OpenFOAM을 활용한 산업용 연소기 해석 연구 현황

2015 4th OpenFOAM Korea Users' Community Conference (4th OKUCC)

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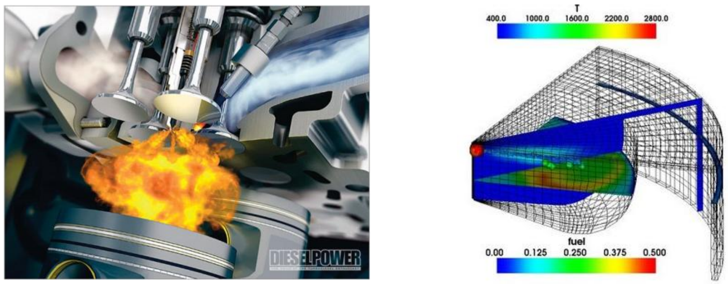
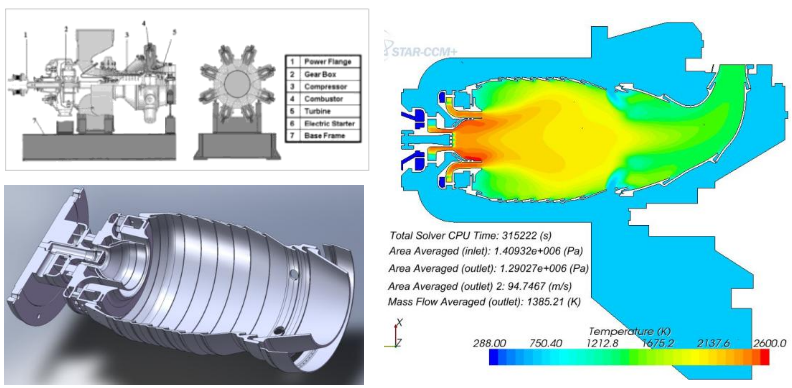
POSTECH
Combustion Laboratory

Introduction

Most industrial combustion devices operate in the regime of turbulent combustion



Diesel engine



Gas turbine

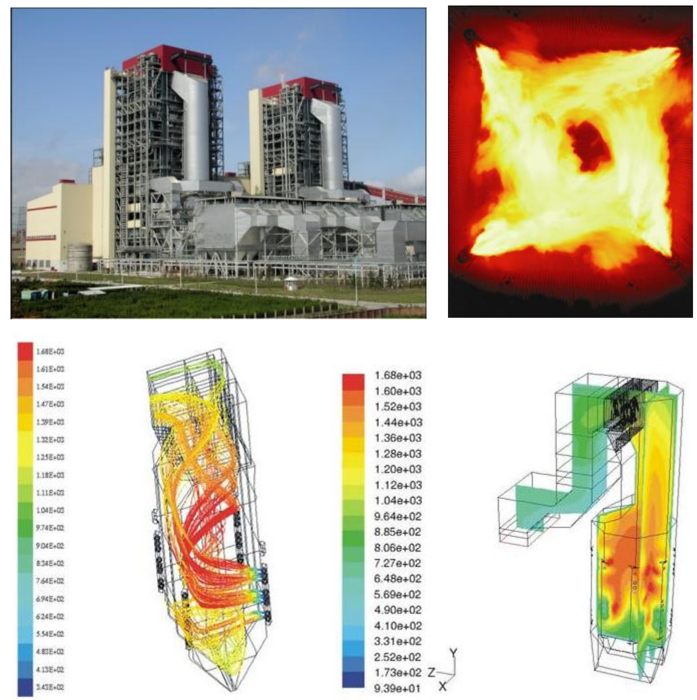


Figure 3.6.2: Particle trajectories in the coal-red boilers with color coded gas temperatures

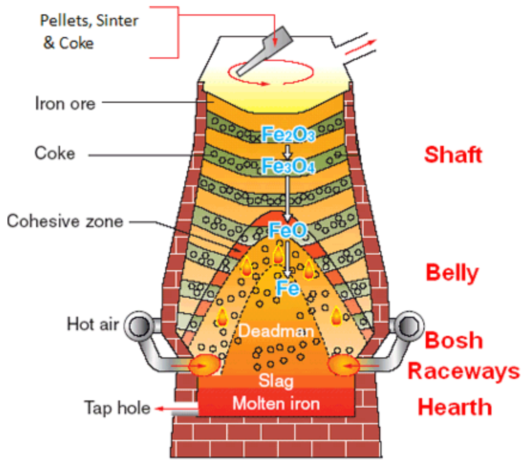
Pulverized coal power plant

CFD analysis of turbulent combustion is a crucial design process to improve performance of practical combustion devices

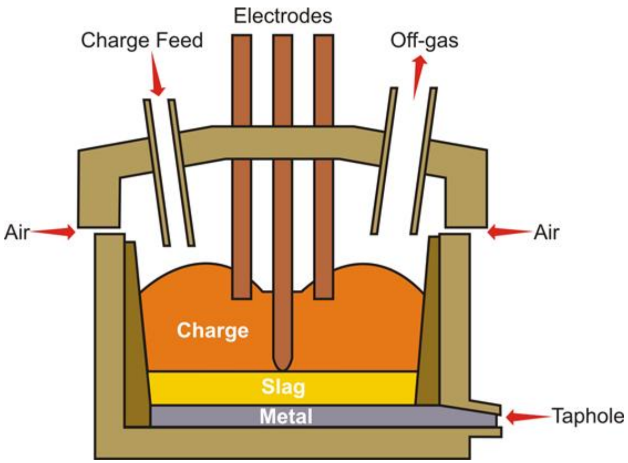
Introduction

Most industrial combustion devices operate in the regime of turbulent combustion

	Transient	**Statistically steady / Steady**
Gas	Spark ignition engine	Gas Turbine / HRSG
Liquid	Compression ignition engine	Heavy-oil furnace
Solid	Blast furnace / Electric arc furnace	FINEX Pulverized coal furnace



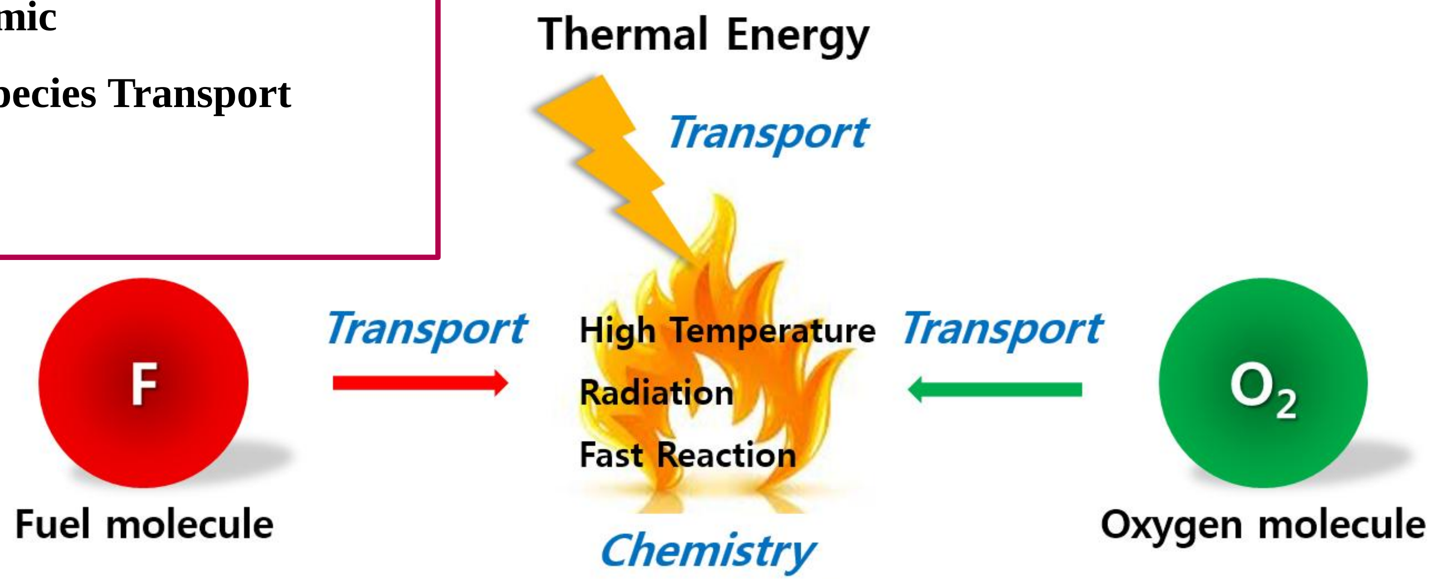
Blast furnace



Electric arc furnace

Basic principle

- **Thermodynamics**
- **Transport**
  - **Fluid Dynamic**
  - **Heat and Species Transport**
- **Chemistry**



$$\sim AT^{\beta}\exp(-E_a/RT)$$

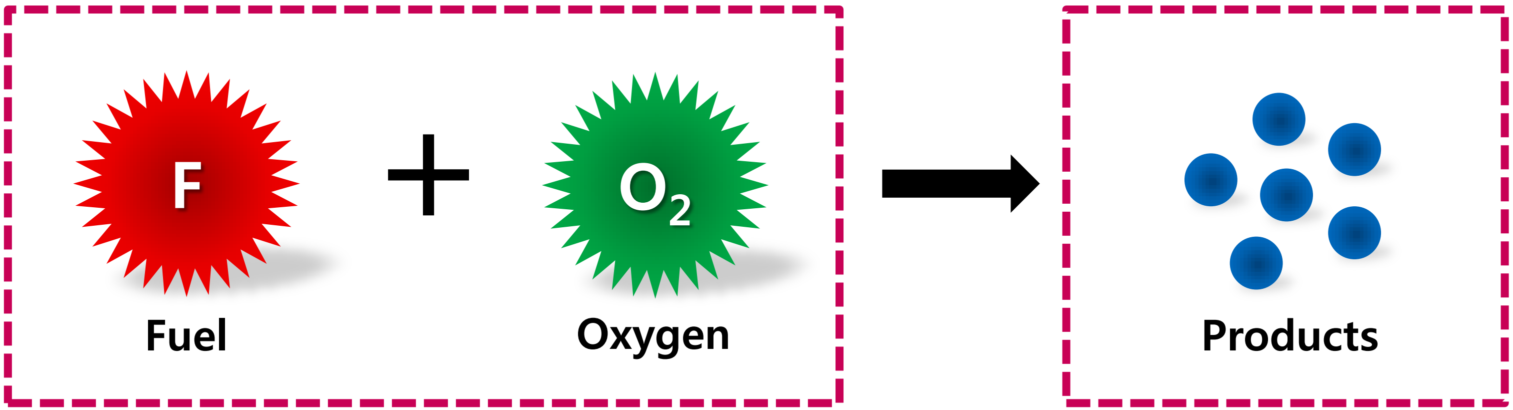
We need both transport and chemistry for combustion to occur.

