CFD Simulation of Dry Low Nox Turbogas Combustion System

L. Bucchieri - Engin Soft
F. Turrini - Fiat Avio

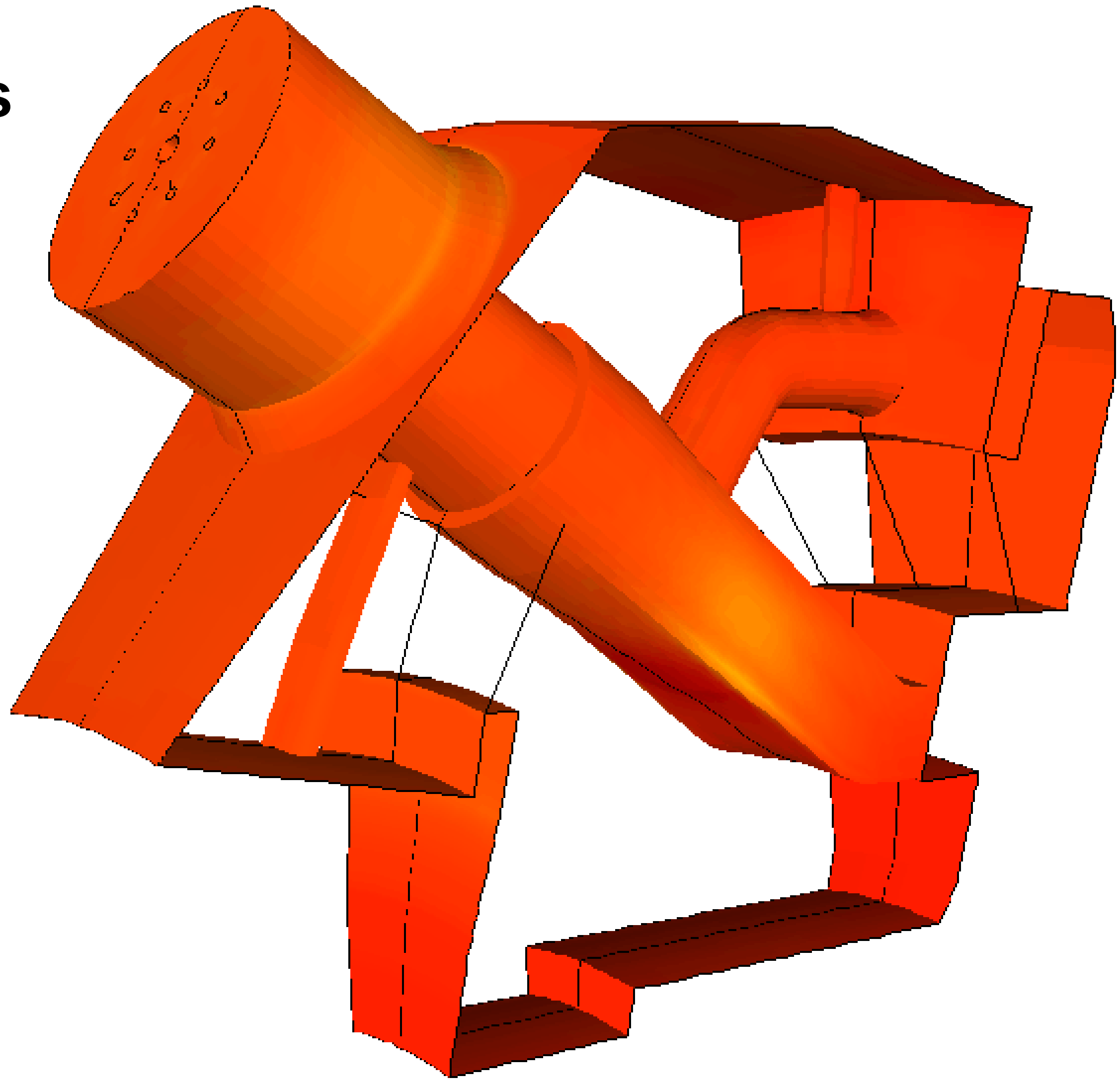
Objectives

- Develop a CFD model for turbogas combustors to calculate and predict:
  - temperature field for liquid and gaseous fuel combustion
  - combustion delay in premix chambers
  - wall heat fluxes on walls
  - emission predictions: Nox and CO

OUTLINE

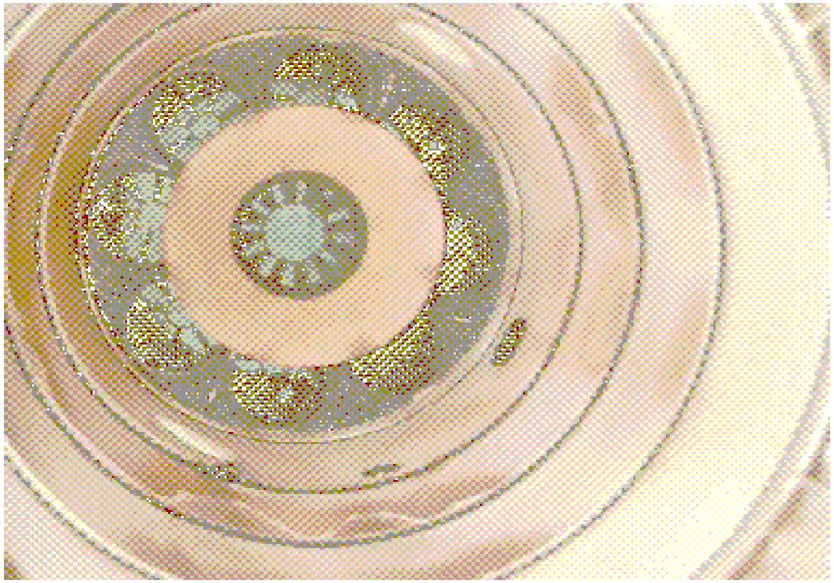
- **DLN: CFD Simulation of sprays and combustion for premixed turbogas**
  - **DLN Combustor Configuration**
  - **CFD Model and Boundary conditions**
  - **CFD Preliminary analysis and Validations of Lean Premixed Prevaporized Duct**
    - **Aerodynamic Field**
    - **Droplet trajectories and vaporization**
  - **CFD Preliminary Combustion Analysis**
    - **EBU OIL model**
    - **EBU gas model**
  - **CFD model development**
    - **4 step kinetic model**

8 LPP ducts
1 Pilot

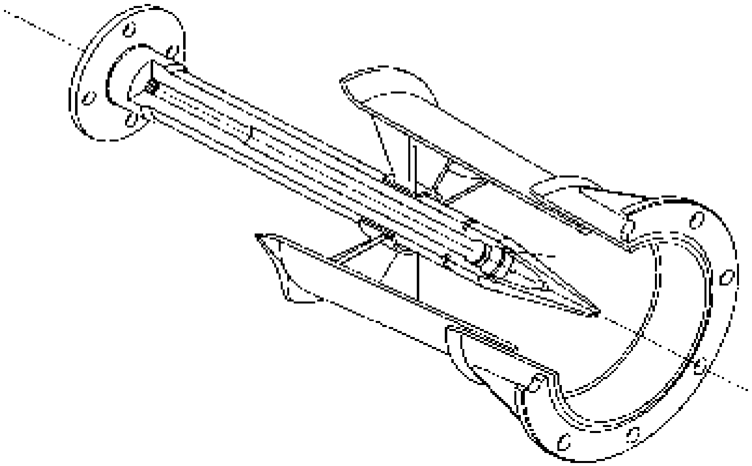


Combustor can and transition duct

Basket inside view looking against flow



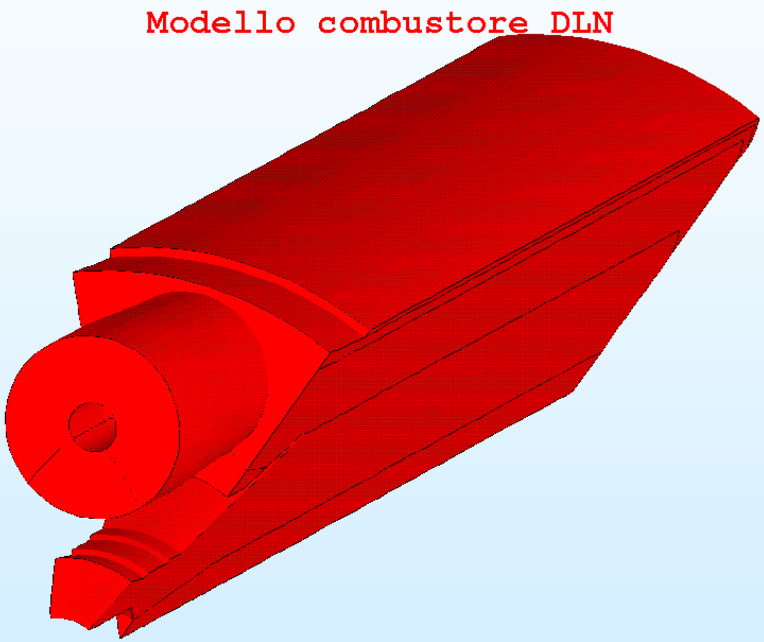
Premixing Duct view
- swirlers
- injectors

