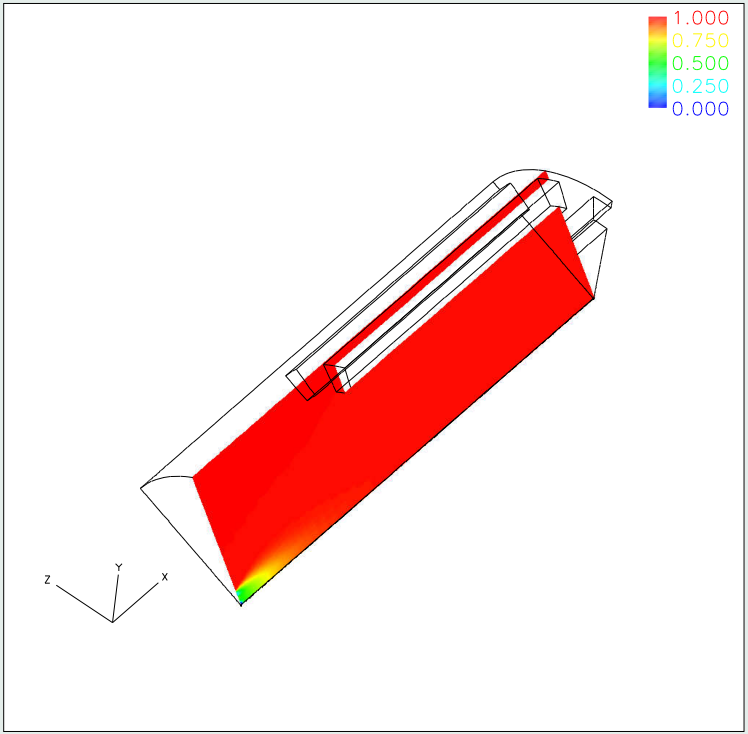
22. Axial velocity distribution (Wunning expt)



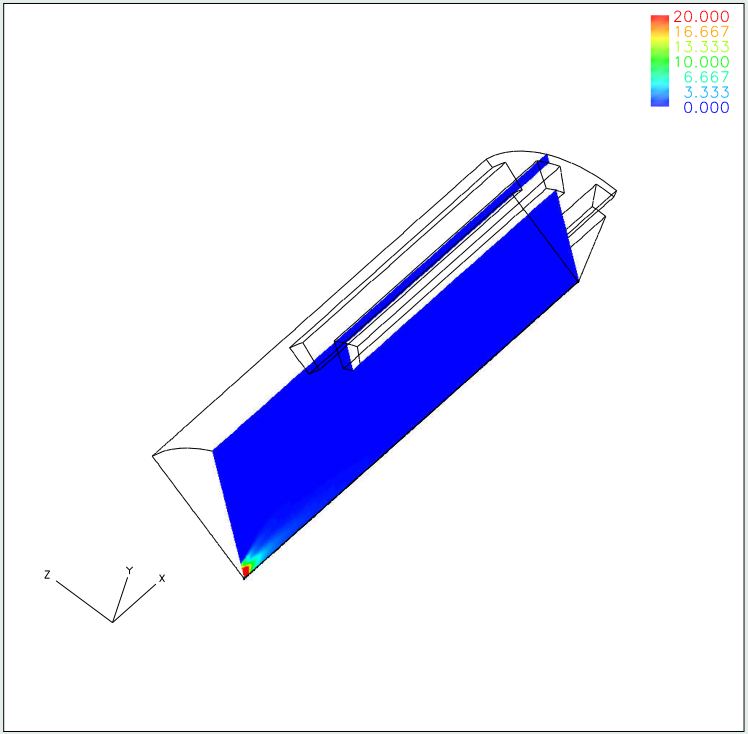
23. Mixture fraction distribution (Wunning expt)



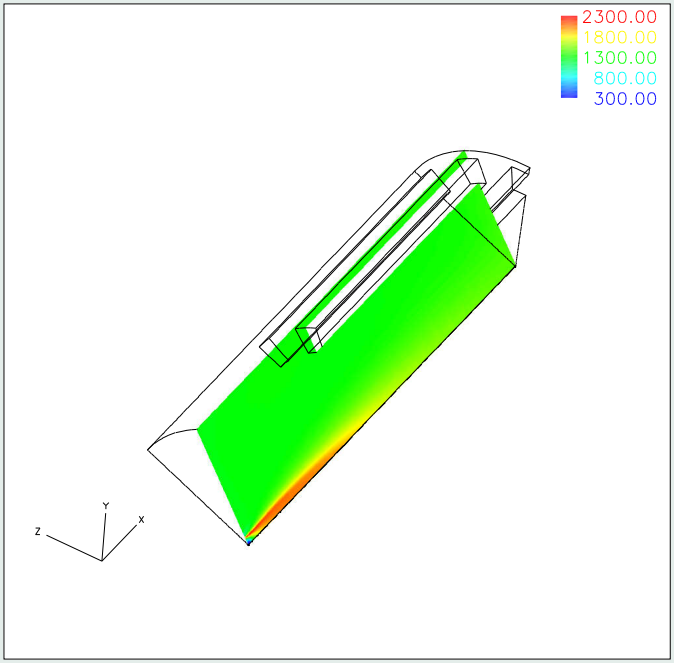
24. Distribution of reaction progress variable (Wunning expt)



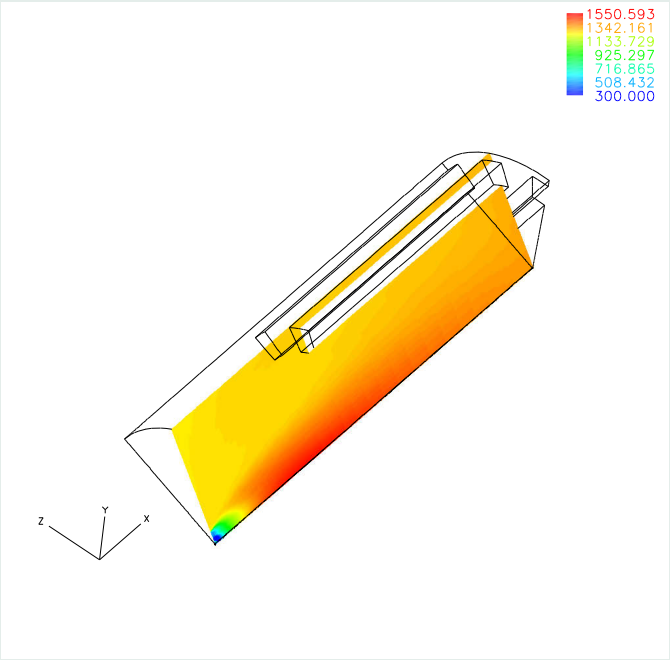
25. Distribution of scalar dissipation rate χ (Wunning expt)



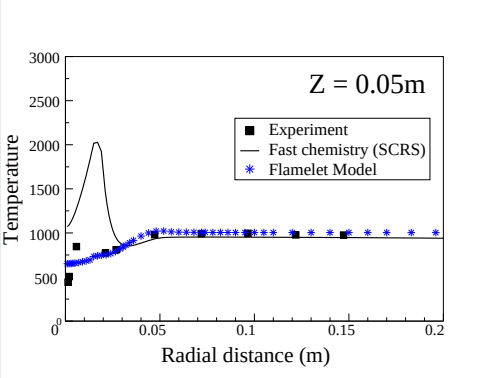
26. Temperature distribution with fast chemistry model (Wunning expt)

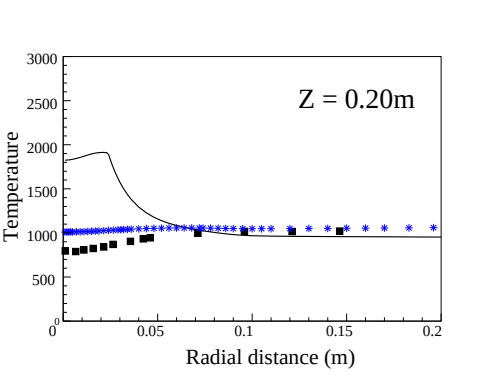


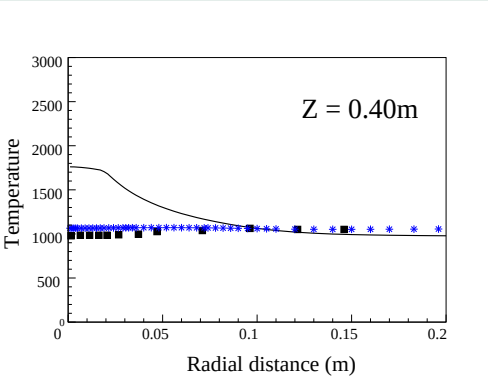
27. Temperature distribution with flamelet-progress variable model (Wunning expt)