$$\tau_{comb} \sim \tau_{trans} + \tau_{chem}$$

Usually $\tau_{chem} \ll \tau_{trans}$ (fast chemistry or equilibrium assumption)

Combustion

Thermodynamics



Initial state

'Frozen composition'

Final state

'Equilibrium'

How to relate initial and final states?

- **1st law – Energy Conservation** Chemical energy ▶ Sensible energy
- **2nd law – Direction** $dS \geq \frac{\delta Q}{T}$ One way only (IS→FS)

Turbulent Combustion

⇩

Large Fluctuations of all Scalar and Vector Quantities

⇩

Problems both in Measurement and Computation

Governing equations

- **Favre Averaged Conservation Eqs with Nonlinear Terms**

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_k} \bar{\rho} \tilde{\mathrm{v}}_k = 0$$

$$\frac{\partial}{\partial t} \bar{\rho} \tilde{Y}_i + \frac{\partial}{\partial x_k} \bar{\rho} \widetilde{\mathrm{v}_k Y_i} = -\frac{\partial}{\partial x_k} \overline{J_{ik}} + \overline{\dot{\mathrm{w}}_i}$$

Nonlinear Reaction Term

$$\frac{\partial}{\partial t} \bar{\rho} \tilde{\mathrm{v}}_i + \frac{\partial}{\partial x_k} \bar{\rho} \widetilde{\mathrm{v}_k \mathrm{v}_i} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_k} \overline{\tau_{ik}} + \overline{g_i}$$

$$\frac{\partial}{\partial t} \bar{\rho} \tilde{h} + \frac{\partial}{\partial x_k} \bar{\rho} \widetilde{\mathrm{v}_k h} = \frac{\partial \bar{p}}{\partial t} + \frac{\partial}{\partial x_k} [\frac{\mu}{\sigma} \frac{\partial \bar{h}}{\partial x_k} + \mu \sum_{i=1}^{N} (\frac{1}{Sc_i} - \frac{1}{\sigma}) \overline{h_i \frac{\partial Y_i}{\partial x_k}}]$$

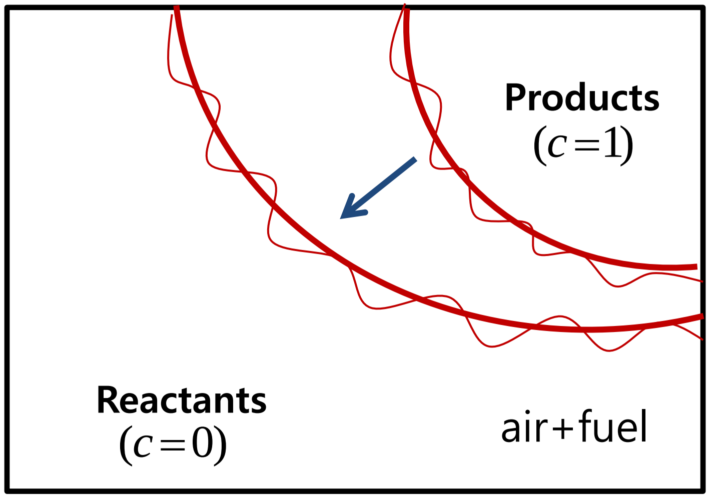
$$\bar{p} = \bar{\rho} R \tilde{T}$$

$$\tilde{h} = h(\tilde{Y}_i,\ \bar{p},\ \tilde{T})$$

Nonlinear Convection Term

Combustion

Premixed Flame



- Reaction Progress Variable

$$c = \frac{\sum_i a_i \left(Y_i - Y_i^u\right)}{\sum_i a_i (Y_i^{eq} - Y_i^u)} = \frac{Y_c}{Y_c^{eq}}$$

^{u} : unburnt reactant

^{eq} : chemical equilibrium

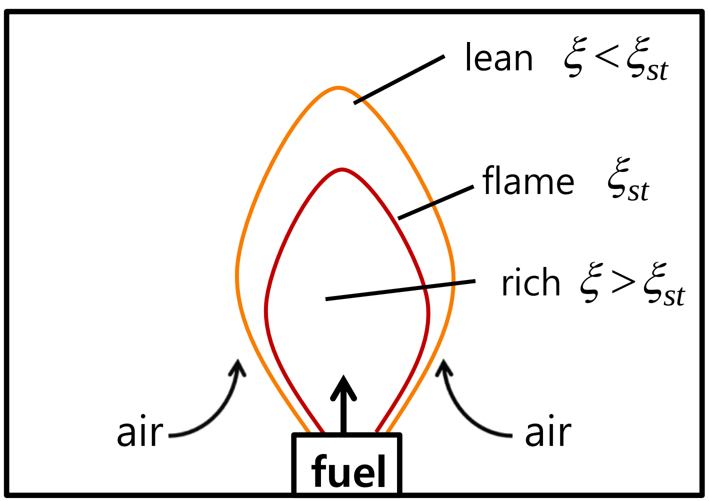
Y_i : i-th species mass fraction

a_i : constant

$c = 0$ where the mixture is unburnt

$c = 1$ where the mixture is burnt

Nonpremixed Flame



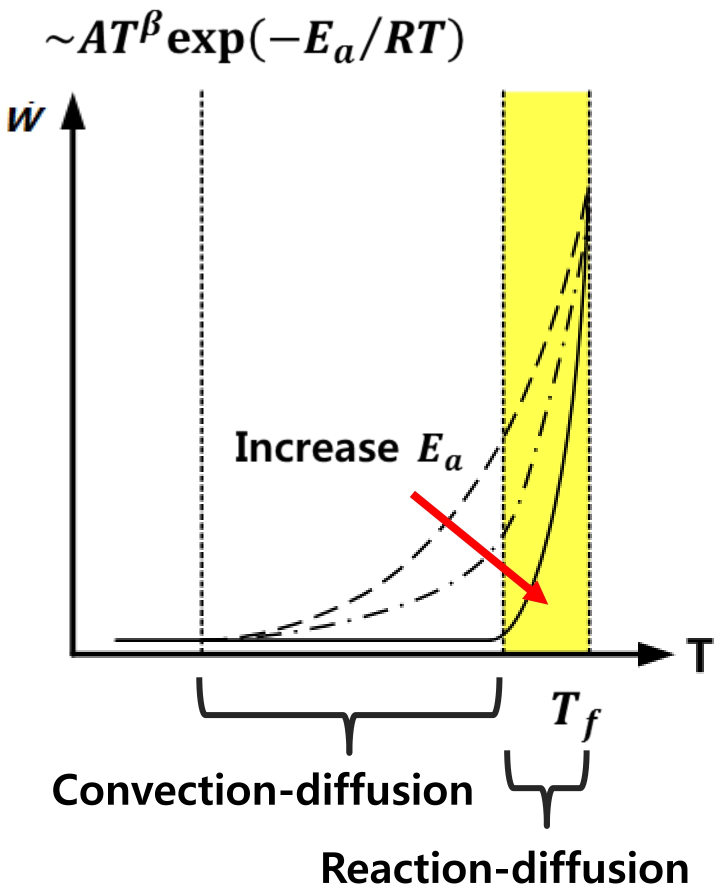
- Mixture Fraction

$$\xi = \frac{\text{mass originating from fuel stream}}{\text{mass of mixture}}$$