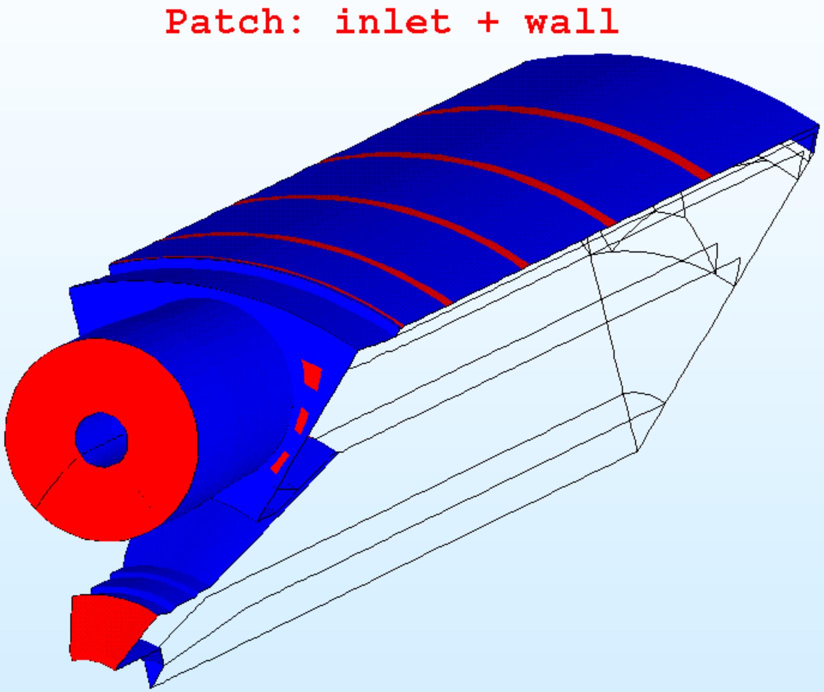


Model Boundary Conditions

- **Spray simulation requires: particle tracking, evaporation and mixing**
  - **Lagrangian particle tracking model with evaporation**
  - **Mass fraction equation of evaporated fuel for mixing**
  - **Fundamentally important to have accurate atomization data for boundary conditions (particle sizes and distribution, Rossin Rammler etc..)**
- **Mixing in premix chamber and validation of DSM**
  - **Initially only the premix chamber is simulated and validated by Differential Stress Model over K-Epsilon for turbulence**
  - **Valid assumption because from thermocouple measurements, $T_{wallpremix}=T_{airinlet}$ hence nothing burns in premix chamber**

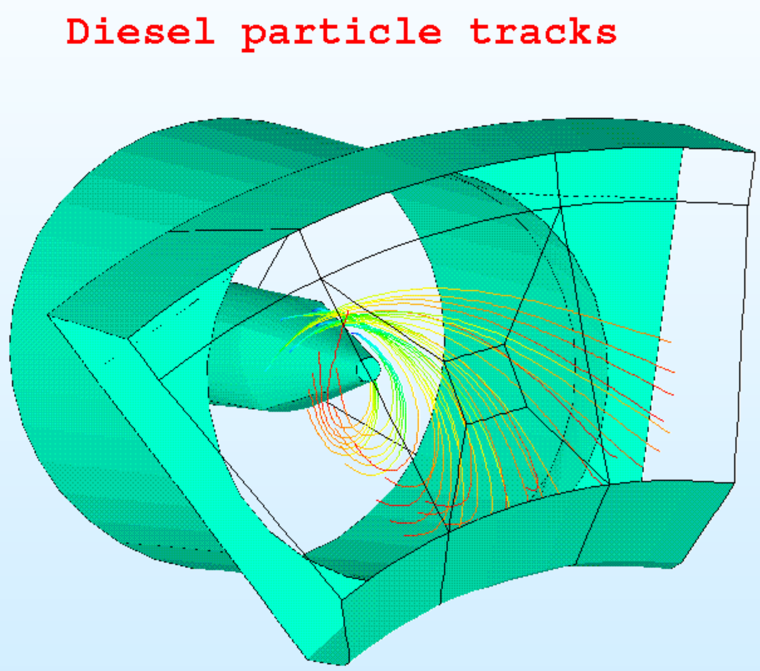
Model Boundary Conditions





Preliminary analysis Spray

- Numerical modeling
  - multiblock hexahedral optimized mesh
  - AMG solver for key equations (pressure, enthalpy)
  - coupling of heat and mass transfer by the lagrangian particle tracking and the fluid model



Preliminary analysis: Spray

- Spray model (Antoine equation)

$$P_{vap} = e^{\left(A - \frac{B}{T - C}\right)}$$

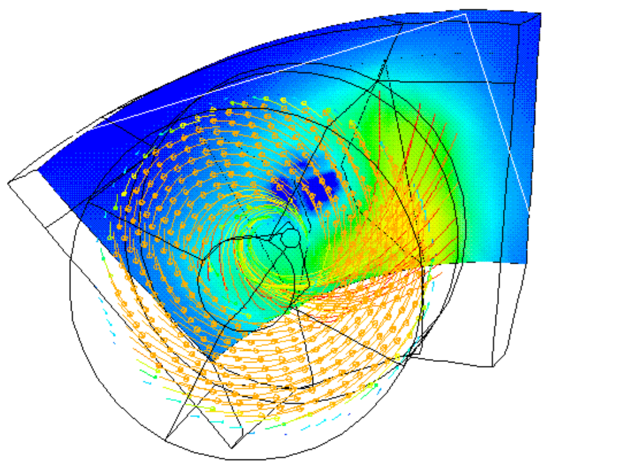
- Rossin Rammler Parameters
  - SDM 30 microns
  - Exponential 5
  - Based on atomization assumption

Preliminary analysis: Spray

- Spray procedure in CFX4
  - Underelax particles to 0.5
  - AMG on Pressure and Enthalpy
  - 20 couplings between particles and 100 flow iterations: total 2000
  - Underelax viscosity for turbulence oscillations into momentum equations