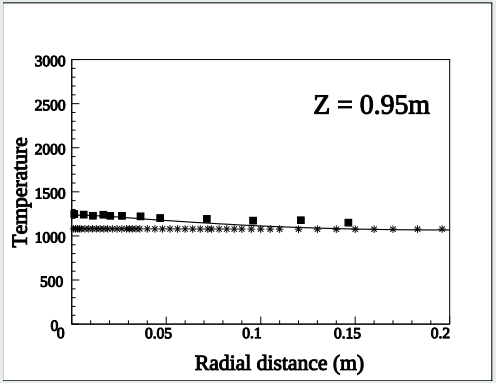


28. Radial temperature distribution simulation & measurements (Wunning expt)

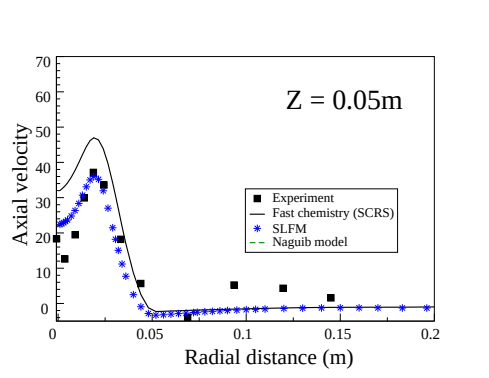


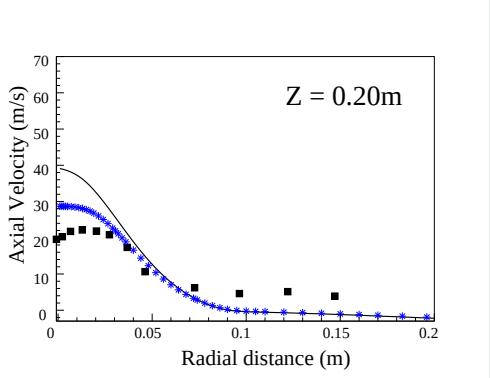


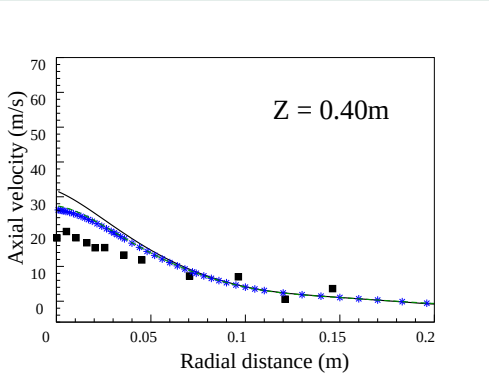


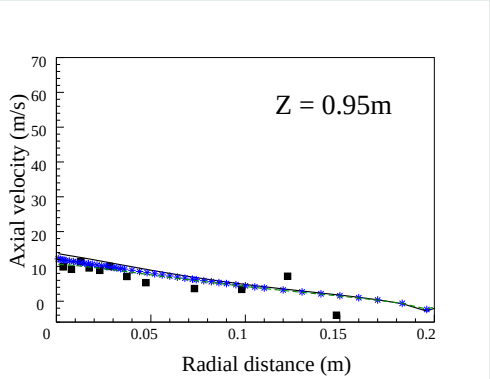


29. Radial axial velocity distribution simulation & measurments (Wunning)









30. Discussion of result

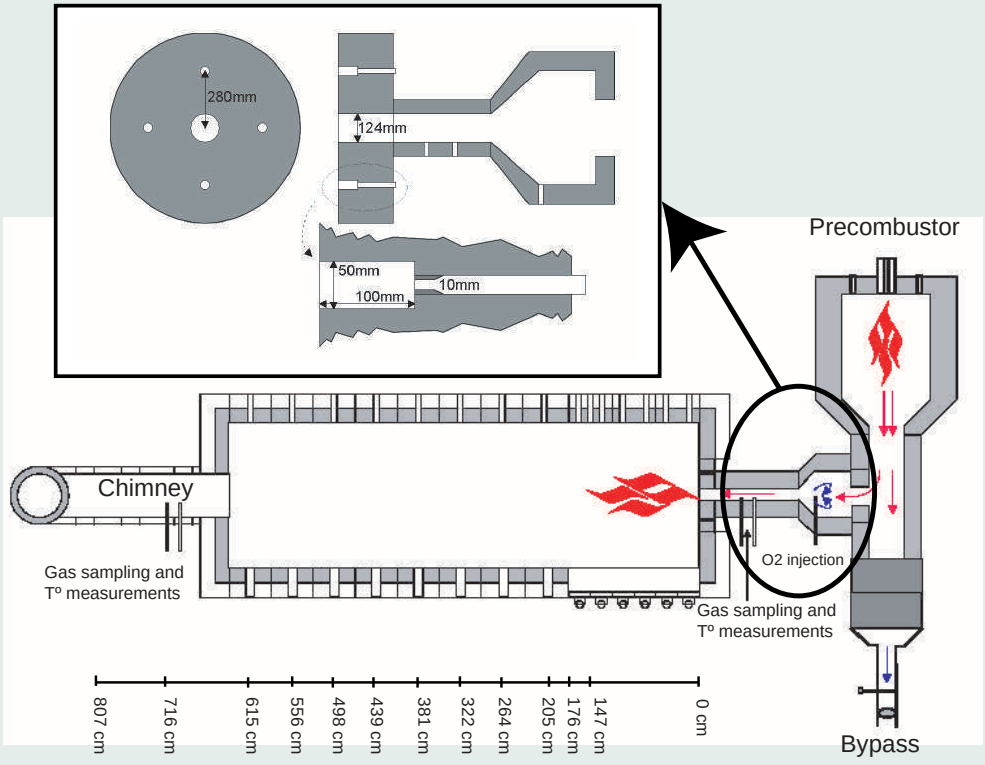
- Fast chemistry combustion model is suitable for FLOX except near burner region where high jet velocity strains the stoichiometric mixture fraction surface.

- Flamelet model shows better predictability in the near burner region due to accountability of strain effects on the flamelet.

- Predictions show that fast chemistry combustion model may not be applicable to flameless oxidation, therefore to confirm this result other flameless oxidation experiment is simulated

31. HITAC experiment by IFRF

IFRF Furnace

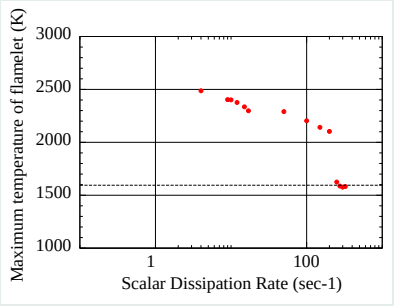


32. Discretised mesh and computational details HITAC simualtion

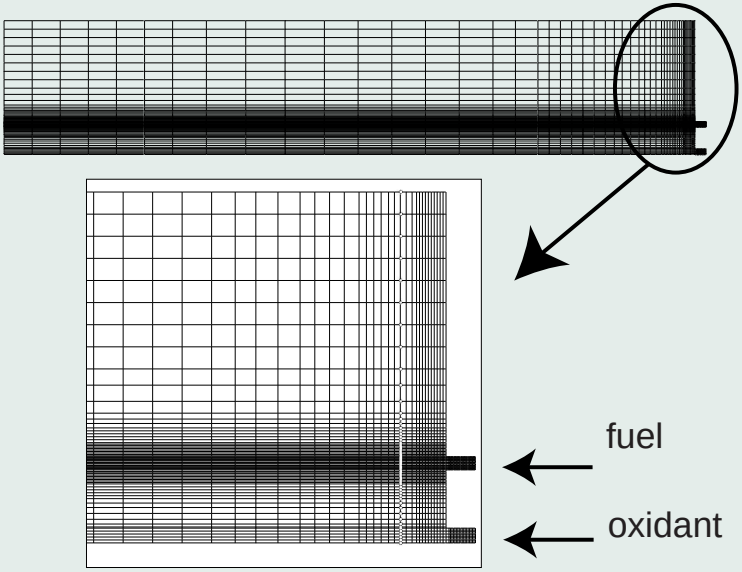
Computational details

Mesh size: 72x75x21 (180° sector)
Standard k-ϵ model
Non-equilibrium diffusion radiation model
Combustion models:

1. Fast chemistry model
2. Flamelet model



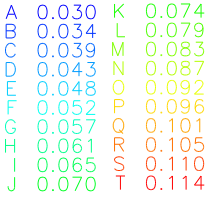
Extinction limit of flamelet at $\chi_{st} \approx 200 s^{-1}$

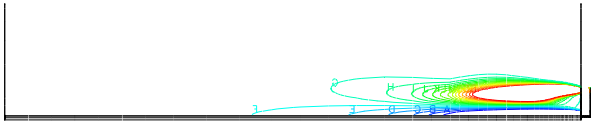


33. Experimental conditions of IFRF experiment

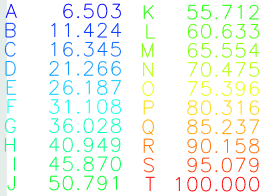
	Flow rate Kg/h	Temp °C	Enthalpy MW	Composition % vol
Natural Gas	47	25	0.58	CH_4 87.8%; C_2H_6 4.6%; $C0_2$ 1.65%; C_3H_8 1.6%; C_4H_10 0.5%;N_2 3.7%
Vitiated air	830	1300	0.35	H_20 15%; O_2 19.5%; N_2 59.1%; CO_2 6.4%
Furnace exit gases	877	1220	0.38	O_2 1.6%; N_2 54.4 %; H_2O 29.6%; CO_2 14.4%;

34. HITAC simulation: Mixture fraction and strain rate distribution





Mixture fraction field



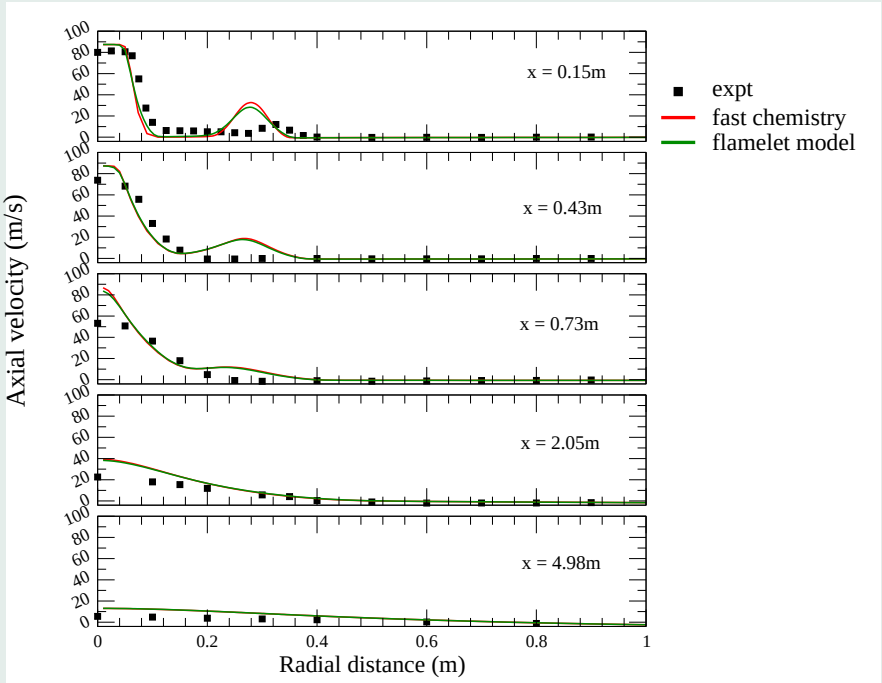
Strain rate field with Flamelet model

35. HITAC simulation: Temperature distribution

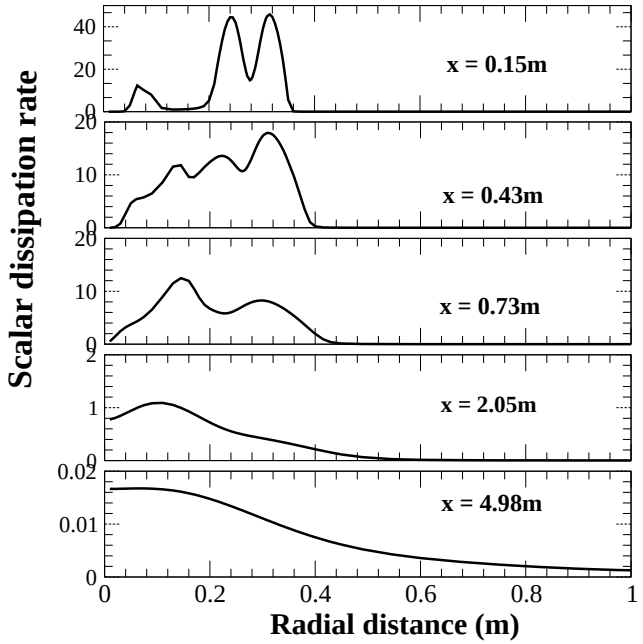
Temperure field with Flamelet model

Temperature field with Fast chemistry

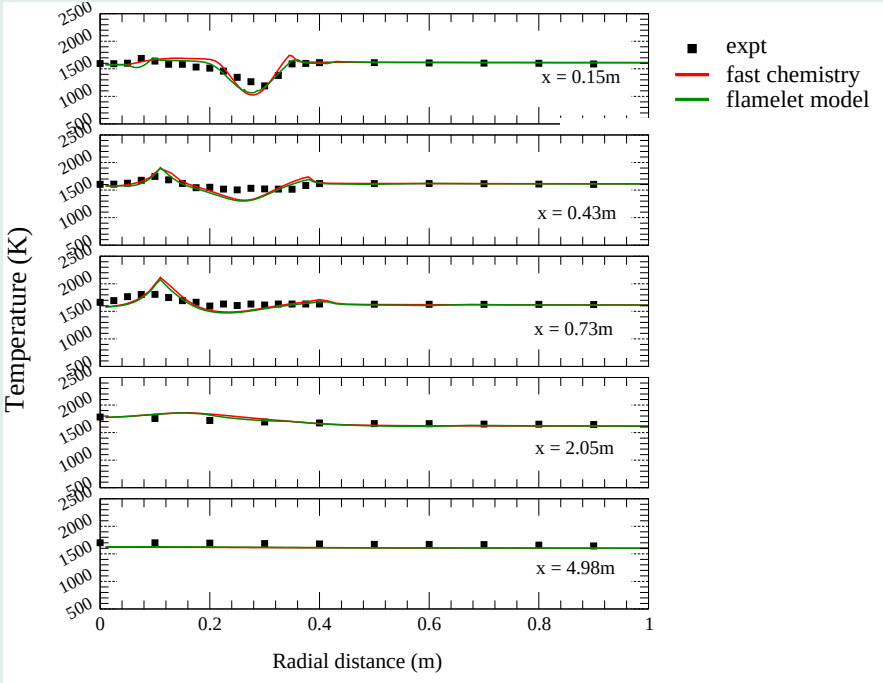
36. HITAC simulations: Radial axial velocity distribution prediction & measurements