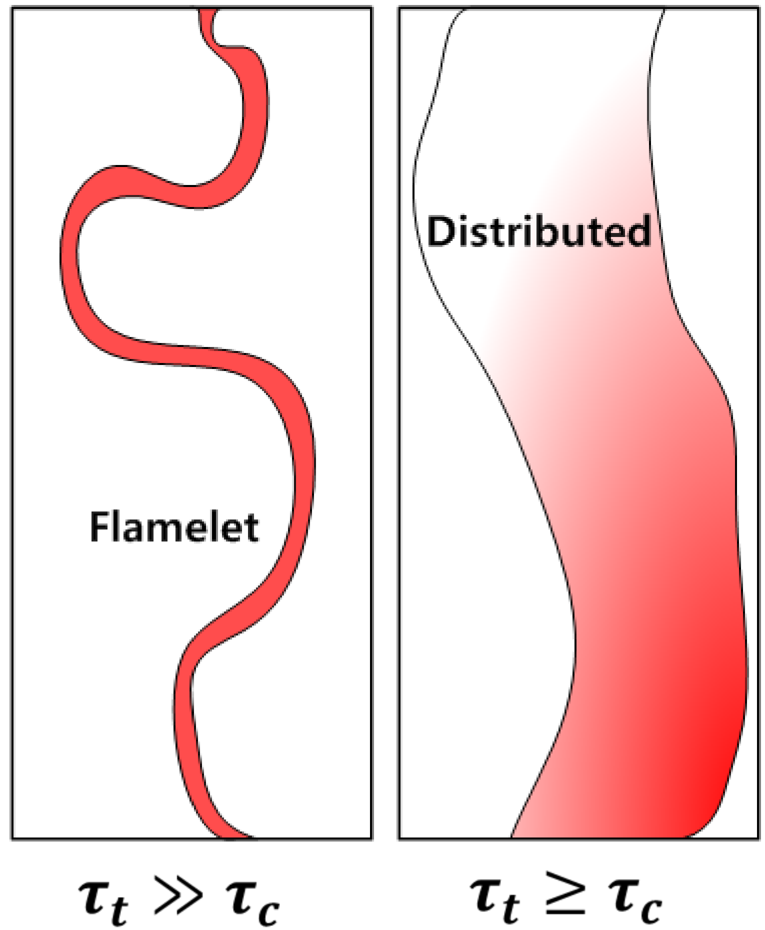
$$= \frac{m_{fuel}}{m_{fuel} + m_{oxidizer}}$$

Why Is Reaction Localized in Space?

Large Activation Energy



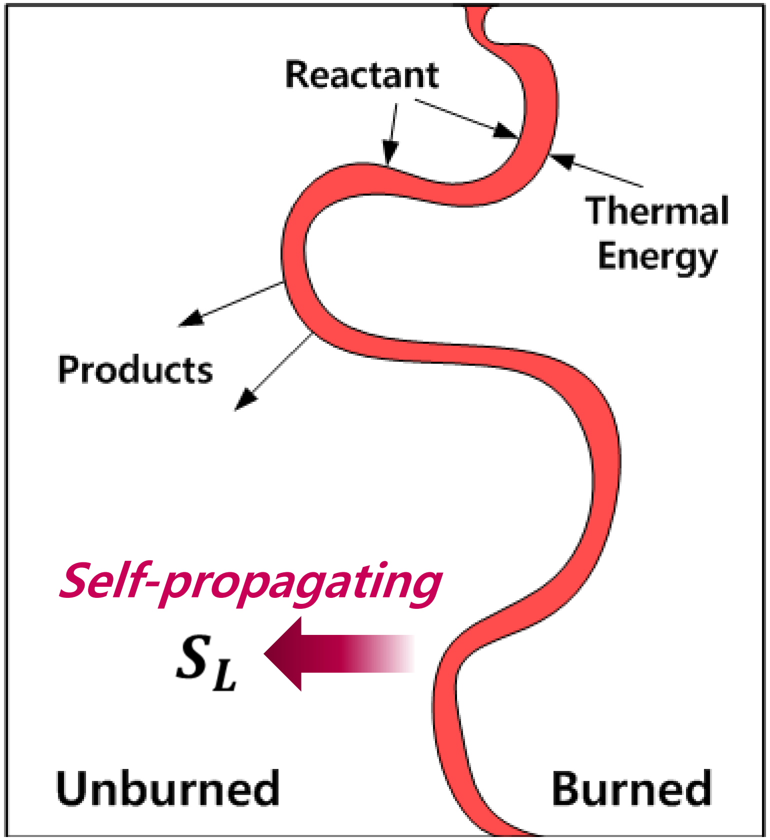
Chemistry Faster than Mixing



Laminar Flamelet Regime

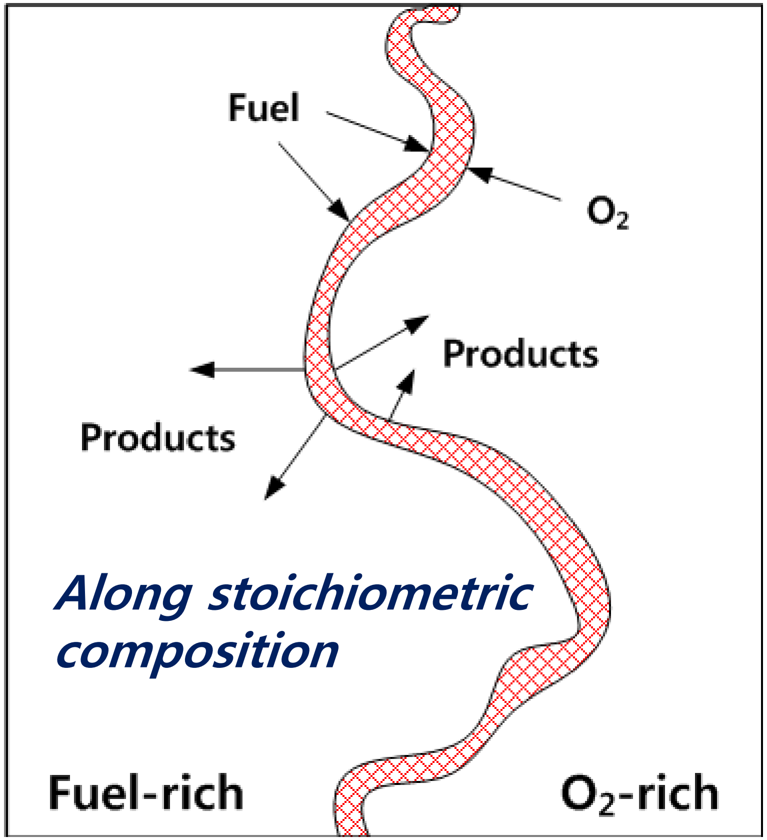
Premixed combustion

Homogeneous F/A mixture



Nonpremixed combustion

F/A separate at mixing



Turbulent Nonpremixed Flames

Conditional Moment Closure Model

Implementation strategies

- **Open source CFD toolbox, OpenFOAM, is coupled with Lagrangian CMC routine**

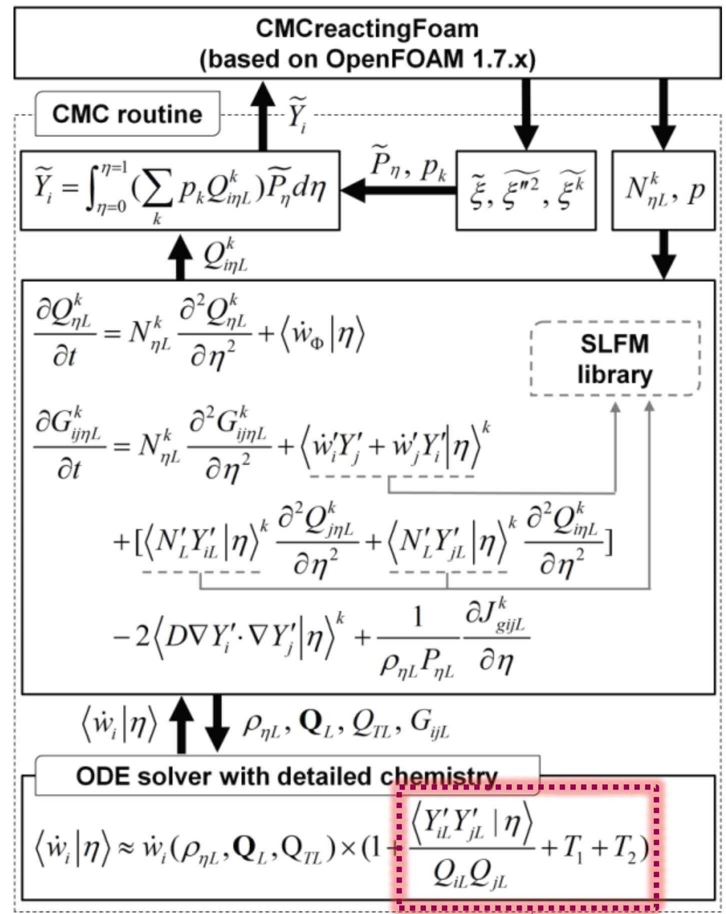
- **OpenFOAM solves flow and mixing field in the physical space,**
  - **Favre mean mass, momentum, energy, turbulence**
  - **Favre mean mixture fraction and its variance**

- **Lagrangian CMC routine solves conditionally averaged equations in the mixture fraction space**
  - **Conditional mean mass fractions and enthalpy**
  - **Conditional variances and covariances (2nd order CMC, $G_{ij\eta L} \equiv \langle Y'_i Y'_j \mid \eta \rangle$)**

- **Source terms of chemical reaction are integrated by stiff ordinary differential equation solver, SIBS, with GRI 3.0 mechanism.**

- **Correction is made up to the second order terms in Taylor expansion of the Arrhenius reaction rate for the following four rate limiting steps**

$$H + O_2 \rightarrow OH + O$$
$$CO + OH \rightarrow CO_2 + H$$
$$CH_4 + H \rightarrow CH_3 + H_2$$
$$H + O_2 + M \rightarrow HO_2 + M$$



Schematic diagram of interaction between OpenFOAM and CMC routines

Second order correction terms

Basic Flame - Sandia Flame D & E

Case description

Sandia/TUD Piloted CH_4/Air Jet Flames

Fuel : 25% CH_4, 75% Air (% vol.)