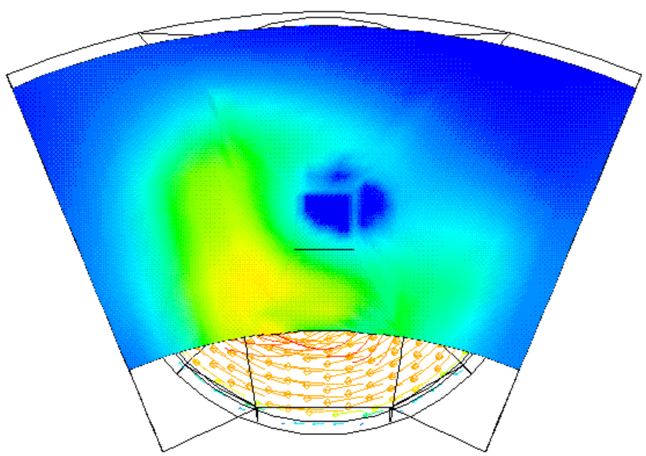
Preliminary analysis: Spray

Diesel particle tracks



Swirl inlet + vaporized fuel

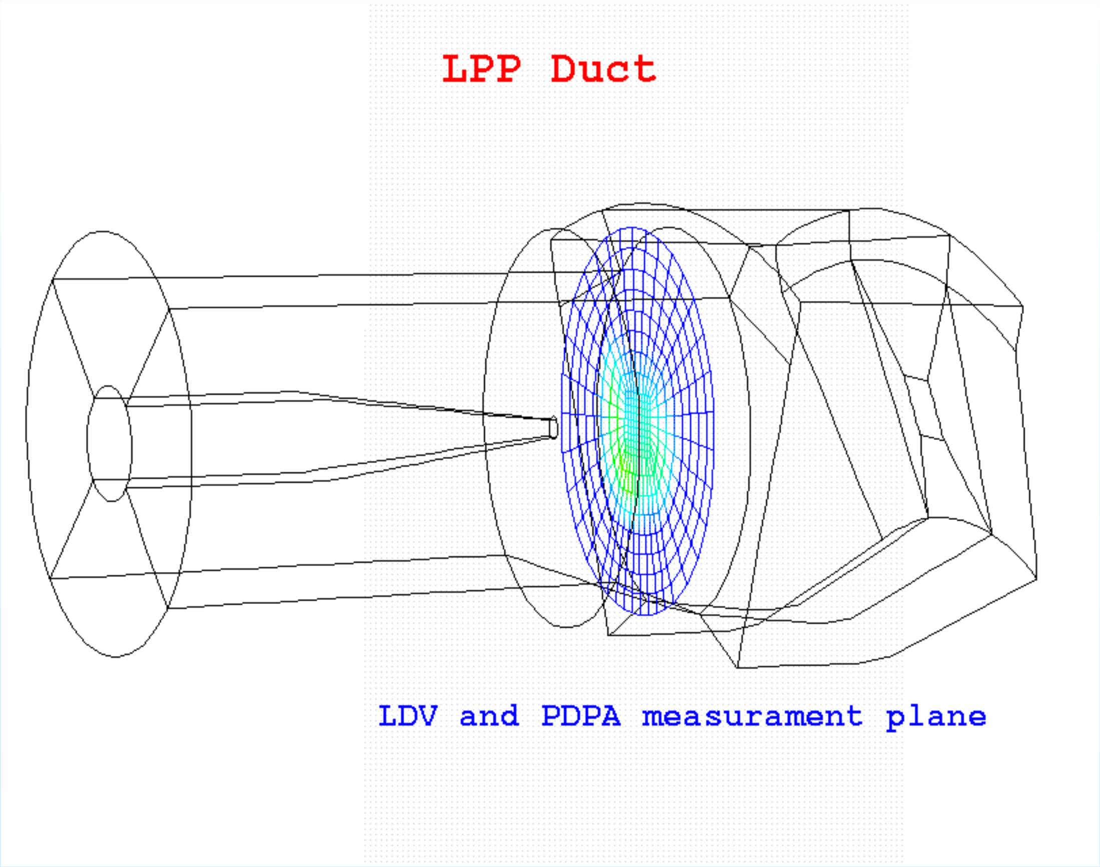
Diesel particle tracks



diesel mass fraction

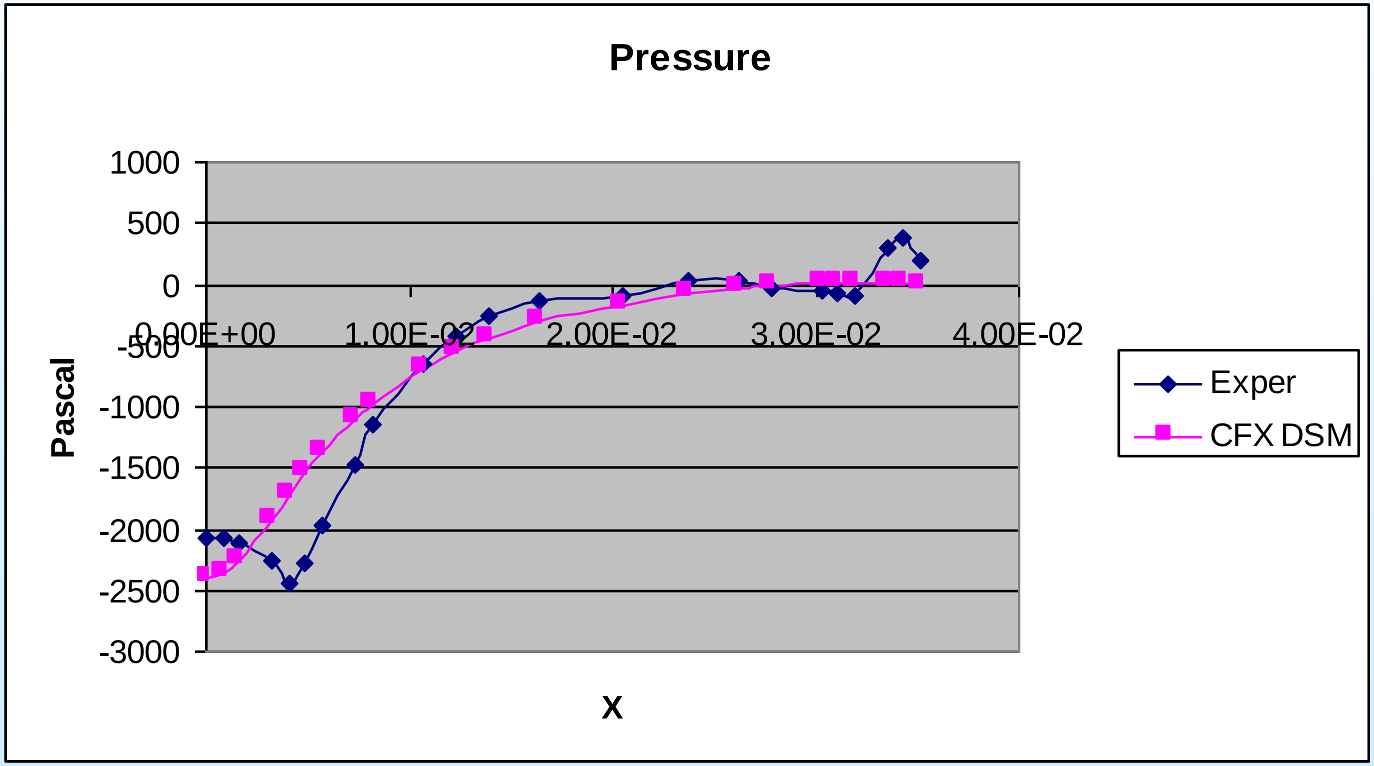
Experimental data

- Experimental set up
  - LDV Laser Doppler
  - Velocimetry
  - PDPA Phase Droplet
  - Particle Analyzer



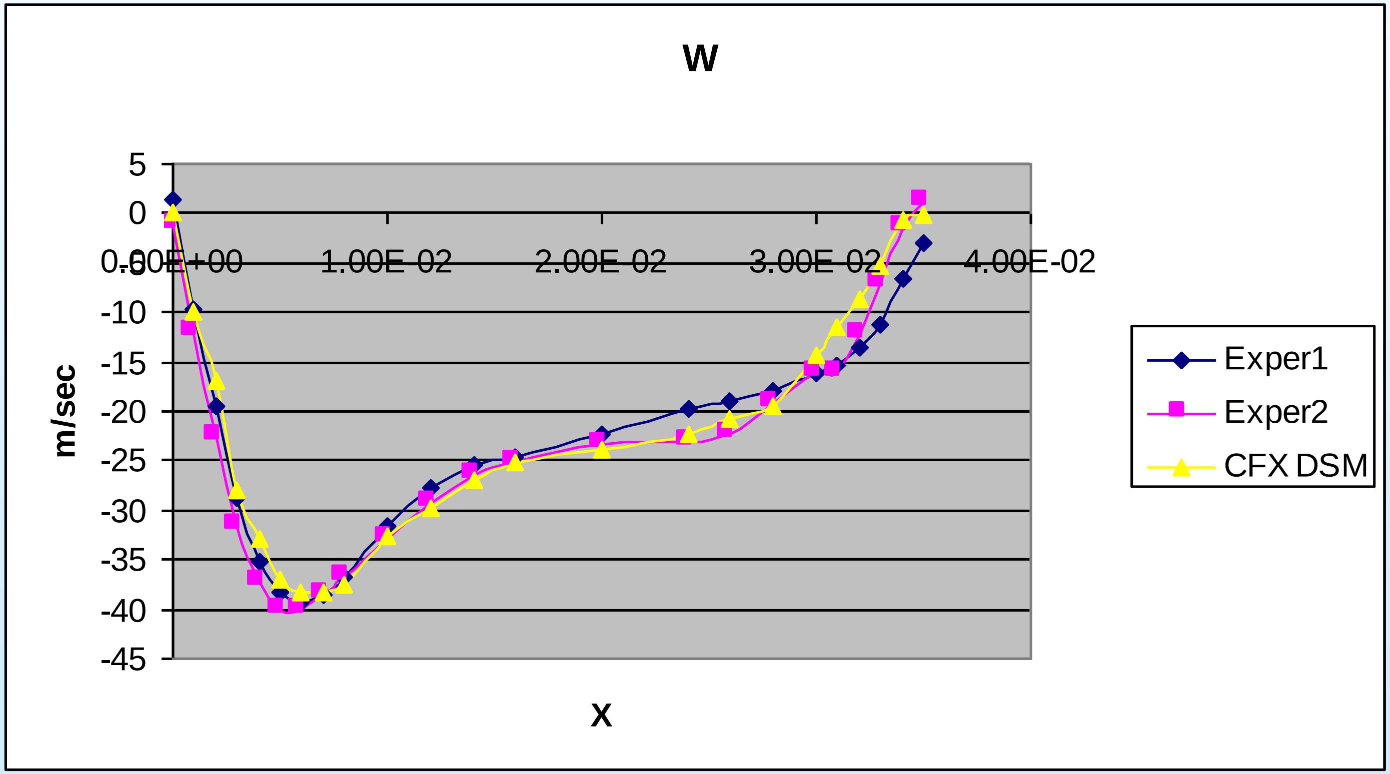
CFD results validation

Pressure profile, exit premix Cone



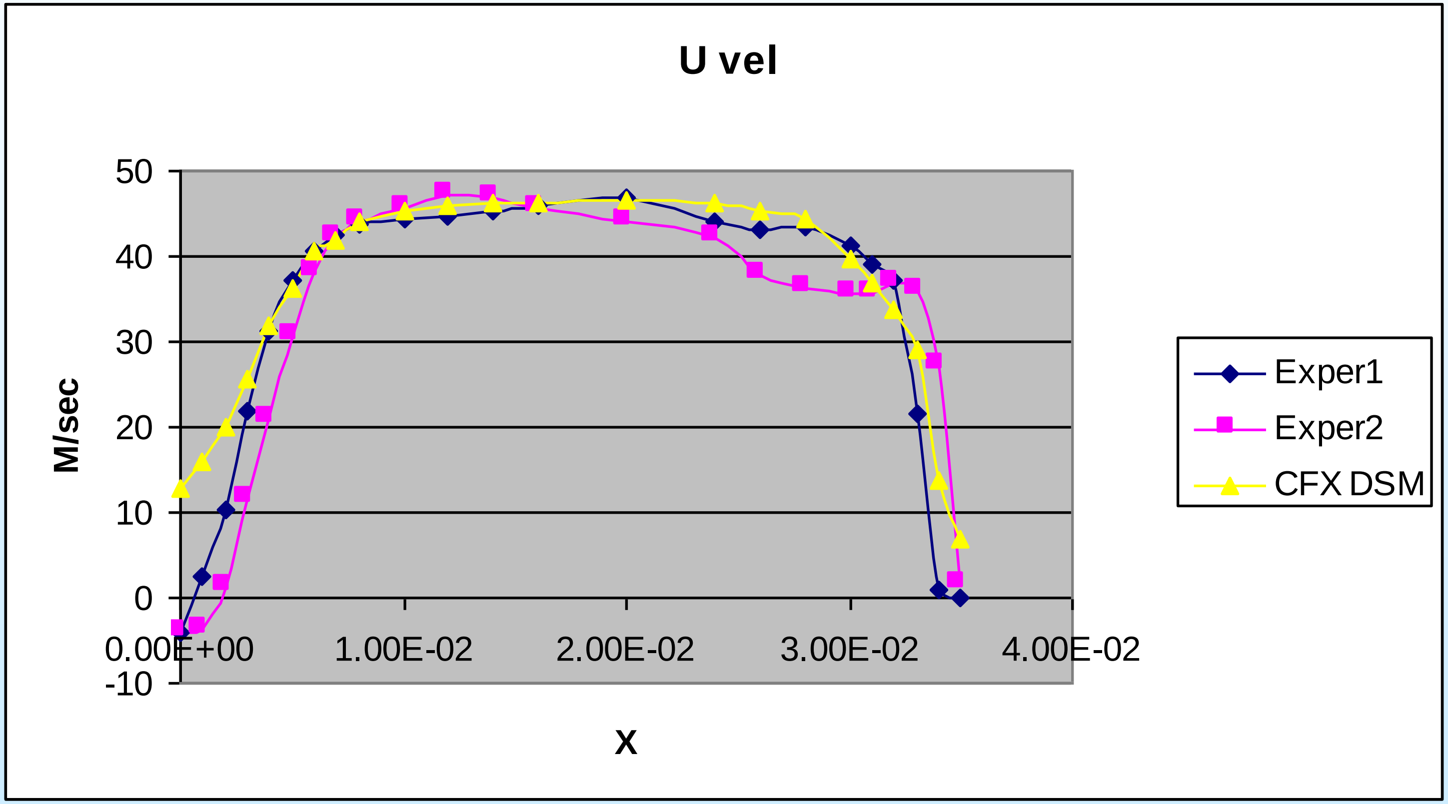
CFD results validation

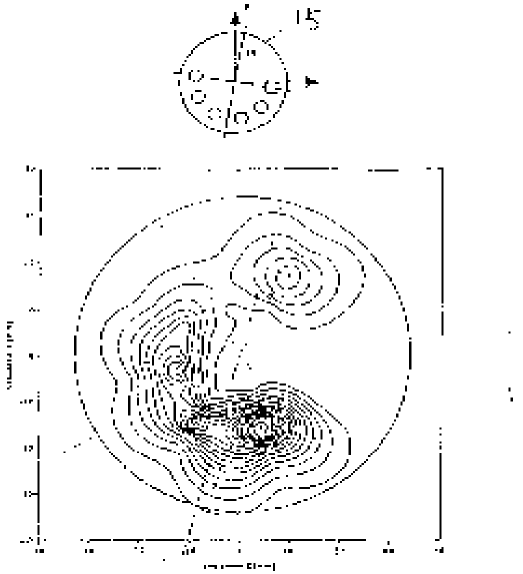
Swirl velocity profile, exit premix Cone