37. HITAC simulations: Radial scalar dissipation rate distribution prediction & measurements

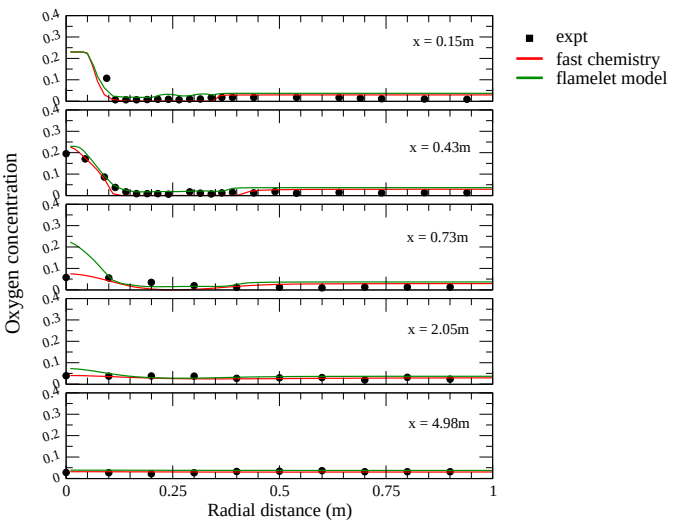


38. HITAC simulations: Radial temperature distribution prediction & measurements

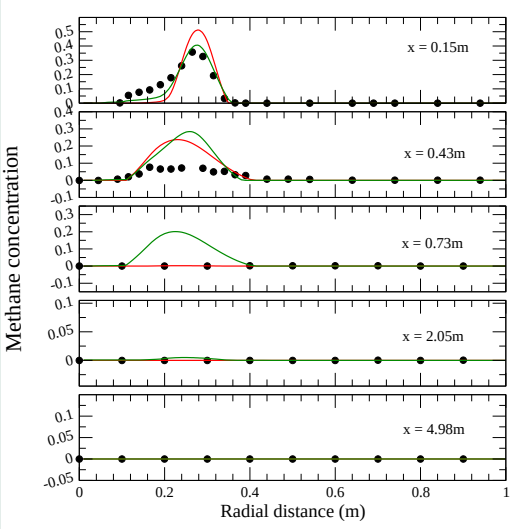


39. HITAC simulations: Radial Oxygen and fuel distribution prediction & measurements

Oxygen concentration

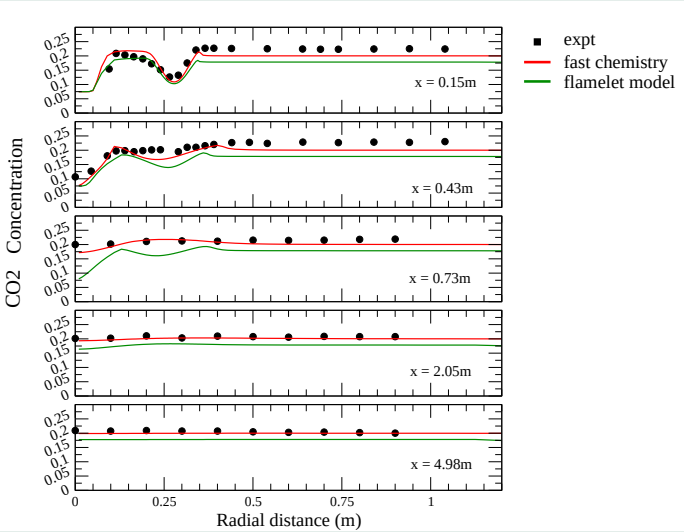


Fuel concentration

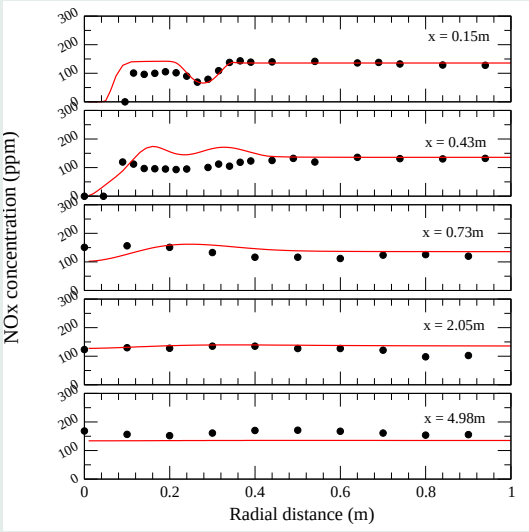


40. HITAC simulations: Radial CO_2 and NO_x distribution prediction & measurements

CO_2 concentration



NO_x concentration



41. Discussion of result

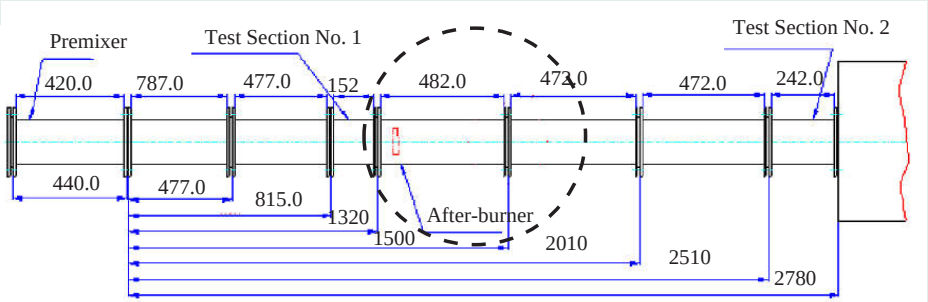
- The fast chemistry and flamelet combustion models temperature predictions agree with the temperature field except near the stoichiometric mixture fraction surface, where temperature is slightly overpredicted by 250K

- Flamelet model predicts little or no influence of strain on the chemical reactions, the predicted field of local scalar dissipation rate is much lower than the predicted extinction limit of $\chi_{st} \approx 200 s^{-1}$

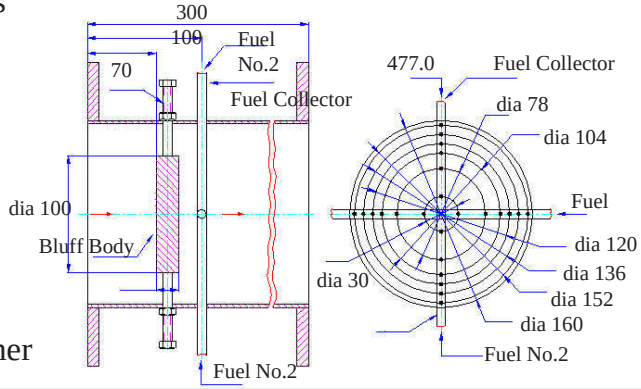
- The level of preheating and the method of recirculation of flue gases could explain why strain is not important in the HITAC experiment. The preheat temperature is higher in the HITAC experimnet than the FLOX experiment. The higher preheat temperature raises the flamelet temperature and hence reduces local quenching effects due to strain.

42. FLOX experiment by Technion

Technion FLOX device



Technion flameless oxidation device

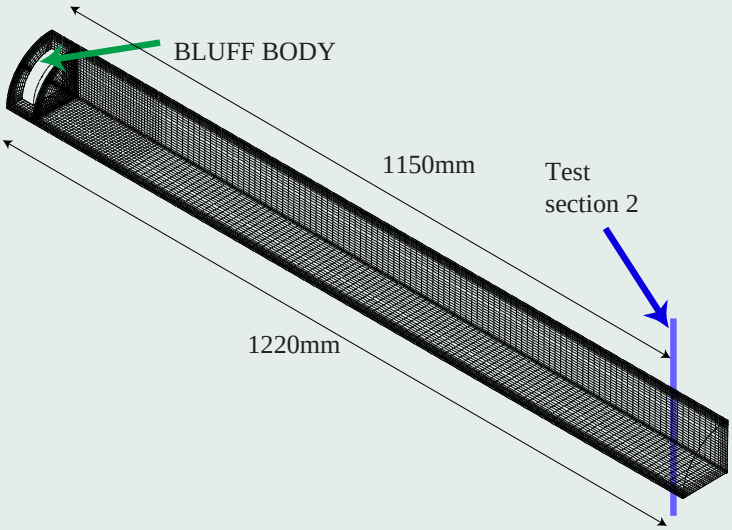


Technion afterburner

43. Discretised mesh and computational details (Technion predictions)

Computational details

Mesh size: 153x37x30 (90° sector)
Standard k-ϵ model
Non-equilibrium diffusion radiation model
Combustion models:
1. Fast chemistry model
2. flamelet model



Oxidant

Stream velocity $= 23.071 \text{ms}^{-1}$
Composition $= 0.108\ O_2; 0.794\ N_2; 0.098\ CO_2$
Temperature $= 1278.05\text{K}$

Fuel

Stream velocity $= 37.910 \text{ms}^{-1}$
Composition $= 0.431\ C_3H_8; 0.569\ C_4H_{10}$
Temperature $= 298\text{K}$