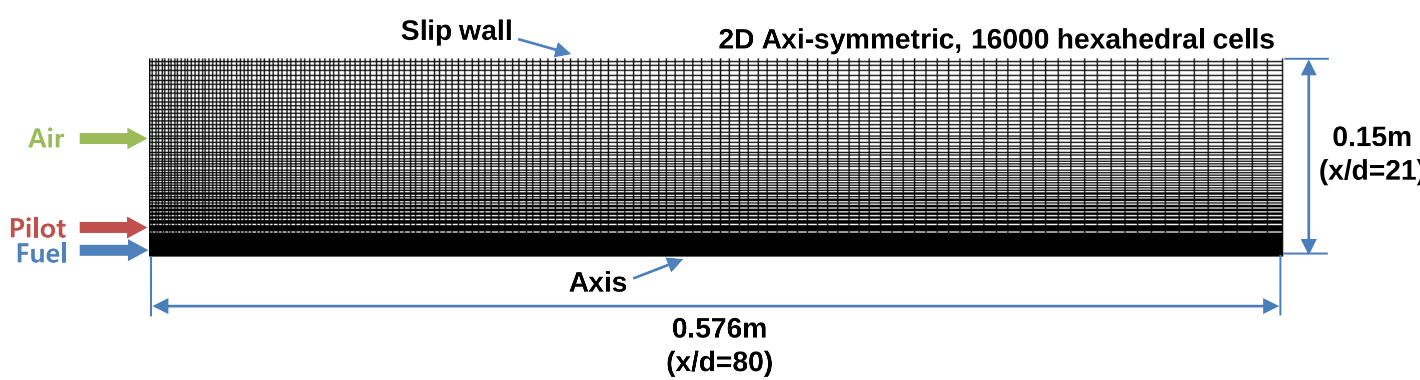
Stoichiometric mixture fraction = 0.351

Nozzle diameter = 7.2mm, Pilot diameter = 18.2mm

Fuel Temp = 294K, Pilot Temp = 1880K, Coflow Temp = 291K

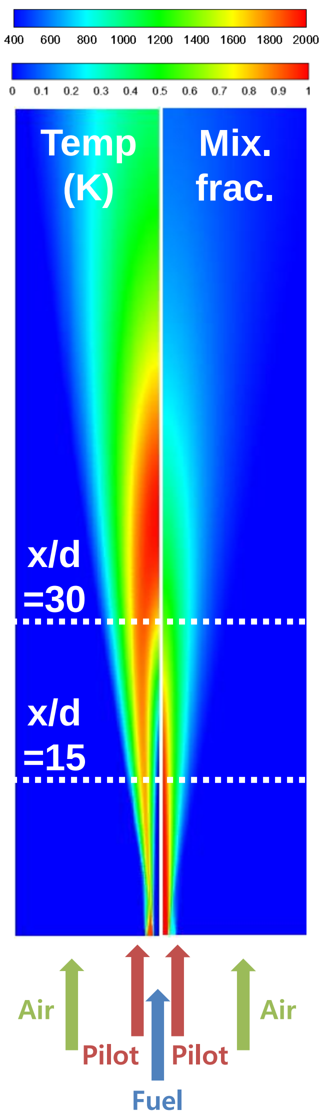
Flame D	Flame E
Fuel velocity = 49.6m/s	Fuel velocity = 74.4m/s
Pilot velocity = 11.4m/s	Pilot velocity = 17.1m/s
Reynolds number = 22,400	Reynolds number = 33,600

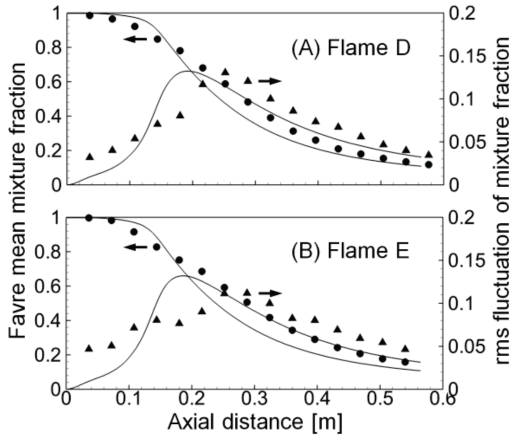
R. S. Barlow and J. H. Frank, Proc. Combust. Inst. 27:1087-1095 (1998)
R. S. Barlow, J. H. Frank, A. N. Karpetis and J. Y. Chen, Combust. Flame 143:433-449 (2005)
Ch. Schneider, A. Dreizler, J. Janicka, Combust. Flame 135:185-190 (2003)



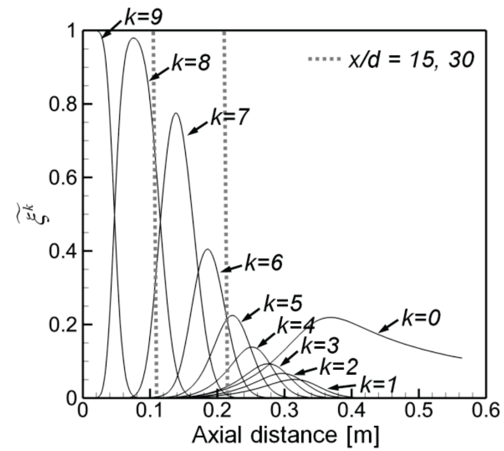
Basic Flame - Sandia Flame D & E

Results

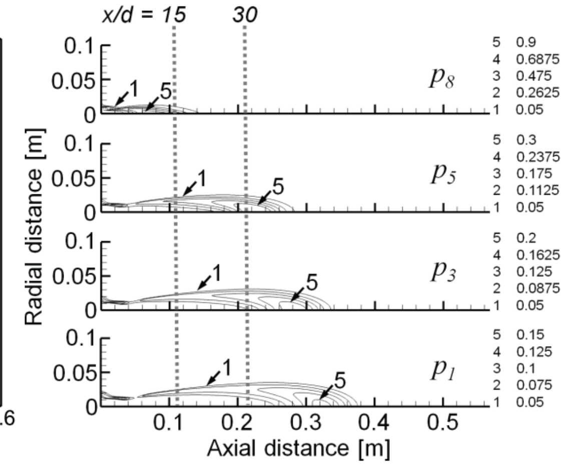




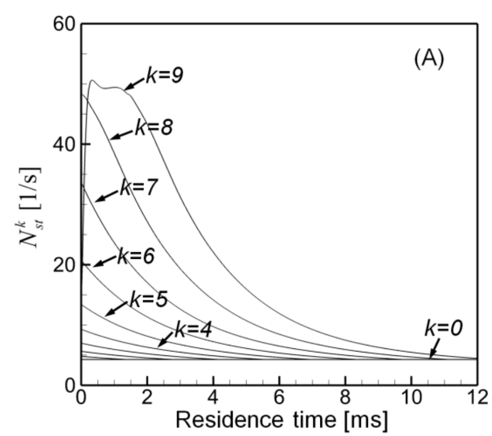
Favre mean mixture fraction and rms fluctuations of mixture fraction along the axis



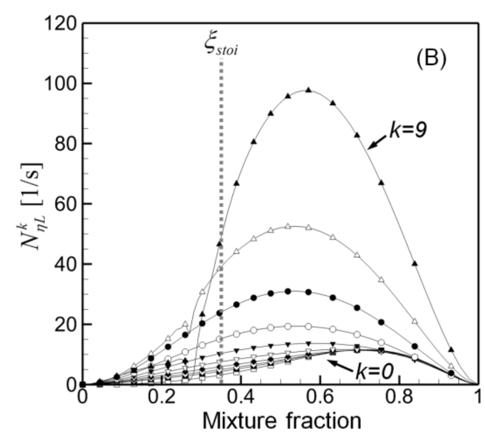
Distribution of ξ^k for ten flame groups along the axis



Axial distribution of p_k for the 1st, 3rd, 5th and 8th flame groups in Flame D



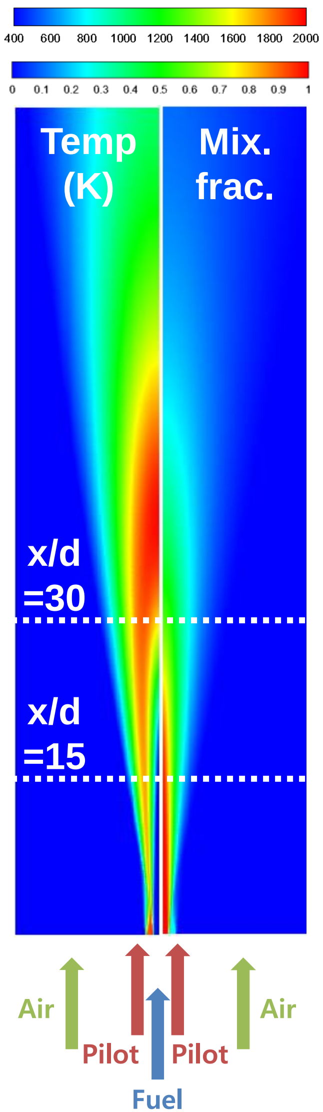
Conditional SDR's at stoichiometry w.r.t. the residence time