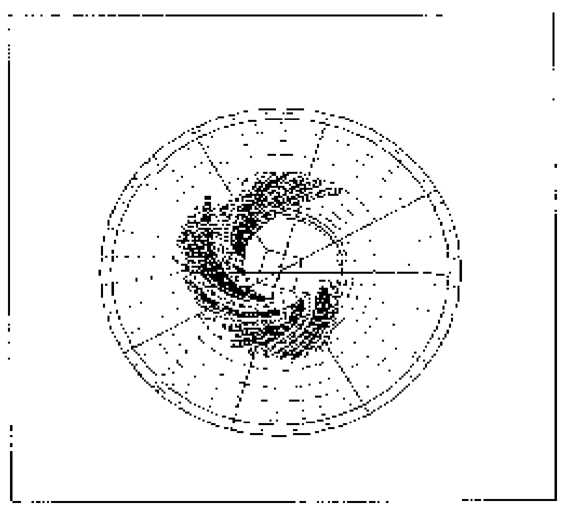
CFD results Validation

Axial velocity profile, Exit premix Cone





Experimental
Droplet distribution (SMD)



Vista frontale

CFX particle trajectories

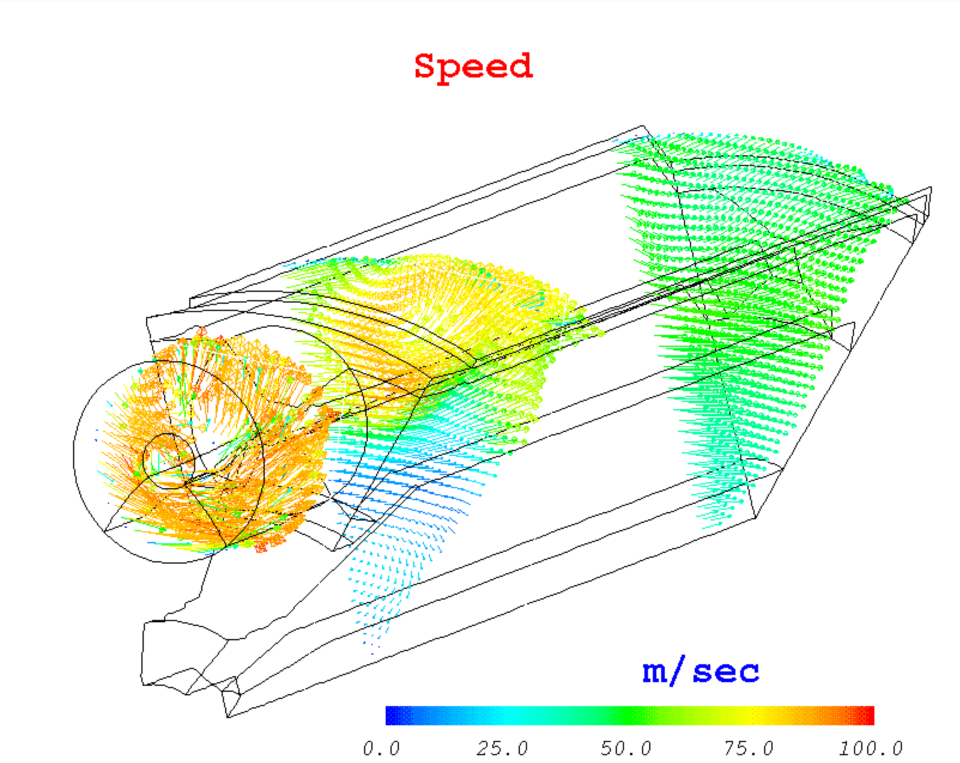
CFD preliminary Combustor analysis

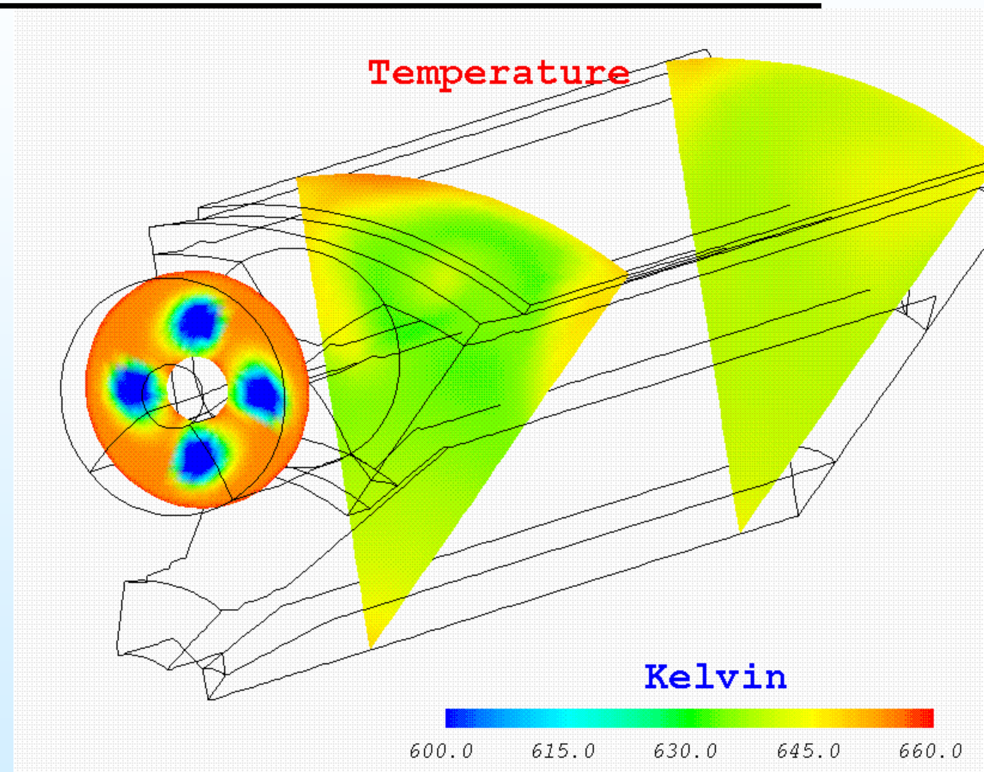
- Dry Low Nox combustor uses two fuels
  - methane
  - oil (heavy diesel)
- First cold flow analysis
- Oil model combustion
  - simulated with Eddy Break Up model with Arrhenius term
  - particles first have to evaporate into a fuel mass fraction which burns
- Methane
  - simulated mixed is burnt with Beta 40 points pdf (no delay in combustion)
  - simulated with EBU and Damkoeler number cutoff (some delay but not correct)

CFD preliminary analysis
Cold Flow

- Cold Flow
  - Compressible and turbulent flow
  - Mach 0.9 injection nozzle for methane
  - AMG solver on Pressure
  - Courant number and High Mach Number Simple algorithm employed
  - Heavy relaxation on Viscosity
  - Deferred correction on K and Epsilon
  - 1000 iterations

CFD Preliminary Analysis
Cold Flow

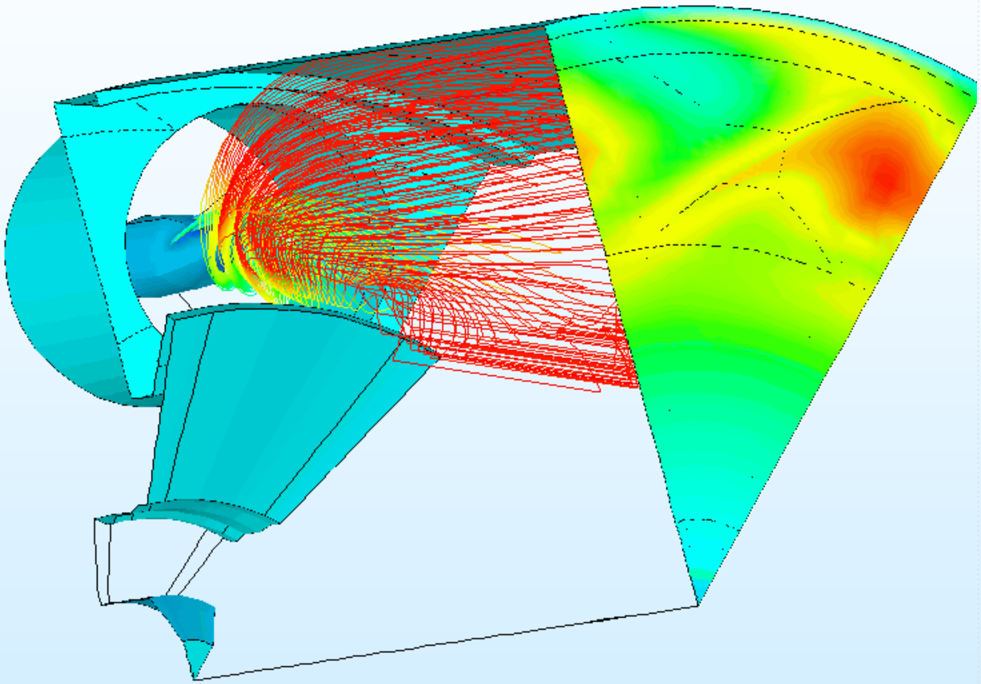


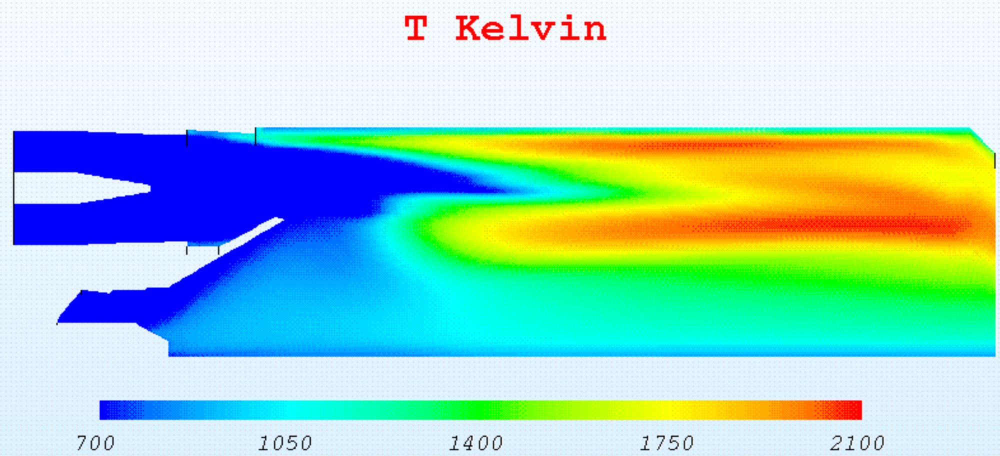


CFD preliminary analysis Combustion

- OIL Model
  - particle vaporization time introduces a delay in combustion which produced combustion after premixing chamber in agreement with experiments
  - OILHM routine changed to include evaporation range over two temperatures
  - 30 couplings of particles versus 200 fluidynamic iterations: total 6000
  - AMG solver on pressure and Enthalpy
  - Heavy relaxation on viscosity and temperature
  - Iterate twice on temperature and scalars