44. High Temperature Reaction Mechanism for Propane and Butane Combustion 36 Species, 200 Reactions (M. Marinov)

C_3H_8 and C_4H_{10} Reaction mechanism

Number	Reaction		A	n	E
1f	$OH + H_2 \rightarrow H + H_2O$		2.140E+08	1.52	14.4
2f	$O + OH \rightarrow O_2 + H$		2.020E+14	-0.40	0
3f	$O + H_2 \rightarrow OH + H$		5.060E+04	2.67	26.3
4f	$H + O_2 + M' \rightarrow HO_2 + M'$	k_0	1.050E+19	-1.26	0
		k_∞	4.520E+13	0.00	0
5f	$OH + HO_2 \rightarrow H_2O + O_2$		2.130E+28	-4.83	14.6
6f	$H + HO_2 \rightarrow 2OH$		1.500E+14	0.00	4.18
7f	$H + HO_2 \rightarrow H_2 + O_2$		8.450E+11	0.65	5.19
8f	$H + HO_2 \rightarrow O + H_2O$		3.010E+13	0.00	7.2
9f	$O + HO_2 \rightarrow O_2 + OH$		3.250E+13	0.00	0
10f	$2OH \rightarrow O + H_2O$		3.570E+04	2.40	-8.84
11f	$2H + M'' \rightarrow H_2 + M''$		1.000E+18	-1.00	0
12f	$2H + H_2 \rightarrow 2H_2$		9.200E+16	-0.60	0
13f	$2H + H_2O \rightarrow H_2 + H_2O$		6.000E+19	-1.25	0
14f	$H + OH + M''' \rightarrow H_2O + M'''$		2.210E+22	-2.00	0
15f	$H + O + M4 \rightarrow OH + M4$		4.710E+18	-1.00	0

C_3H_8 and C_4H_{10} Reaction mechanism

16f	$2O + M5 \rightarrow O_2 + M5$		1.890E+13	0.00	-7.48
17f	$2HO_2 \rightarrow H_2O_2 + O_2$		4.200E+14	0.00	50.1
18f	$2OH + M6 \rightarrow H_2O_2 + M6$	k_0	3.040E+30	-4.63	8.57
		k_∞	1.240E+14	-0.37	0
19f	$H_2O_2 + H \rightarrow HO_2 + H_2$		1.980E+06	2.00	10.2
20f	$H_2O_2 + H \rightarrow OH + H_2O$		3.070E+13	0.00	17.6
21f	$H_2O_2 + O \rightarrow OH + HO_2$		9.550E+06	2.00	16.6
22f	$H_2O_2 + OH \rightarrow H_2O + HO_2$		2.400E+00	4.04	-9.05
23f	$2CH_3 + M7 \rightarrow C_2H_6 + M7$	k_0	1.140E+36	-5.25	7.13
		k_∞	9.220E+16	-1.17	2.66
24f	$CH_3 + H + M8 \rightarrow CH_4 + M8$	k_0	3.310E+30	-4.00	8.82
		k_∞	2.140E+15	-0.40	0
25f	$CH_4 + H \rightarrow CH_3 + H_2$		2.200E+04	3.00	36.6
26f	$CH_4 + OH \rightarrow CH_3 + H_2O$		4.190E+06	2.00	10.7
27f	$CH_4 + O \rightarrow CH_3 + OH$		6.920E+08	1.56	35.5
28f	$CH_4 + HO_2 \rightarrow CH_3 + H_2O_2$		1.120E+13	0.00	103
29f	$CH_3 + HO_2 \rightarrow CH_4 + O_2$		3.000E+12	0.00	0
30f	$CH_3 + O \rightarrow CH_2O + H$		8.000E+13	0.00	0
31f	$CH_3 + O_2 \rightarrow CH_2O + OH$		2.510E+11	0.00	61.3
32f	$CH_3 + OH \rightarrow S\text{-}CH_2 + H_2O$		2.650E+13	0.00	9.15
33f	$CH_3 + OH \rightarrow CH_2 + H_2O$		3.000E+06	2.00	10.5

C_3H_8 and C_4H_{10} Reaction mechanism

34f	$CH_3 + OH \rightarrow CH_2O + H_2$	2.250E+13	0.00	18
35f	$CH_3 + H \rightarrow CH_2 + H_2$	9.000E+13	0.00	63.2
36f	$CH_3 + M9 \rightarrow CH + H_2 + M9$	6.900E+14	0.00	345
37f	$CH_3 + M10 \rightarrow CH_2 + H + M10$	1.900E+16	0.00	383
38f	$CH_2 + H \rightarrow CH + H_2$	1.000E+18	-1.56	0
39f	$CH_2 + OH \rightarrow CH + H_2O$	1.130E+07	2.00	12.6
40f	$CH_2 + OH \rightarrow CH_2O + H$	2.500E+13	0.00	0
41f	$CH_2 + CO_2 \rightarrow CH_2O + CO$	1.100E+11	0.00	4.18
42f	$CH_2 + O \rightarrow CO + 2H$	5.000E+13	0.00	0
43f	$CH_2 + O \rightarrow CO + H_2$	3.000E+13	0.00	0
44f	$CH_2 + O_2 \rightarrow CH_2O + O$	3.290E+21	-3.30	12
45f	$CH_2 + O_2 \rightarrow CO_2 + 2H$	3.290E+21	-3.30	12
46f	$CH_2 + O_2 \rightarrow CO_2 + H_2$	1.010E+21	-3.30	6.31
47f	$CH_2 + O_2 \rightarrow CO + H_2O$	7.280E+19	-2.54	7.57
48f	$CH_2 + O_2 \rightarrow HCO + OH$	1.290E+20	-3.30	1.19
49f	$CH_2 + CH_3 \rightarrow C_2H_4 + H$	4.000E+13	0.00	0
50f	$2CH_2 \rightarrow C_2H_2 + 2H$	4.000E+13	0.00	0
51f	$CH_2 + HCCO \rightarrow C_2H_3 + CO$	3.000E+13	0.00	0
52f	$S\text{-}CH_2 + M11 \rightarrow CH_2 + M11$	1.000E+13	0.00	0
53f	$S\text{-}CH_2 + CH_4 \rightarrow 2CH_3$	4.000E+13	0.00	0

C_3H_8 and C_4H_{10} Reaction mechanism

54f	$S\text{-}CH_2 + C_2H_6$	$\rightarrow$	$CH_3 + C_2H_5$	1.200E+14	0.00	0
55f	$S\text{-}CH_2 + O_2$	$\rightarrow$	$CO + OH + H$	7.000E+13	0.00	0
56f	$S\text{-}CH_2 + H_2$	$\rightarrow$	$CH_3 + H$	7.000E+13	0.00	0
57f	$S\text{-}CH_2 + O$	$\rightarrow$	$CO + 2H$	3.000E+13	0.00	0
58f	$S\text{-}CH_2 + OH$	$\rightarrow$	$CH_2O + H$	3.000E+13	0.00	0
59f	$S\text{-}CH_2 + H$	$\rightarrow$	$CH + H_2$	3.000E+13	0.00	0
60f	$S\text{-}CH_2 + CO_2$	$\rightarrow$	$CH_2O + CO$	3.000E+12	0.00	0
61f	$S\text{-}CH_2 + CH_3$	$\rightarrow$	$C_2H_4 + H$	2.000E+13	0.00	0
62f	$S\text{-}CH_2 + CH_2CO$	$\rightarrow$	$C_2H_4 + CO$	1.600E+14	0.00	0
63f	$CH + O_2$	$\rightarrow$	$HCO + O$	3.300E+13	0.00	0
64f	$CH + O$	$\rightarrow$	$CO + H$	5.700E+13	0.00	0
65f	$CH + OH$	$\rightarrow$	$HCO + H$	3.000E+13	0.00	0
66f	$CH + CO_2$	$\rightarrow$	$HCO + CO$	3.400E+12	0.00	2.89
67f	$CH + H_2O$	$\rightarrow$	$CH_2O + H$	1.170E+15	-0.75	0
68f	$CH + CH_2O$	$\rightarrow$	$CH_2CO + H$	9.460E+13	0.00	-2.15
69f	$CH + CH_2$	$\rightarrow$	$C_2H_2 + H$	4.000E+13	0.00	0
70f	$CH + CH_3$	$\rightarrow$	$C_2H_3 + H$	3.000E+13	0.00	0
71f	$CH + CH_4$	$\rightarrow$	$C_2H_4 + H$	6.000E+13	0.00	0
72f	$CH_2O + OH$	$\rightarrow$	$HCO + H_2O$	3.430E+09	1.18	-1.87
73f	$CH_2O + H$	$\rightarrow$	$HCO + H_2$	2.190E+08	1.77	12.6
74f	$CH_2O + M12$	$\rightarrow$	$HCO + H + M12$	3.310E+16	0.00	339