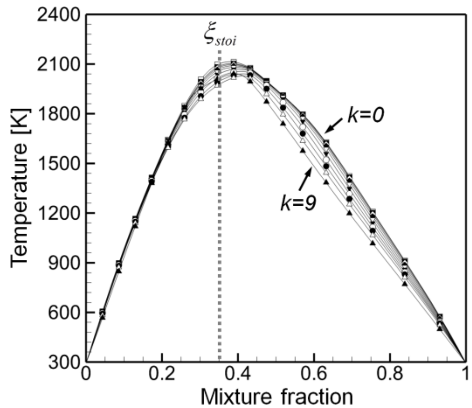


Conditional SDR's for ten flame groups in Flame D

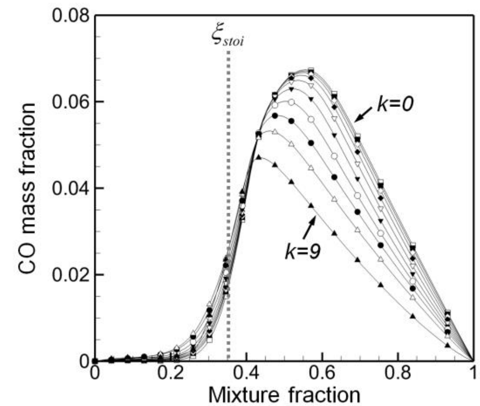
Basic Flame - Sandia Flame D & E

Results

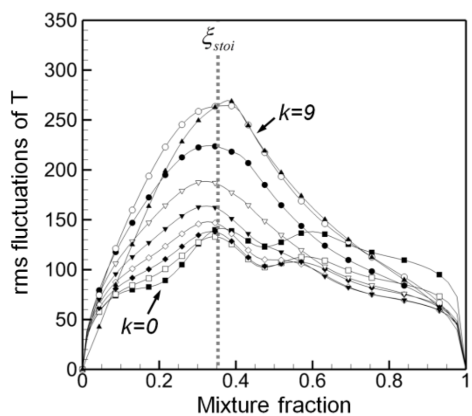




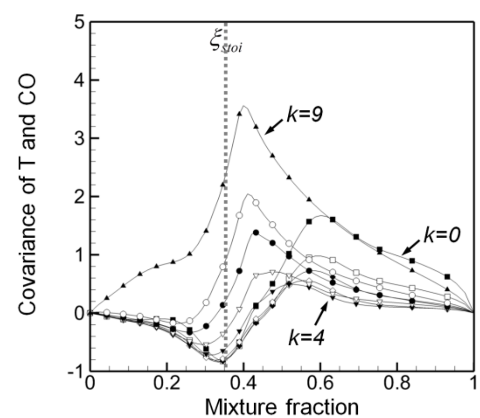
Conditional temperature for ten flame groups in Flame D



Conditional CO mass fraction for ten flame groups in Flame D



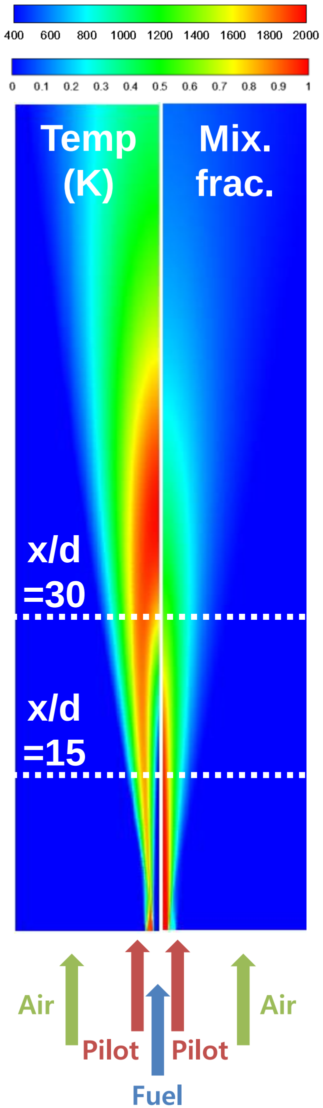
Conditional rms fluctuations of T for ten flame groups in Flame D