DLN: combustion EBU oil

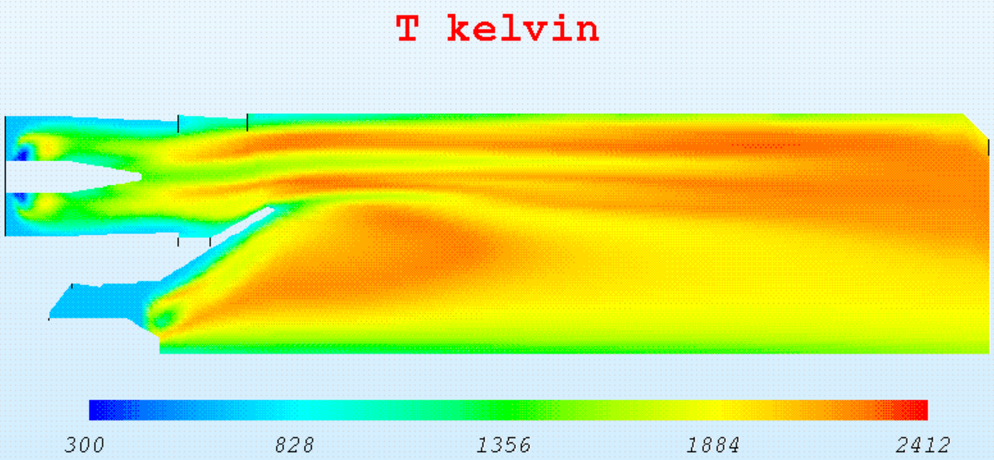


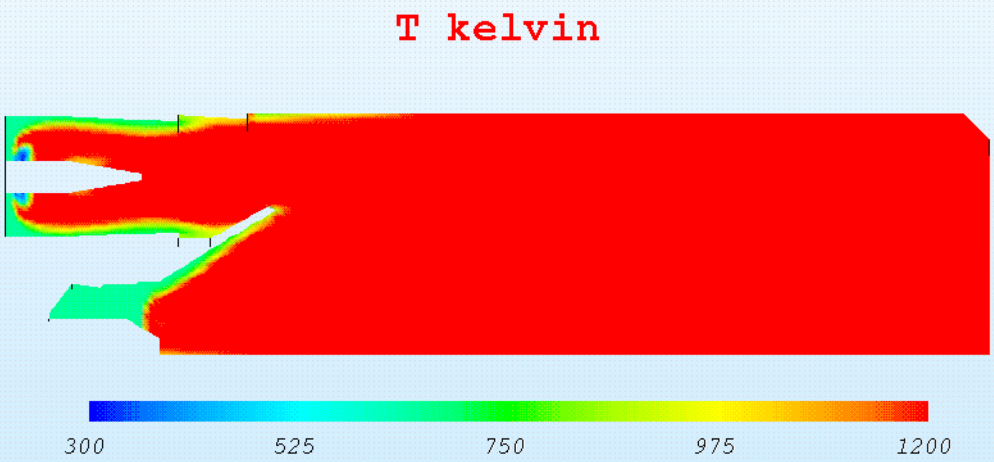


CFD preliminary analysis Combustion

- Gas Model
  - AMG solver on pressure and Enthalpy
  - Heavy relaxation on viscosity and temperature
  - Iterate twice on temperature and combustion scalars
  - Arrhenius term and Damkoheler cutoff
    - varied several times
    - methane burns too quickly
    - practically no combustion delay
    - unsatisfactory results

DLN: combustion EBU gas





DLN: 4 step

- Ran both 2 step and 4 step model
- 2 step reduced kinetic scheme (6 species, N_2 in background)
  - 1 $CH_4+3/2O_2 \rightarrow CO + 2H_2O$
  - 2 $CO + 1/2O_2 \leftrightarrow CO_2$
- 4 step reduced kinetic scheme (7 species, N_2 in background)
  - 1 $CH_4+1/2O_2 \rightarrow CO + 2H_2$
  - 2 $CH_4 + H_2O \rightarrow CO + 3H_2$
  - 3 $H_2+1/2O_2 \leftrightarrow H_2O$
  - 4 $CO + H_2O \leftrightarrow CO_2 + H_2$

ENGIN SOFT

DLN: 4step

FiatAvio

- Generic reaction formulation

- A pre-exponential factor
- β temperature exponent
- Ea activation energy
- X_i species concentration
- a_i forward rate exponent

$$R = A\,T^{\beta} e^{-Ea/RT} \prod_{i=1}^{Ns} [X_i]^{\alpha_i}$$

DLN: 4step

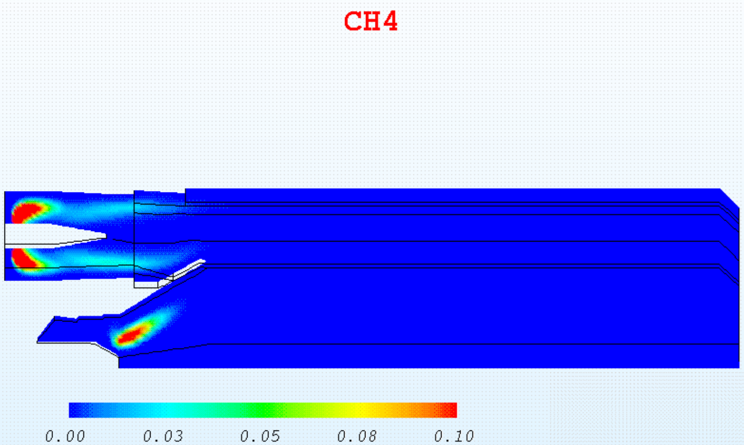
- Reaction constants

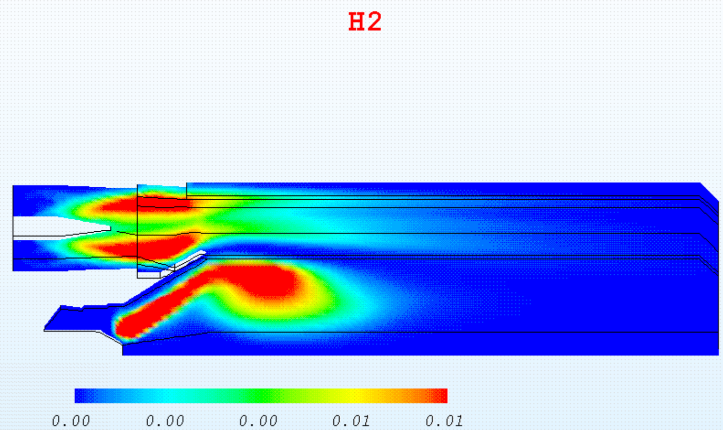
	A	β	Ea	CH_4	O_2	H_2O	H_2	CO
R1	**0.44e+12**	**0**	**1.258e+8**	**0.5**	**1.25**			
R2	**0.3e+9**	**0**	**1.258e+8**	**1.0**		**1.0**		
R3	**0.68e+16**	**-1**	**1.676e+8**		**2.25**	**-1.0**	**1.0**	
R4	**0.275e+10**	**0**	**8.38e+7**			**1.0**		**1.0**

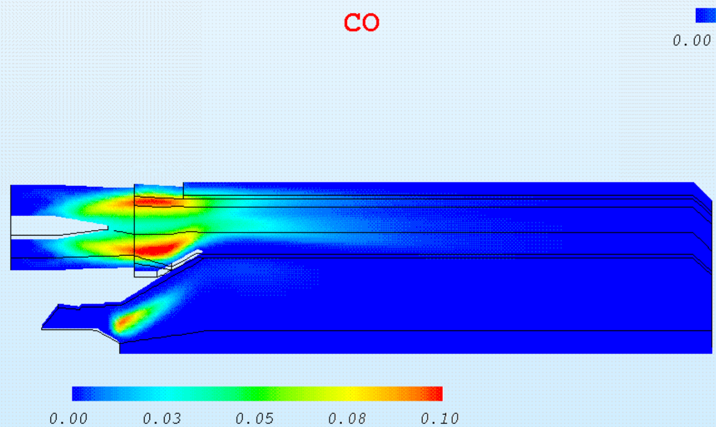
DLN: 4step

- 2 step model did not give right delay
- 4 step model gave almost right delay with standard literature constants
- 2 step sequential reactions and easy to converge
- 4 step competing reactions not so easy to converge
  - impossible to converge unless iterating twice on 6 species and temperature
  - CPU time approximately 3 times higher than EBU
  - problems with backward reaction rates