C_3H_8 and C_4H_{10} Reaction mechanism

75f	$CH_2O + O \rightarrow HCO + OH$	1.800E+13	0.00	12.9
76f	$HCO + O_2 \rightarrow HO_2 + CO$	7.580E+12	0.00	1.72
77f	$HCO + M13 \rightarrow H + CO + M13$	1.860E+17	-1.00	71.1
78f	$HCO + OH \rightarrow H_2O + CO$	1.000E+14	0.00	0
79f	$HCO + H \rightarrow CO + H_2$	1.190E+13	0.25	0
80f	$HCO + O \rightarrow CO + OH$	3.000E+13	0.00	0
81f	$HCO + O \rightarrow CO_2 + H$	3.000E+13	0.00	0
82f	$CO + OH \rightarrow CO_2 + H$	9.420E+03	2.25	-9.84
83f	$CO + O + M14 \rightarrow CO_2 + M14$	6.170E+14	0.00	12.6
84f	$CO + O_2 \rightarrow CO_2 + O$	2.530E+12	0.00	200
85f	$CO + HO_2 \rightarrow CO_2 + OH$	5.800E+13	0.00	96
86f	$C_2H_6 + CH_3 \rightarrow C_2H_5 + CH_4$	5.500E-01	4.00	34.7
87f	$C_2H_6 + H \rightarrow C_2H_5 + H_2$	5.400E+02	3.50	21.8
88f	$C_2H_6 + O \rightarrow C_2H_5 + OH$	3.000E+07	2.00	21.4
89f	$C_2H_6 + OH \rightarrow C_2H_5 + H_2O$	7.230E+06	2.00	3.62
90f	$C_2H_5 + H \rightarrow C_2H_4 + H_2$	1.250E+14	0.00	33.5
91f	$C_2H_5 + H \rightarrow 2CH_3$	3.000E+13	0.00	0
92f	$C_2H_5 + H \rightarrow C_2H_6$	1.000E+14	0.00	0
93f	$C_2H_5 + OH \rightarrow C_2H_4 + H_2O$	4.000E+13	0.00	0
94f	$C_2H_5 + O \rightarrow CH_3 + CH_2O$	1.000E+14	0.00	0

C_3H_8 and C_4H_{10} Reaction mechanism

95f	$C_2H_5 + HO_2$	$\rightarrow$	$CH_3 + CH_2O + OH$		3.000E+13	0.00	0
96f	$C_2H_5 + O_2$	$\rightarrow$	$C_2H_4 + HO_2$		3.000E+20	-2.86	28.3
97f	$C_2H_4 + H$	$\rightarrow$	$C_2H_3 + H_2$		3.360E-07	6.00	7.08
98f	$C_2H_4 + OH$	$\rightarrow$	$C_2H_3 + H_2O$		2.020E+13	0.00	24.8
99f	$C_2H_4 + O$	$\rightarrow$	$CH_3 + HCO$		1.020E+07	1.88	0.749
100f	$C_2H_4 + CH_3$	$\rightarrow$	$C_2H_3 + CH_4$		6.620E+00	3.70	39.8
101f	$C_2H_4 + H + M15$	$\rightarrow$	$C_2H_5 + M15$	k_0	1.112E+34	-5.00	18.6
				k_∞	1.080E+12	0.45	7.62
102f	$C_2H_4 + M16$	$\rightarrow$	$C_2H_2 + H_2 + M16$	k_0	1.500E+15	0.00	232
				k_∞	1.800E+13	0.00	318
103f	$C_2H_4 + M17$	$\rightarrow$	$C_2H_3 + H + M17$	k_0	1.400E+15	0.00	342
				k_∞	2.000E+16	0.00	460
104f	$C_2H_3 + H$	$\rightarrow$	$C_2H_2 + H_2$		4.000E+13	0.00	0
105f	$C_2H_3 + O$	$\rightarrow$	$CH_2CO + H$		3.000E+13	0.00	0
106f	$C_2H_3 + O_2$	$\rightarrow$	$CH_2O + HCO$		1.700E+29	-5.31	27.2
107f	$C_2H_3 + O_2$	$\rightarrow$	$C_2H_2 + HO_2$		2.120E-06	6.00	39.7
108f	$C_2H_3 + OH$	$\rightarrow$	$C_2H_2 + H_2O$		2.000E+13	0.00	0
109f	$C_2H_3 + C_2H$	$\rightarrow$	$2C_2H_2$		3.000E+13	0.00	0
110f	$C_2H_3 + CH$	$\rightarrow$	$CH_2 + C_2H_2$		5.000E+13	0.00	0
111f	$C_2H_3 + CH_3$	$\rightarrow$	$C_2H_2 + CH_4$		2.000E+13	0.00	0
112f	$2C_2H_3$	$\rightarrow$	$C_2H_4 + C_2H_2$		1.450E+13	0.00	0

C_3H_8 and C_4H_{10} Reaction mechanism

113f	$C_2H_2 + OH \rightarrow C_2H + H_2O$		3.370E+07	2.00	58.6
114f	$C_2H_2 + OH \rightarrow CH_2CO + H$		2.180E-04	4.50	-4.18
115f	$C_2H_2 + OH \rightarrow CH_3 + CO$		4.830E-04	4.00	-8.37
116f	$C_2H_2 + O \rightarrow CH_2 + CO$		6.120E+06	2.00	7.95
117f	$C_2H_2 + O \rightarrow C_2H + OH$		3.160E+15	-0.60	62.8
118f	$C_2H_2 + CH_3 \rightarrow C_2H + CH_4$		1.810E+11	0.00	72.3
119f	$C_2H_2 + O_2 \rightarrow HCCO + OH$		4.000E+07	1.50	126
120f	$C_2H_2 + M18 \rightarrow C_2H + H + M18$		4.200E+16	0.00	448
121f	$C_2H_2 + H + M19 \rightarrow C_2H_3 + M19$	k_0	2.250E+40	-7.27	27.5
		k_∞	3.110E+11	0.58	10.8
122f	$CH_2CO + O \rightarrow CO_2 + CH_2$		1.750E+12	0.00	5.65
123f	$CH_2CO + H \rightarrow CH_3 + CO$		7.000E+12	0.00	12.6
124f	$CH_2CO + M20 \rightarrow CH_2 + CO + M20$	k_0	3.600E+15	0.00	248
		k_∞	3.000E+14	0.00	297
125f	$C_2H + H_2 \rightarrow C_2H_2 + H$		4.090E+05	2.39	3.62
126f	$C_2H + O \rightarrow CH + CO$		5.000E+13	0.00	0
127f	$C_2H + O_2 \rightarrow 2CO + H$		9.040E+12	0.00	-1.91
128f	$C_2H + C_2H_2 \rightarrow C_4H_2 + H$		9.640E+13	0.00	0
129f	$HCCO + H \rightarrow S\text{-}CH_2 + CO$		1.000E+14	0.00	0
130f	$HCCO + O \rightarrow H + 2CO$		8.000E+13	0.00	0
131f	$HCCO + O \rightarrow CH + CO_2$		2.950E+13	0.00	4.66

C_3H_8 and C_4H_{10} Reaction mechanism

132f	$HCCO + O_2 \rightarrow HCO + CO + O$	2.500E+08	1.00	0
133f	$HCCO + O_2 \rightarrow CO_2 + HCO$	2.400E+11	0.00	-3.57
134f	$HCCO + CH \rightarrow C_2H_2 + CO$	5.000E+13	0.00	0
135f	$2HCCO \rightarrow C_2H_2 + 2CO$	1.000E+13	0.00	0
136f	$C_3H_8 + M21 \rightarrow C_2H_5 + CH_3 + M21$ k_0	7.237E+27	-2.88	282
	k_∞	7.900E+22	-1.80	371
137f	$C_3H_8 + O_2 \rightarrow I\text{-}C_3H_7 + HO_2$	4.000E+13	0.00	203
138f	$C_3H_8 + O_2 \rightarrow N\text{-}C_3H_7 + HO_2$	4.000E+13	0.00	215
139f	$C_3H_8 + HO_2 \rightarrow N\text{-}C_3H_7 + H_2O_2$	4.760E+04	2.55	69
140f	$C_3H_8 + HO_2 \rightarrow I\text{-}C_3H_7 + H_2O_2$	9.640E+03	2.60	58.2
141f	$C_3H_8 + OH \rightarrow N\text{-}C_3H_7 + H_2O$	3.160E+07	1.80	3.91
142f	$C_3H_8 + OH \rightarrow I\text{-}C_3H_7 + H_2O$	7.080E+06	1.90	-0.665
143f	$C_3H_8 + O \rightarrow N\text{-}C_3H_7 + OH$	3.730E+06	2.40	23
144f	$C_3H_8 + O \rightarrow I\text{-}C_3H_7 + OH$	5.480E+05	2.50	13.1
145f	$C_3H_8 + H \rightarrow I\text{-}C_3H_7 + H_2$	1.300E+06	2.40	18.7
146f	$C_3H_8 + H \rightarrow N\text{-}C_3H_7 + H_2$	1.330E+06	2.54	28.3
147f	$C_3H_8 + CH_3 \rightarrow N\text{-}C_3H_7 + CH_4$	9.040E-01	3.65	29.9
148f	$C_3H_8 + CH_3 \rightarrow I\text{-}C_3H_7 + CH_4$	1.510E+00	3.46	22.9
149f	$C_3H_8 + C_2H_3 \rightarrow I\text{-}C_3H_7 + C_2H_4$	1.000E+03	3.10	36.9
150f	$C_3H_8 + C_2H_3 \rightarrow N\text{-}C_3H_7 + C_2H_4$	6.000E+02	3.30	43.9