Conditional covariance of T and CO for ten flame groups in Flame D

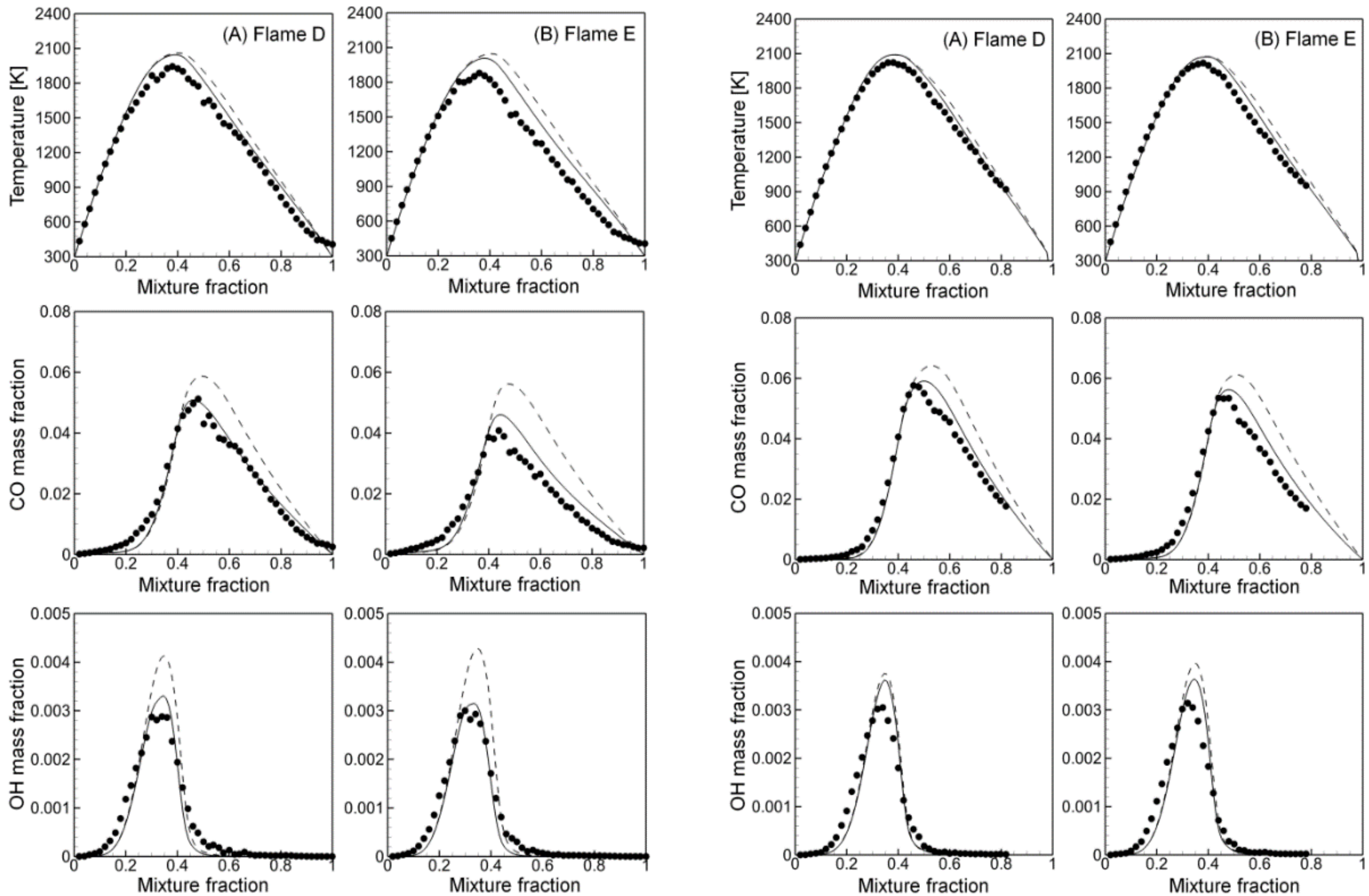
Basic Flame - Sandia Flame D & E

Results



x/d=15

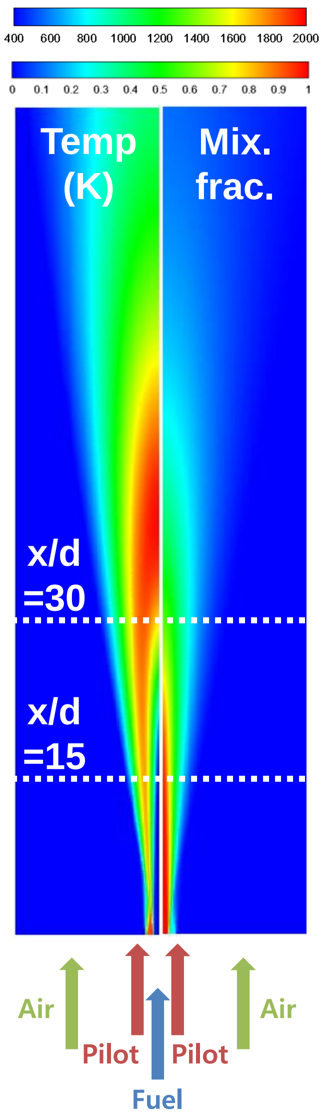
x/d=30

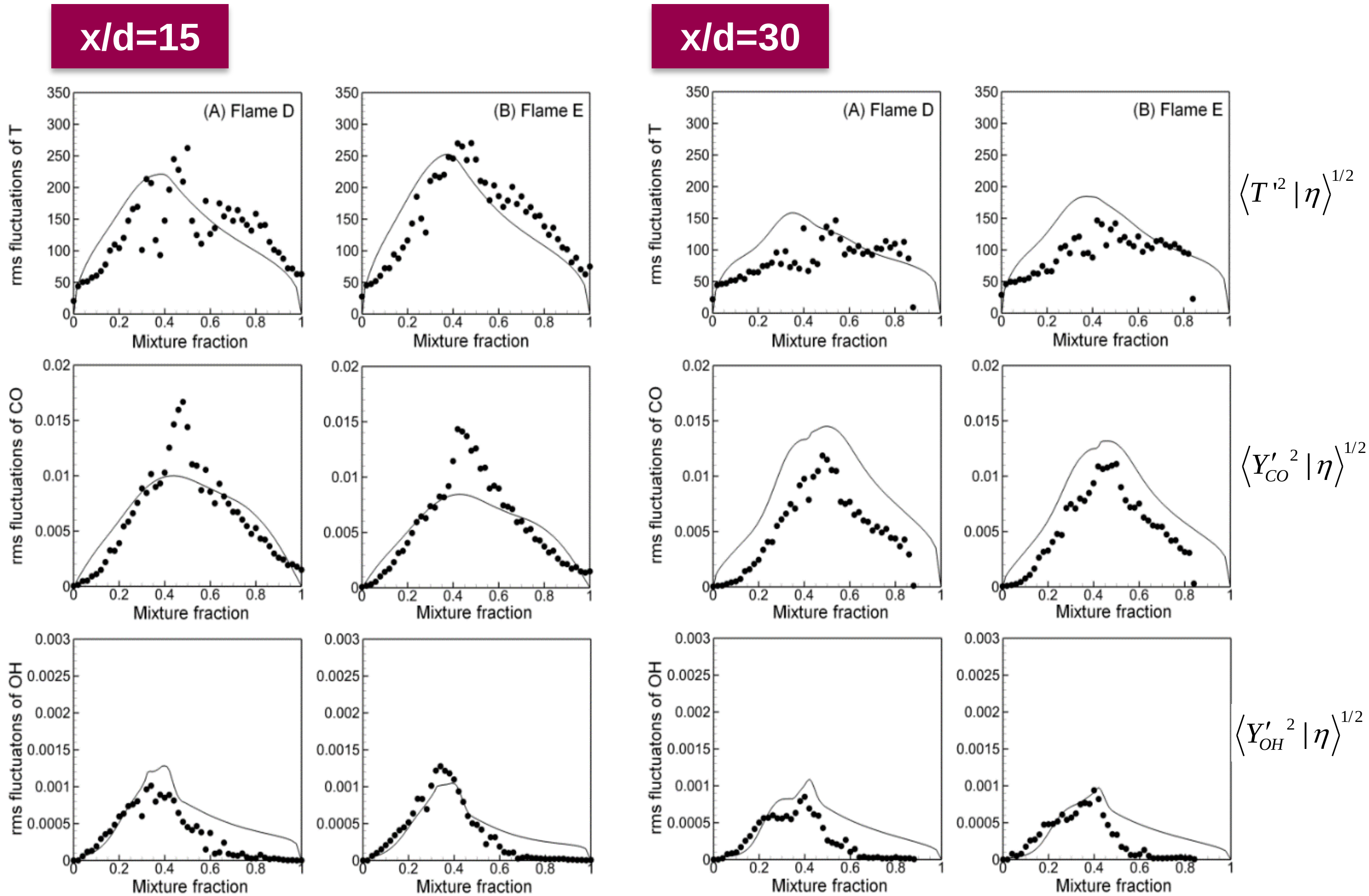


Measured and predicted T, conditional mass fractions at x/d=15, 30 in Flame D and E (symbols, measurement; lines, prediction)

Basic Flame - Sandia Flame D & E

Results

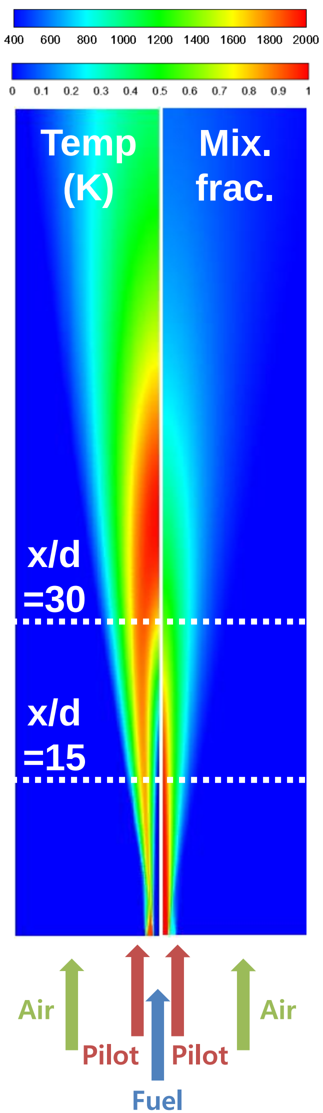


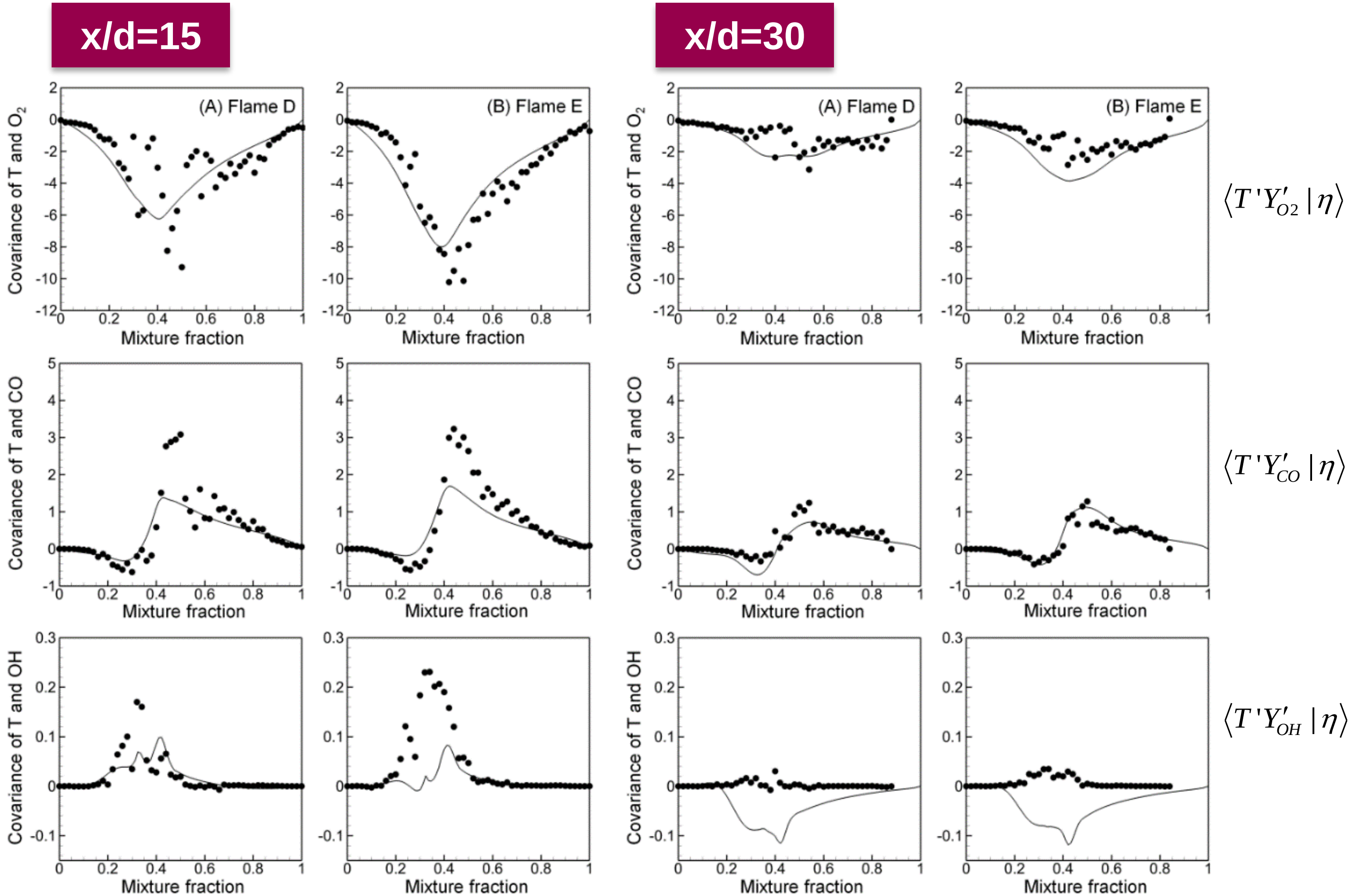


Measured and predicted conditional rms fluctuations at x/d=15, 30 in Flame D and E (symbols, measurement; lines, prediction)

Basic Flame - Sandia Flame D & E

Results





Measured and predicted conditional covariances at x/d=15, 30 in Flame D and E (symbols, measurement; lines, prediction)

Steady Laminar Flamelet Model

Model description

- Turbulent flame modeled as an ensemble of thin, laminar, locally 1-D flamelet structures
- Reacting scalars mapped from physical space to mixture fraction space

SLFM Library (Q_i, Q_h, T)

- Contains Q_i, Q_h and T distributions in mixture fraction space
- **Parameterized in terms of scalar dissipation rate (SDR)**
- Usually **pre-calculated** by in-house code or other tools (OpenFOAM?)

$$0 = \langle N|\eta\rangle \frac{\partial^2 Q_\eta}{\partial \eta^2} + \langle \dot{w}_\eta|\eta\rangle$$