DLN: 4 step

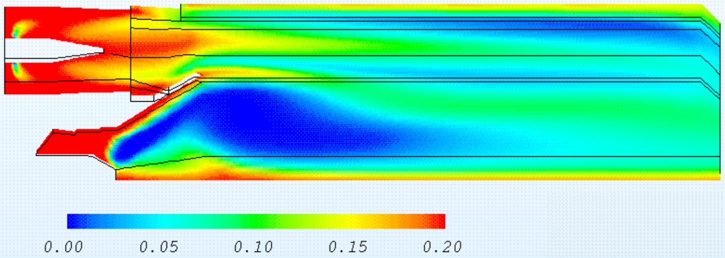

CH4
0.00
0.03
0.05
0.08
0.10


H2
0.00
0.00
0.00
0.01
0.01

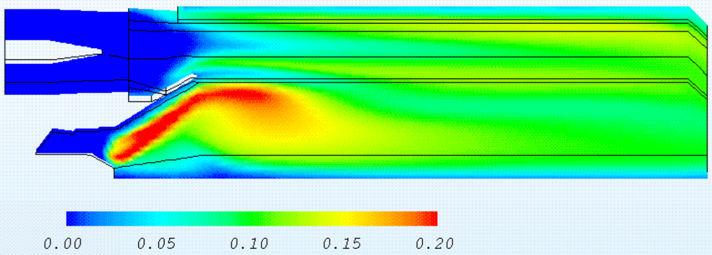

CO
0.00
0.03
0.05
0.08
0.10

DLN: 4 step

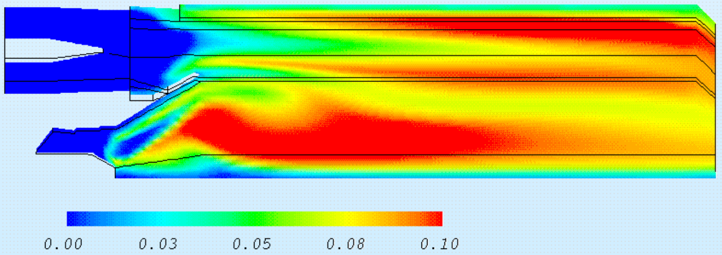
O_2



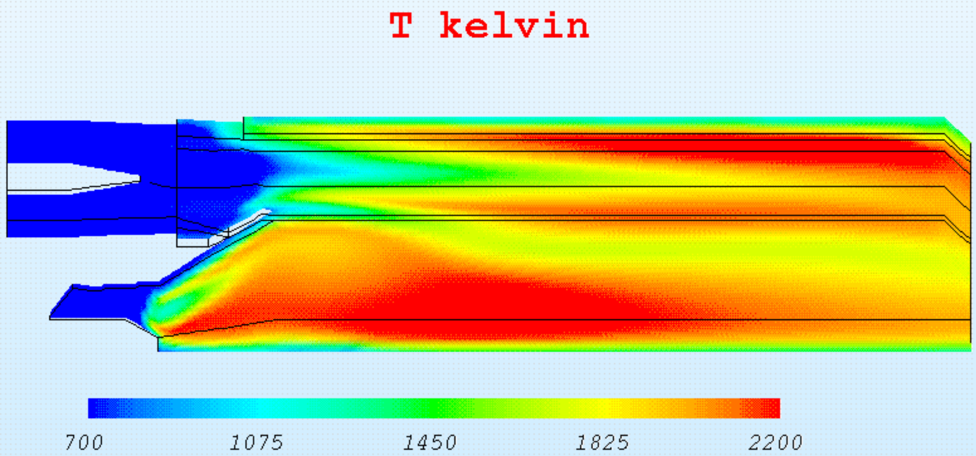
CO_2



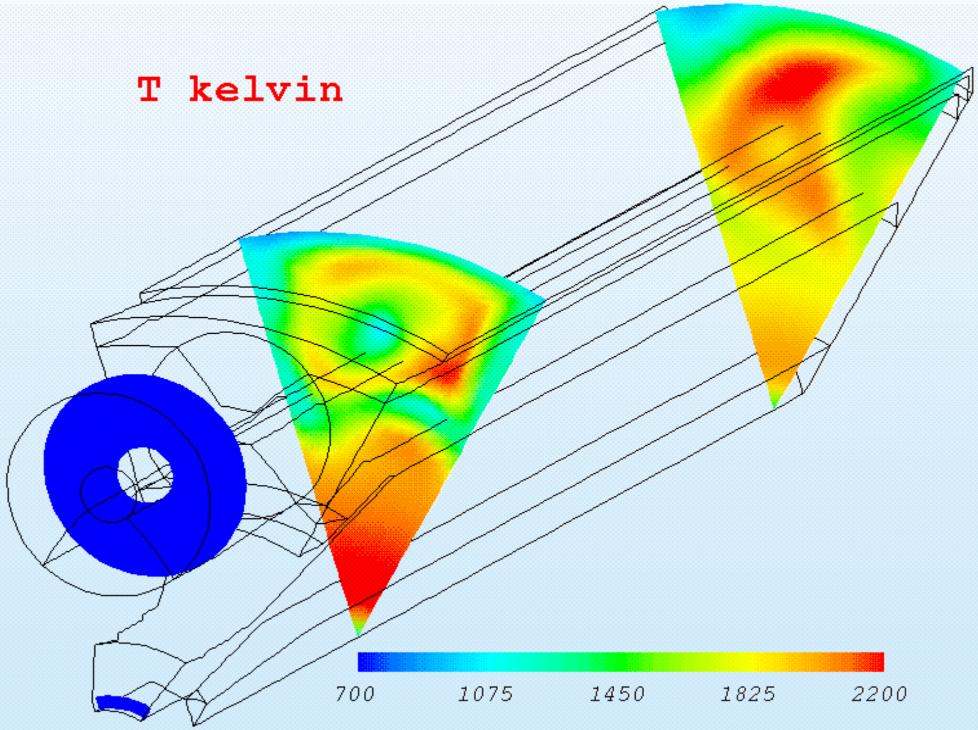
H_2O



DLN: 4 step

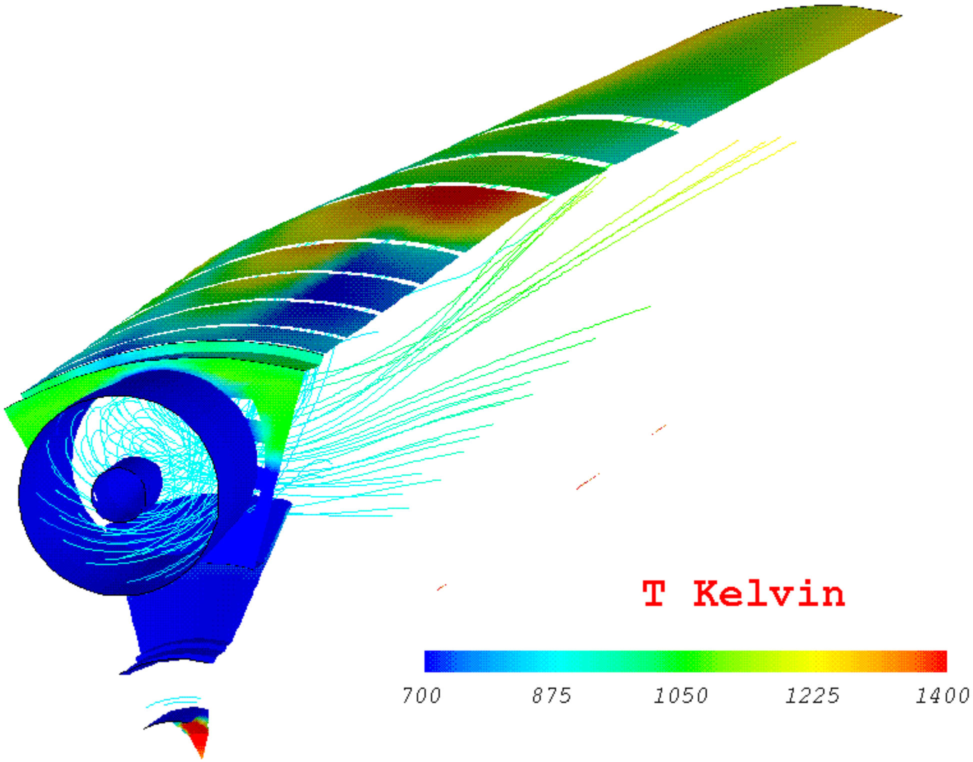


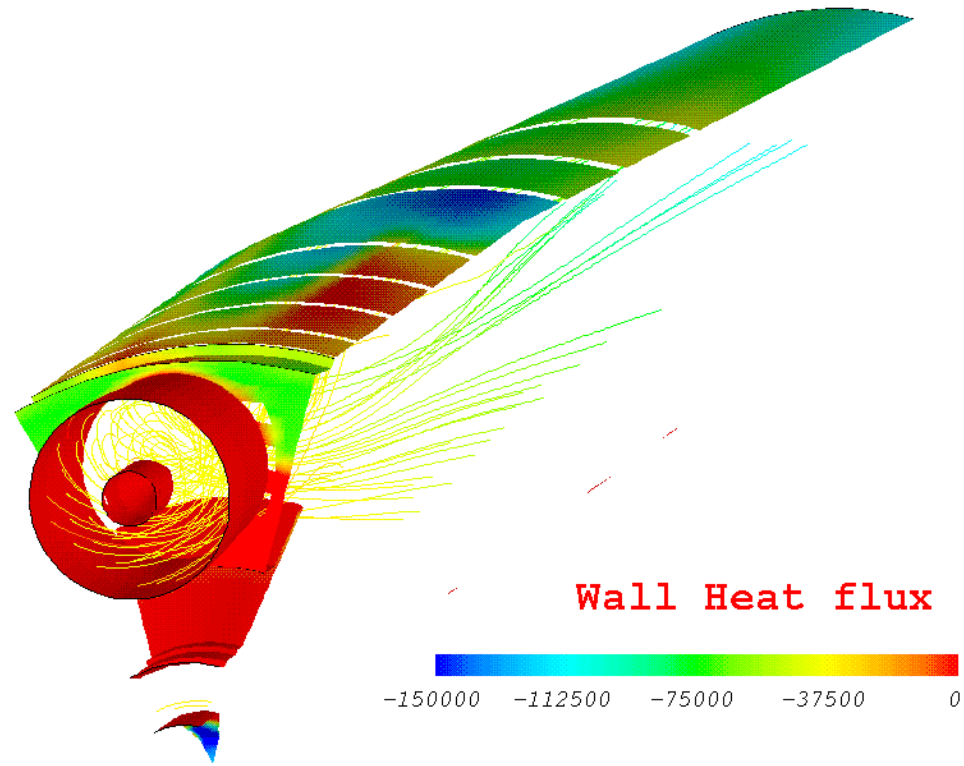
T kelvin
700
1075
1450
1825
2200



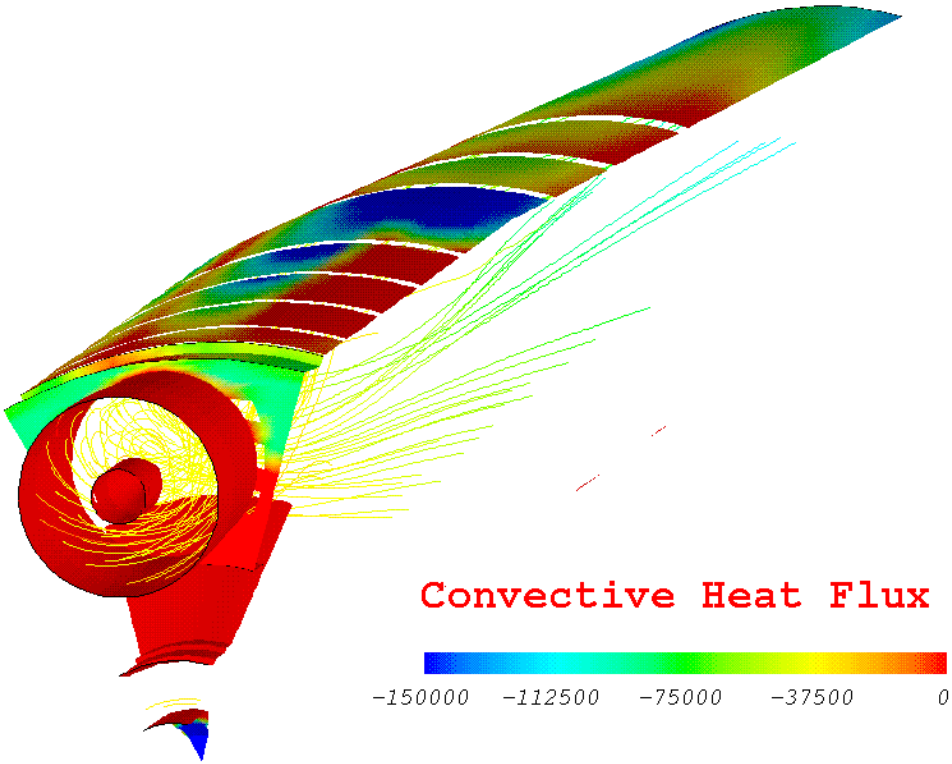
T kelvin
700
1075
1450
1825
2200

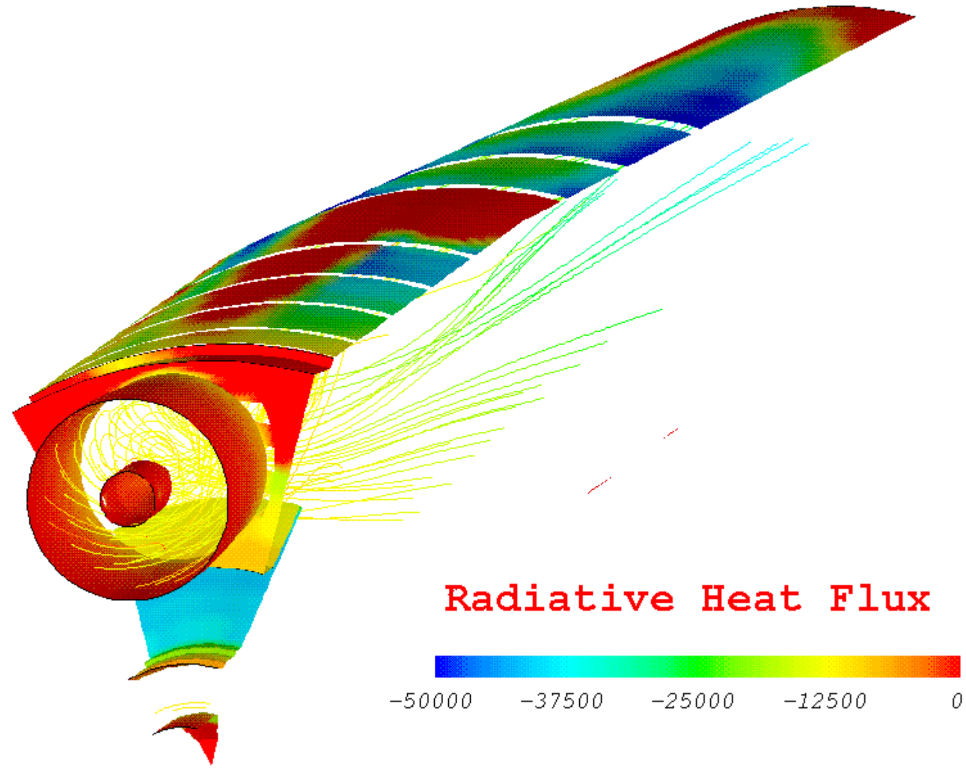
DLN: 4 step


T Kelvin
700
875
1050
1225