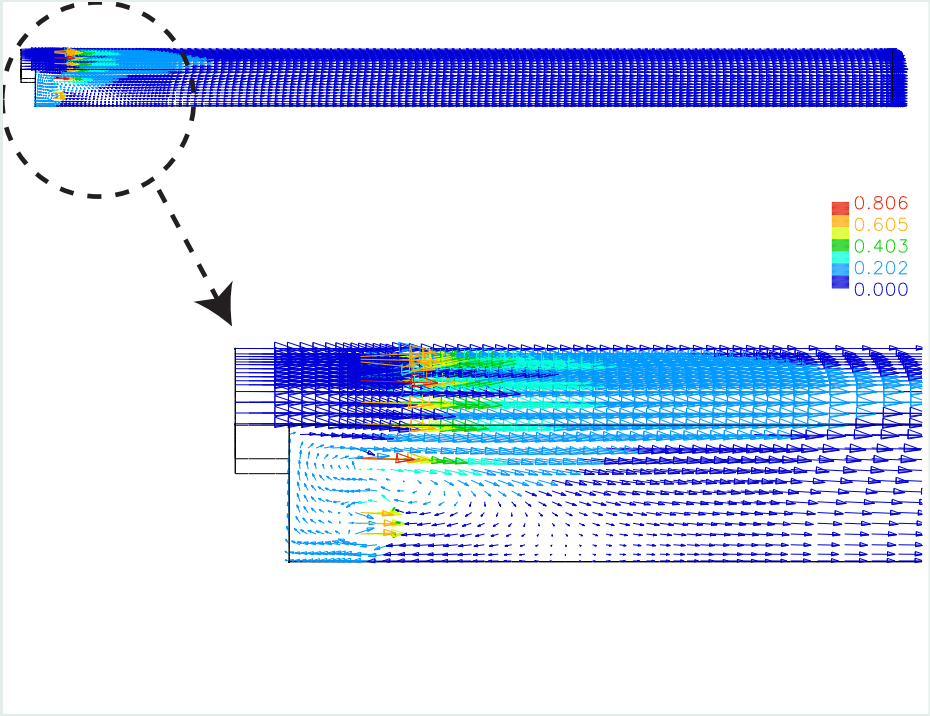
C_3H_8 and C_4H_{10} Reaction mechanism

151f	$C_3H_8 + C_2H_5 \rightarrow I\text{-}C_3H_7 + C_2H_6$	1.510E+00	3.46	31.3
152f	$C_3H_8 + C_2H_5 \rightarrow N\text{-}C_3H_7 + C_2H_6$	9.030E-01	3.65	38.2
153f	$N\text{-}C_3H_7 + M22 \rightarrow C_2H_4 + CH_3 + M22$ k_0	5.485E+49	-10.00	150
	k_∞	1.230E+13	-0.10	126
154f	$N\text{-}C_3H_7 + O_2 \rightarrow C_3H_6 + HO_2$	3.580E+09	0.00	-14.8
155f	$I\text{-}C_3H_7 + O_2 \rightarrow C_3H_6 + HO_2$	6.100E+20	-2.86	33.1
156f	$C_3H_6 + H + M23 \rightarrow I\text{-}C_3H_7 + M23$ k_0	1.640E+54	-11.10	39.2
	k_∞	5.700E+09	1.16	3.66
157f	$C_3H_6 \rightarrow C_2H_2 + CH_4$	2.500E+12	0.00	293
158f	$C_3H_6 \rightarrow A\text{-}C_3H_4 + H_2$	3.000E+13	0.00	335
159f	$C_3H_6 + OH + O_2 \rightarrow CH_3HCO + CH_2O + OH$	3.000E+10	0.00	-34.6
160f	$C_3H_6 + O \rightarrow C_2H_5 + HCO$	1.580E+07	1.76	-5.09
161f	$C_3H_6 + H \rightarrow C_2H_4 + CH_3$	7.230E+12	0.00	5.45
162f	$A\text{-}C_3H_4 + O \rightarrow C_2H_4 + CO$	1.340E+07	1.88	0.749
163f	$A\text{-}C_3H_4 \rightarrow P\text{-}C_3H_4$	1.480E+13	0.00	253
164f	$P\text{-}C_3H_4 + O \rightarrow C_2H_4 + CO$	1.500E+13	0.00	8.8
165f	$P\text{-}C_3H_4 + H \rightarrow CH_3 + C_2H_2$	5.120E+10	1.00	8.62
166f	$C_4H_{10} \rightarrow 2C_2H_5$	2.000E+16	0.00	340
167f	$C_4H_{10} \rightarrow N\text{-}C_3H_7 + CH_3$	1.740E+17	0.00	359
168f	$C_4H_{10} \rightarrow P\text{-}C_4H_9 + H$	1.000E+14	0.00	418
169f	$C_4H_{10} \rightarrow S\text{-}C_4H_9 + H$	1.000E+14	0.00	418