+

PDF Library

- Contains probability density function i
- **Parameterized in terms of mixture fraction** and **its variance**
- **Pre-calculated** or calculate on the fly

$$\tilde{P}(\eta) = \frac{\zeta^{\alpha-1}(1-\zeta)^{\beta-1}}{\Gamma(\alpha)\Gamma(\beta)}\Gamma(\alpha+\beta)$$

- Integrate scalars (Yi, T, h …) from SLFM and PDF library, make 3D Look-up table (mf, mfVar, SDR) before calculation
- Solve transport eqns for mixture fraction and its variance
- Find and interpolate scalars from 3D Look-up table for given mixture fraction, variance and SDR
- Correct thermodynamic properties at local position

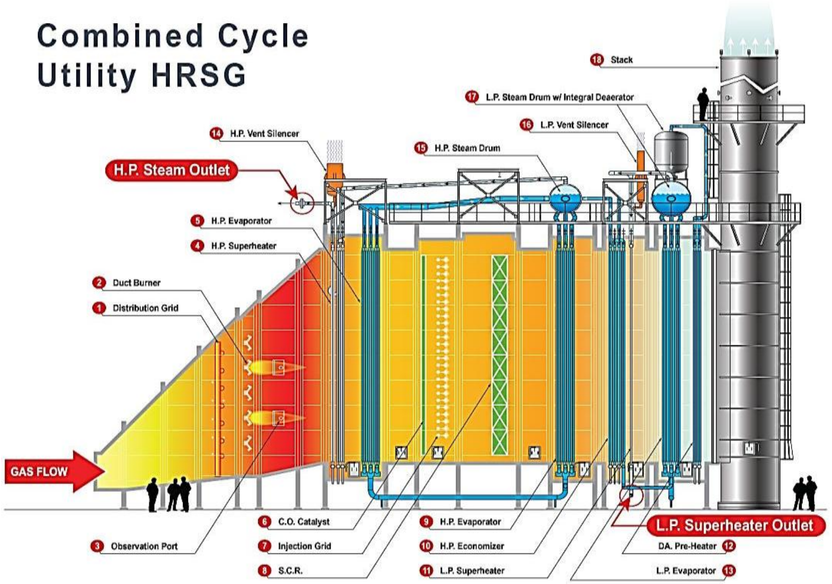
→ **SLFMFoam**

Industrial Furnace - Heat Recovery Steam Generator

Case description

- The HRSG is an energy recovery heat exchanger that recovers heat from a hot gas stream
  It produces steam that can be used in a process (cogeneration)
- The HRSG includes supplemental, or duct firing. These additional burners provide additional energy to the HRSG, which produces more steam and increases the output of the steam turbine
- Generally, duct firing provides electrical output at lower capital cost
  It is therefore often utilized for peaking operations

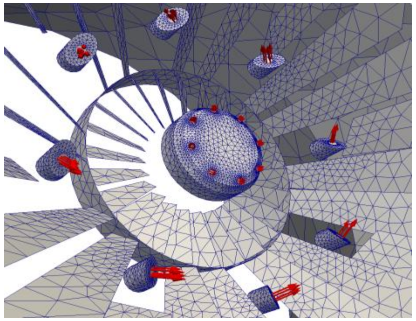
- **Main components of HRSG**
  - **Silencer**
    Attenuates noise level to meet government and site requirements
  - **Integral Deaerator**
    Uses low temperature heat to deaerate feed-water for improved thermal efficiency
  - **CO Catalyst**
    Reduces carbon monoxide in the flue gas
  - **Diverter Valve**
    Modulates steam production in the bypass systems
  - **SCR Catalyst**
    Reduces nitrous oxides in the flue gas
  - **Duct Burner**
    Provides supplementary firing of turbine exhaust to increase unfired steam production



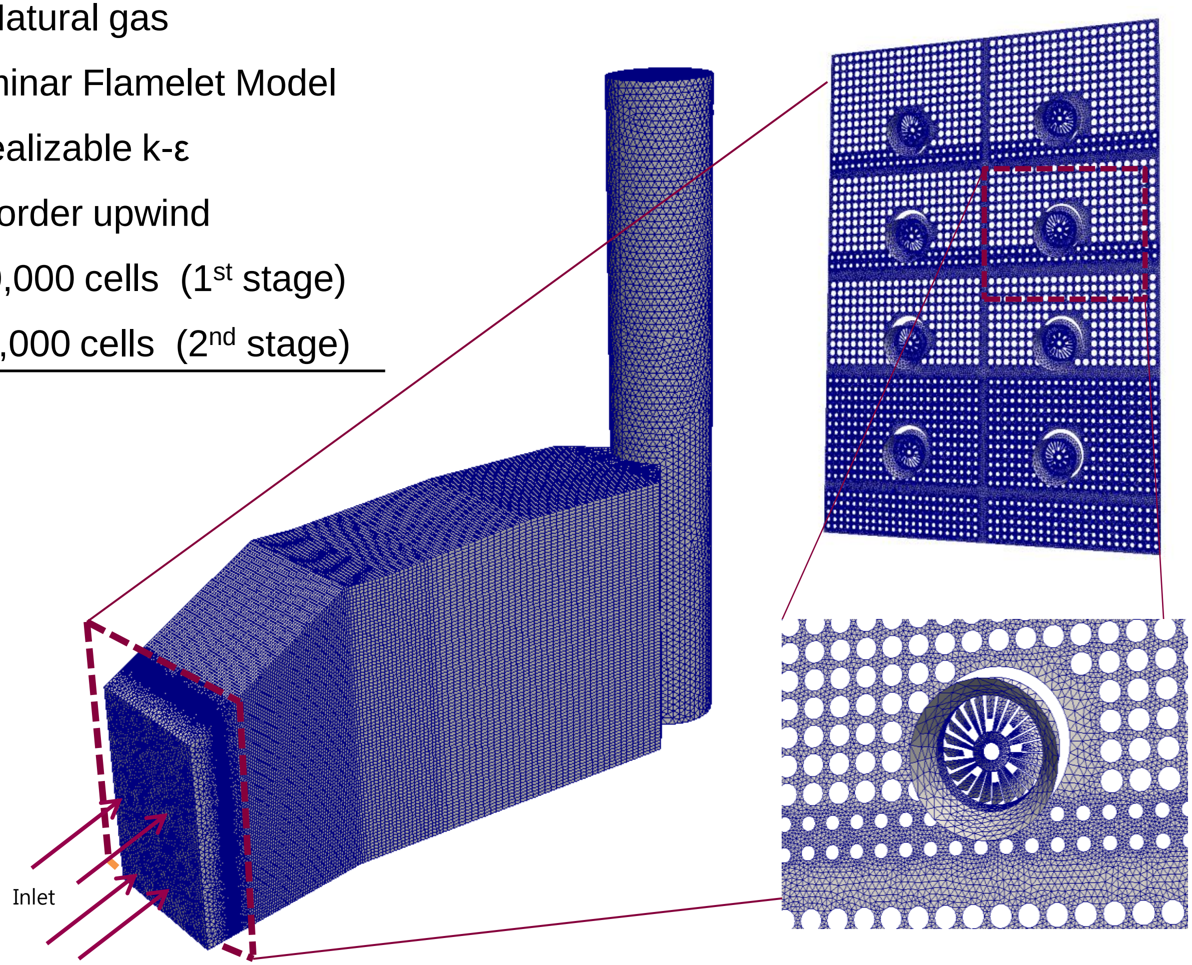
Industrial Furnace - Heat Recovery Steam Generator

Case description

Description	Specification
Fuel	Natural gas
Combustion model	Steady Laminar Flamelet Model
Turbulence model	Realizable k-ε
Discretization	2^{nd} order upwind
Mesh	About 7,000,000 cells (1^{st} stage)
	About 9,000,000 cells (2^{nd} stage)