1400

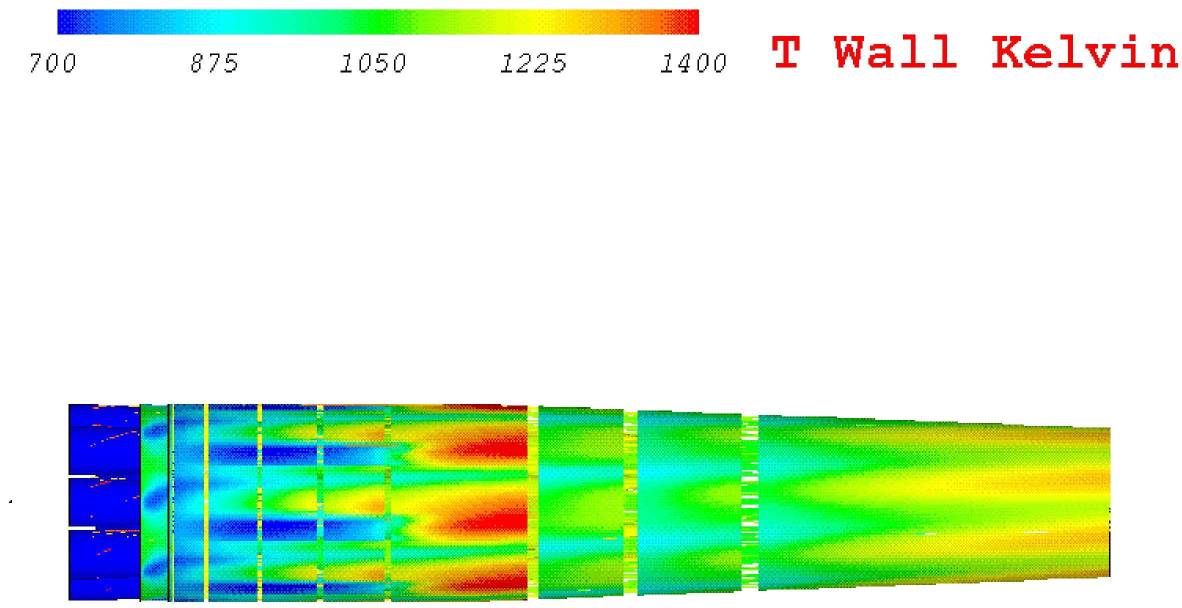

Wall Heat flux
−150000
−112500
−75000
−37500
0

DLN: 4 step

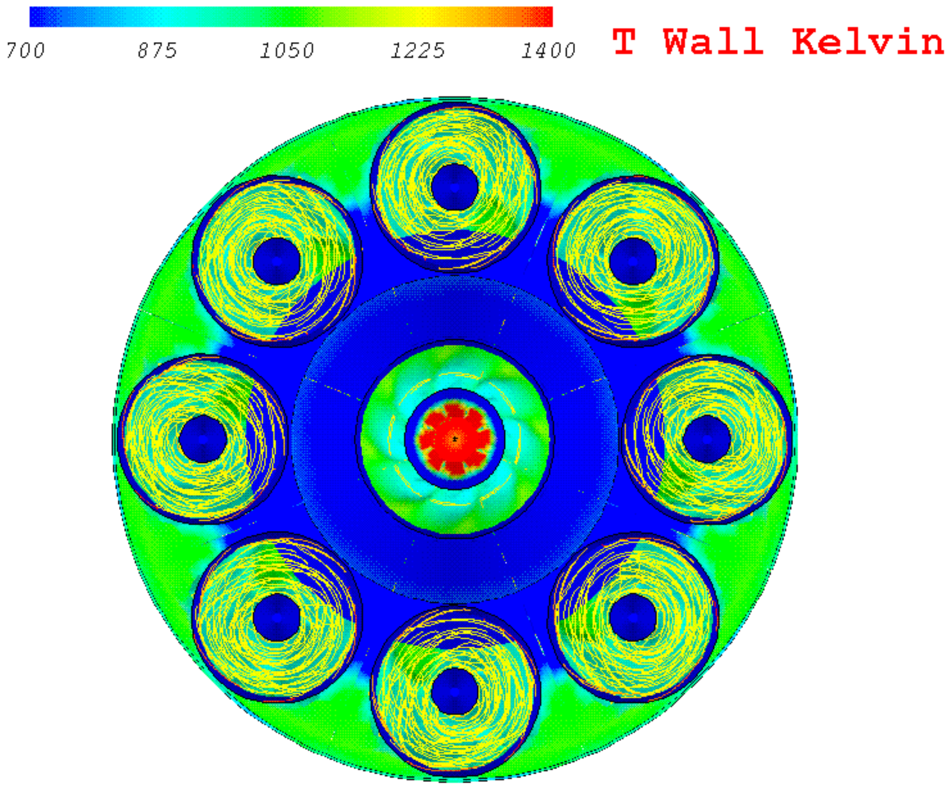

Convective Heat Flux
−150000
−112500
−75000
−37500
0


Radiative Heat Flux
−50000
−37500
−25000
−12500
0

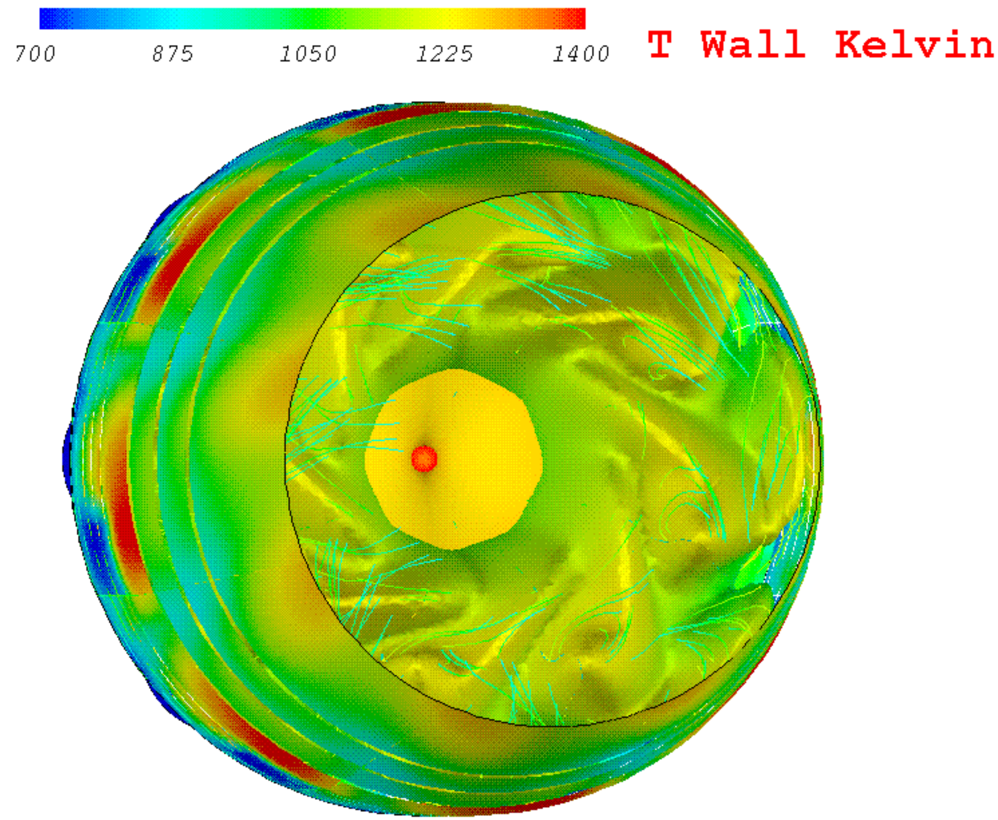
DLN: 4 step



DLN: 4 step

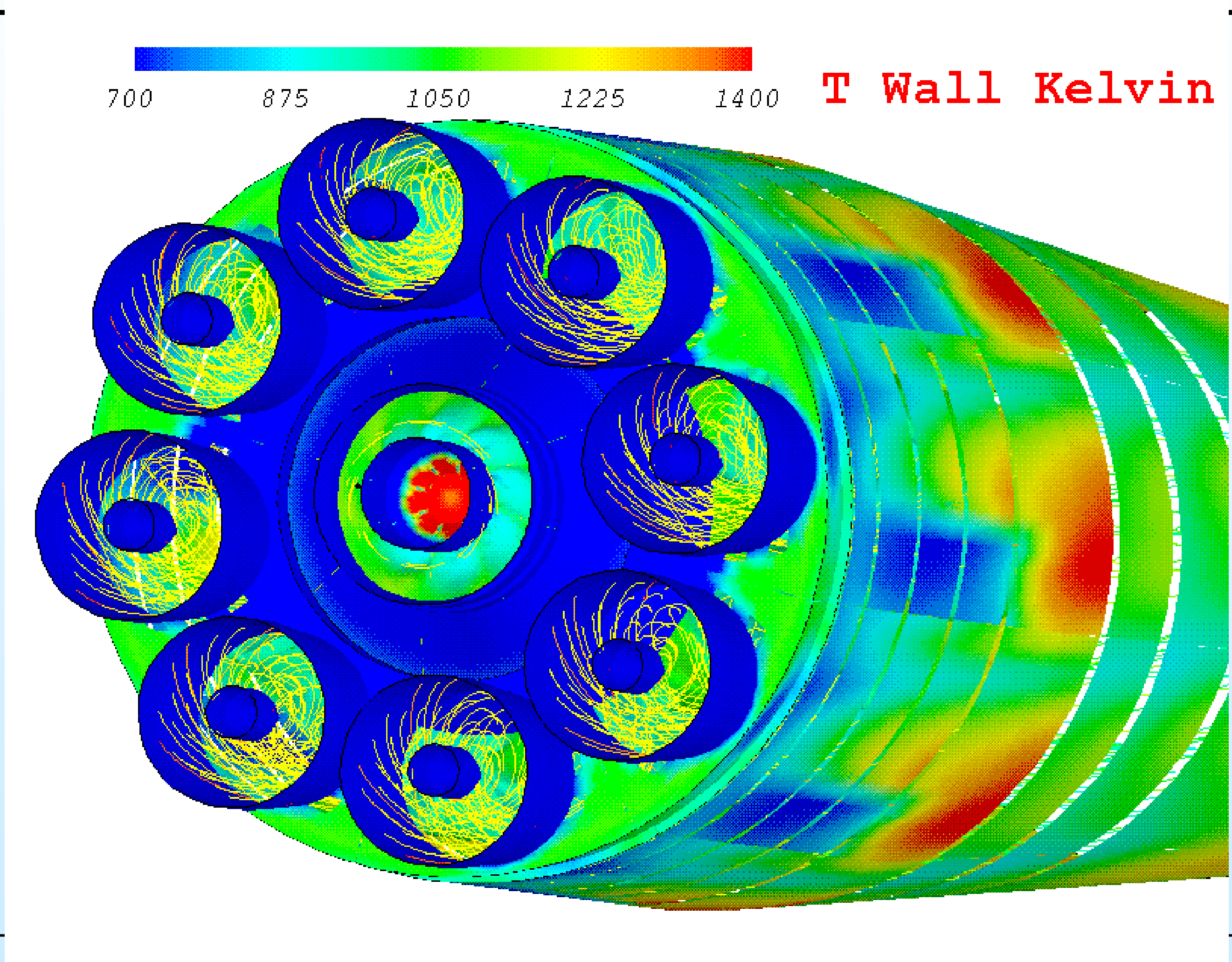


700 875 1050 1225 1400
T Wall Kelvin



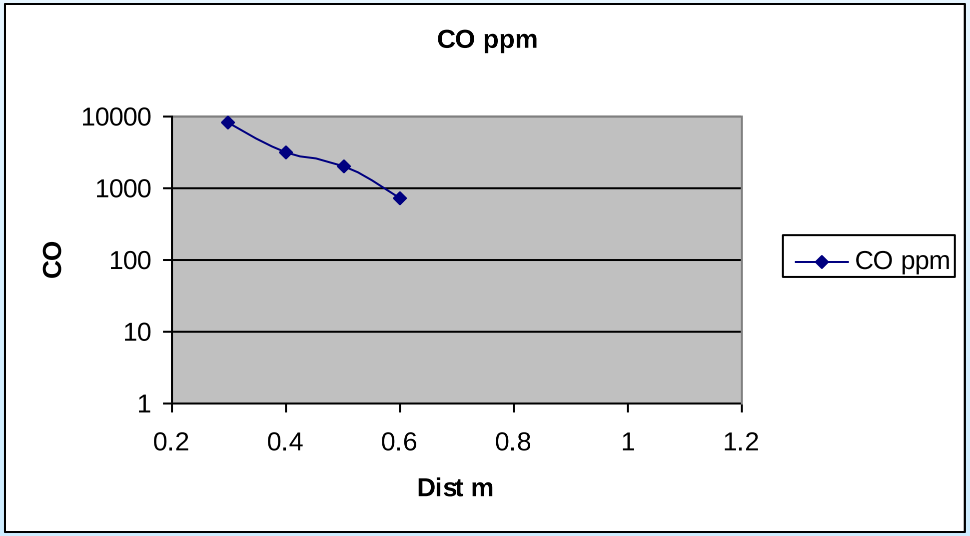
700 875 1050 1225 1400
T Wall Kelvin

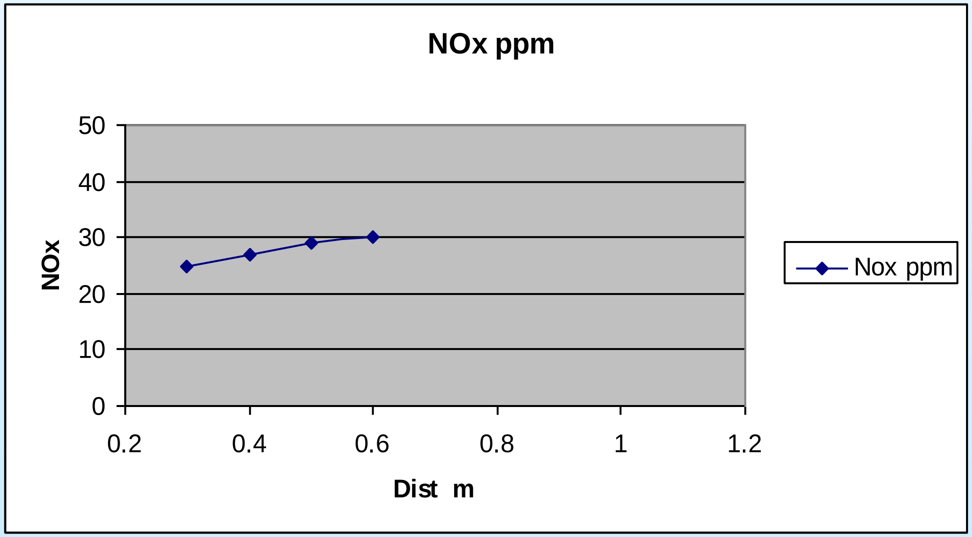
DLN: 4 step



NOX e CO

- Emissions
  - 2 steps overpredicts CO compared to 4step
  - Nox model to be tuned (Clarke & Williams, Malloggi, Oksanen ??)
  - Experimental measuraments (1.2 meters) outside CFD domain (0.6 meters)
  - NOX 50 ppm measured (12. Meters)
  - CO 7 ppm measured





DLN : Conclusions

Conclusion

- RSM model validated mixing data and particle trajectories
- EBU combustion only satisfactory for oil
- 4 step scheme gave reliable combustion delay answers with extra CPU effort and user skill

Further investigations

- combustion stability (off design conditions)
- CO an Nox models to review and validate at transition exit
- test and validate models over a wide range of TURBOGAS cycle operational conditions