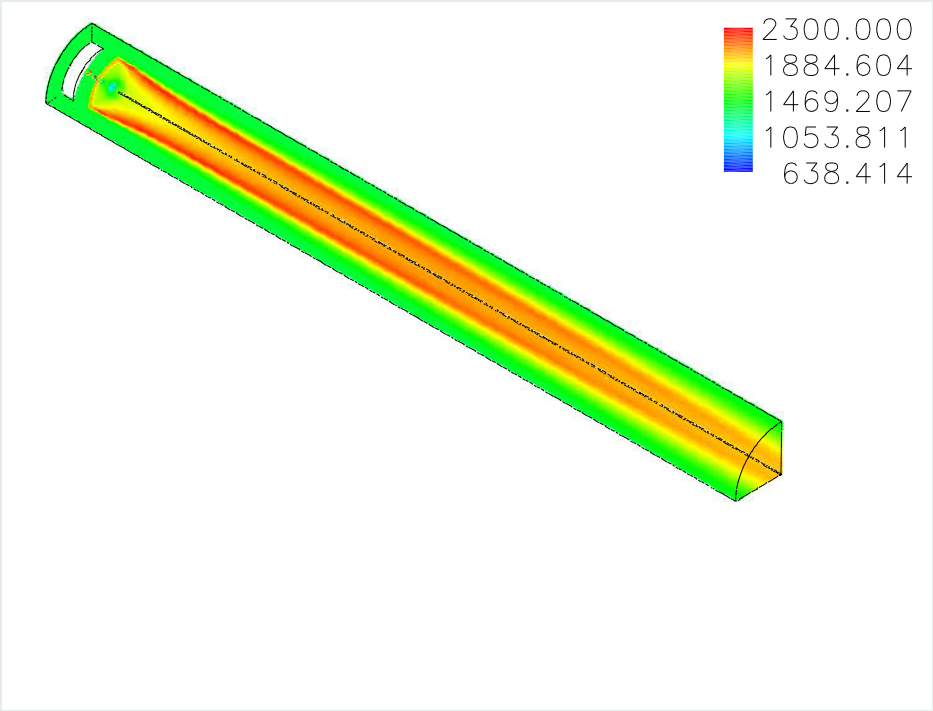
C_3H_8 and C_4H_{10} Reaction mechanism

170f	$C_4H_{10} + O_2 \rightarrow P\text{-}C_4H_9 + HO_2$		2.500E+13	0.00	205
171f	$C_4H_{10} + O_2 \rightarrow S\text{-}C_4H_9 + HO_2$		4.000E+13	0.00	199
172f	$C_4H_{10} + CH_3 \rightarrow P\text{-}C_4H_9 + CH_4$		5.000E+11	0.00	56.9
173f	$C_4H_{10} + CH_3 \rightarrow S\text{-}C_4H_9 + CH_4$		4.300E+11	0.00	43.9
174f	$C_4H_{10} + H \rightarrow P\text{-}C_4H_9 + H_2$		2.840E+05	2.54	25.3
175f	$C_4H_{10} + H \rightarrow S\text{-}C_4H_9 + H_2$		5.680E+05	2.40	15.8
176f	$C_4H_{10} + OH \rightarrow P\text{-}C_4H_9 + H_2O$		4.130E+07	1.73	3.15
177f	$C_4H_{10} + OH \rightarrow S\text{-}C_4H_9 + H_2O$		7.230E+07	1.64	-1.03
178f	$C_4H_{10} + O \rightarrow P\text{-}C_4H_9 + OH$		1.130E+14	0.00	32.8
179f	$C_4H_{10} + O \rightarrow S\text{-}C_4H_9 + OH$		5.620E+13	0.00	21.8
180f	$C_4H_{10} + HO_2 \rightarrow P\text{-}C_4H_9 + H_2O_2$		1.700E+13	0.00	85.6
181f	$C_4H_{10} + HO_2 \rightarrow S\text{-}C_4H_9 + H_2O_2$		1.120E+13	0.00	74.1
182f	$S\text{-}C_4H_9 + M24 \rightarrow C_3H_6 + CH_3 + M24$	k_0	6.323E+58	-12.85	149
		k_∞	2.140E+12	0.65	129
183f	$P\text{-}C_4H_9 + M25 \rightarrow C_2H_5 + C_2H_4 + M25$	k_0	1.897E+55	-11.91	135
		k_∞	1.060E+13	0.00	116
184f	$C_4H_2 + C_2H \rightarrow C_6H_2 + H$		9.600E+13	0.00	0

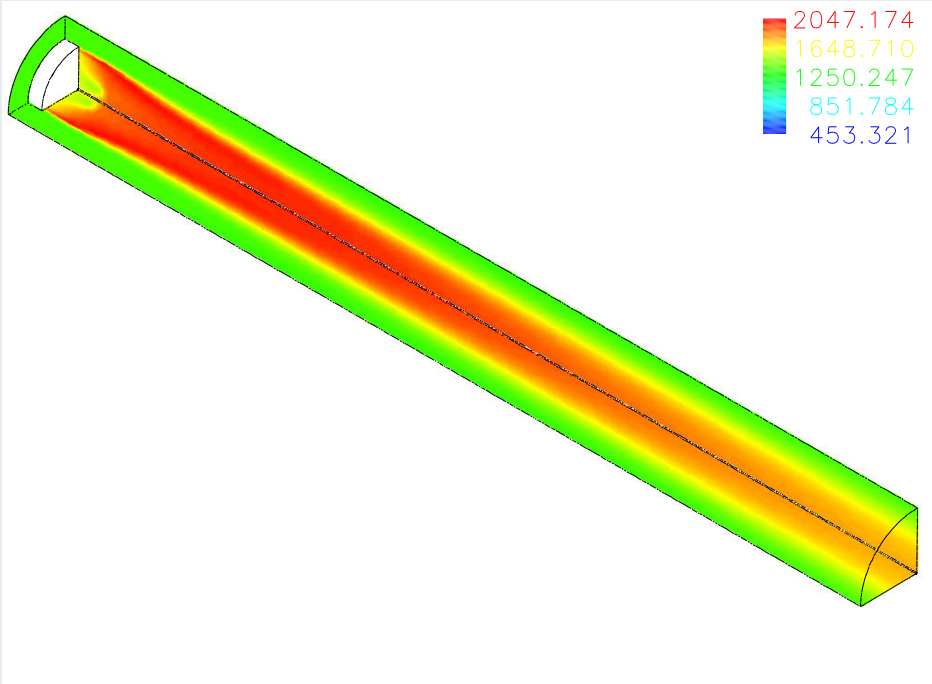
45. Results: velocity vector plot with mixture fraction



46. Results: Temperature distribution (Fast chemistry)

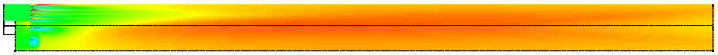


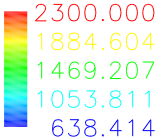
47. Results: Temperature distribution (Flamelet model)



48. Results: Mid-plane temperature distribution (Technion predictions)

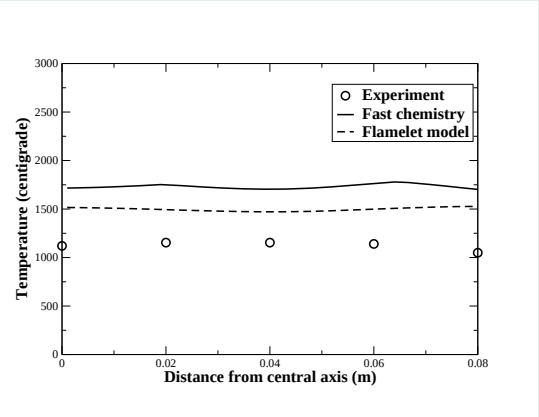
fast chemistry

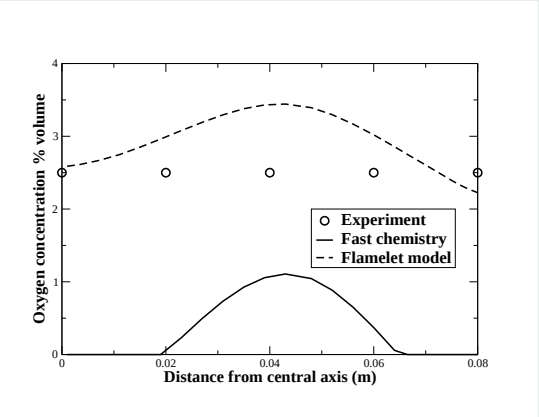




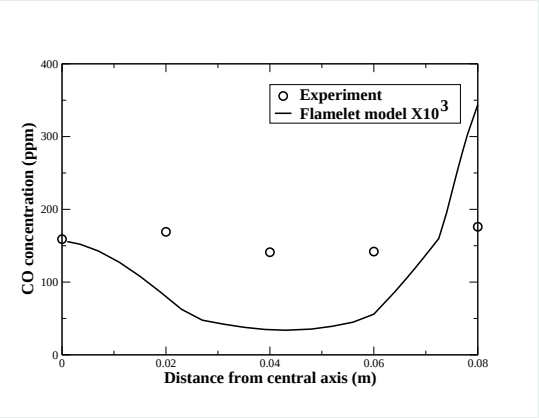
flamelet model

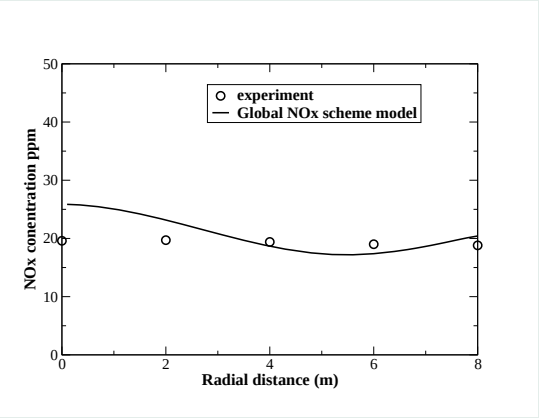
49. Simulation of Technion FLOX device: Predicted & measured Temperature and Oxygen distribution at test section 2





50. Simulation of Technion FLOX device: Predicted & measured NO_x and CO distribution at test section 2





51. Conclusions

- The fast chemistry and flamelet combustion models have been validated against a widerange of experimental data on flameless oxidation.
- The numerical simulations show that the models are comparable with a number of in-furnace measurements of temperature, species concentration, velocity and flue gas emissions and are capable of providing valuable information for temperature and NO_x emissions from flameless oxidation devices in practice.
- Detailed analysis shows that the simple fast chemistry assumption with infinite reaction rate provides a rough description of combustion charateristics, the flamelet model is more sophisticated since it provides comprehensive details of the chemmistry involved.
- The prediction of the NO_x emissions by the global NO_x model are in good agremeent with the measurements.