Fuel nozzle



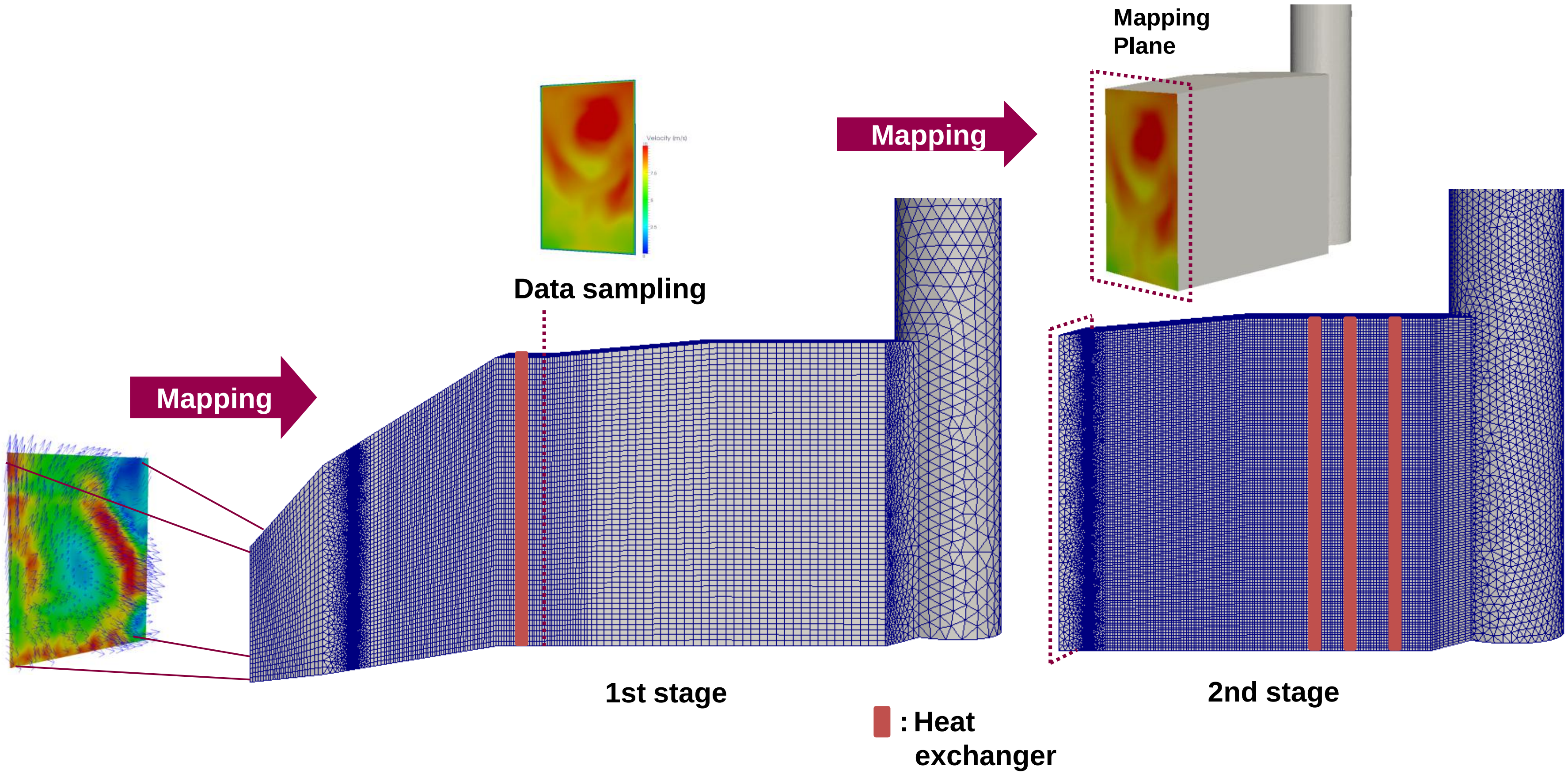
Computational mesh

Perforated wall and Burner

Industrial Furnace - Heat Recovery Steam Generator

Case description

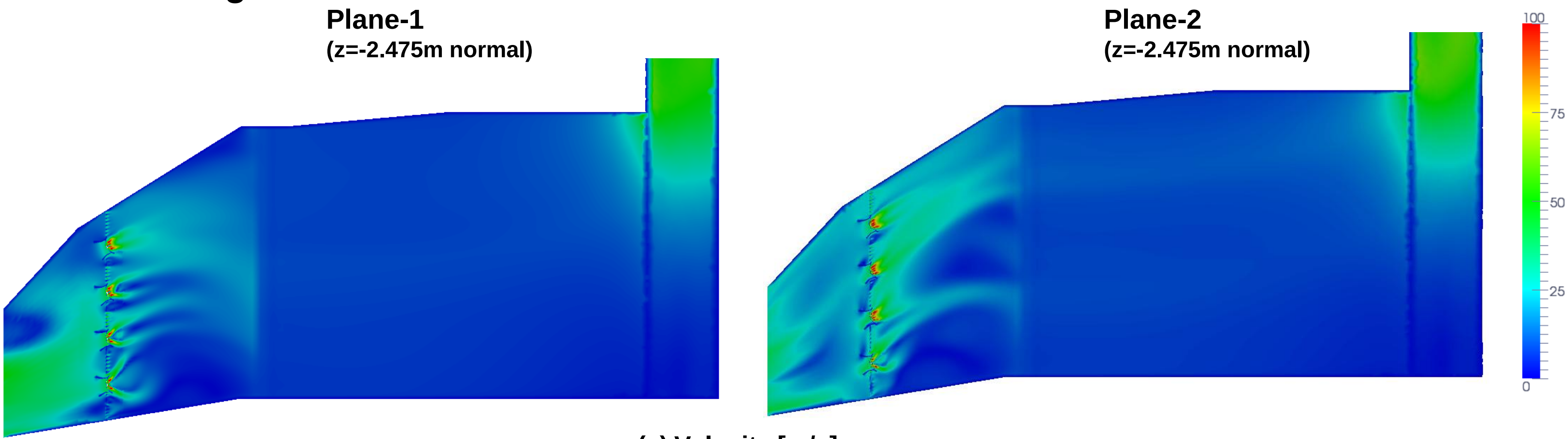
- It is very difficult to analyze a whole system of HRSG at a time
- A whole system is divided into two stages; 1st stage and 2nd stage
- A input of 2nd stage use sampled data from 1st stage result



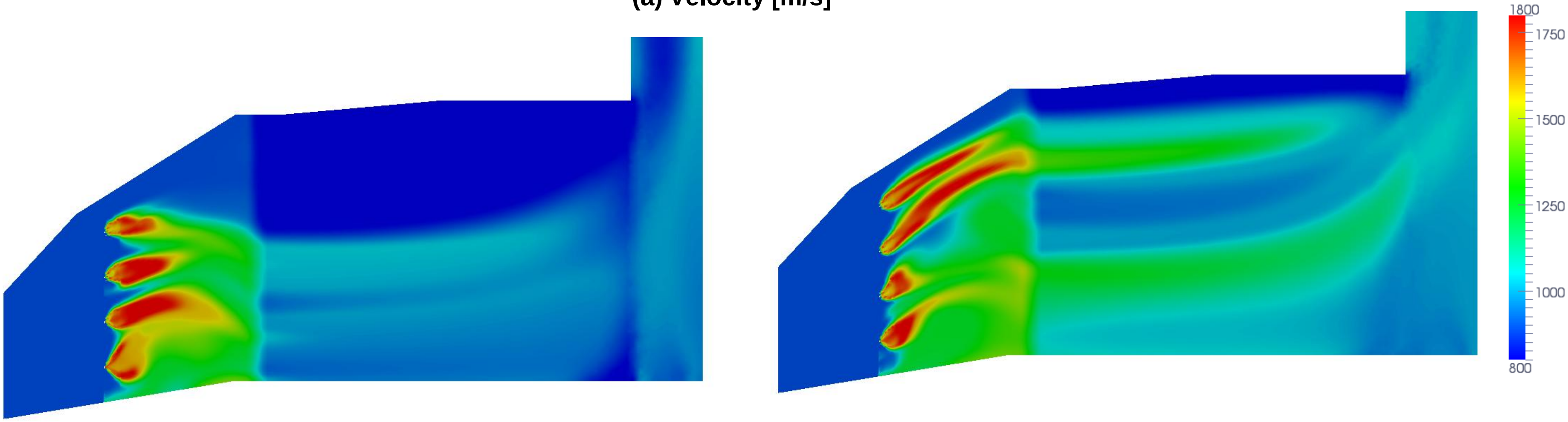
Industrial Furnace - Heat Recovery Steam Generator

Results

- 1st Stage



(a) Velocity [m/s]

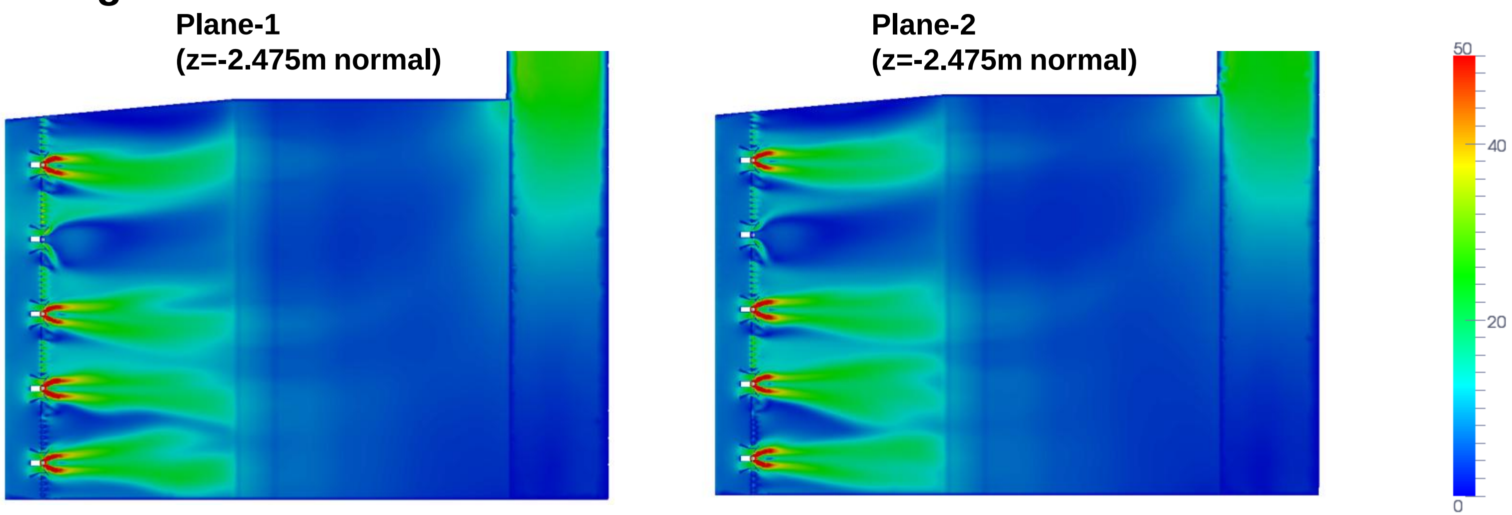


(b) Temperature [K]

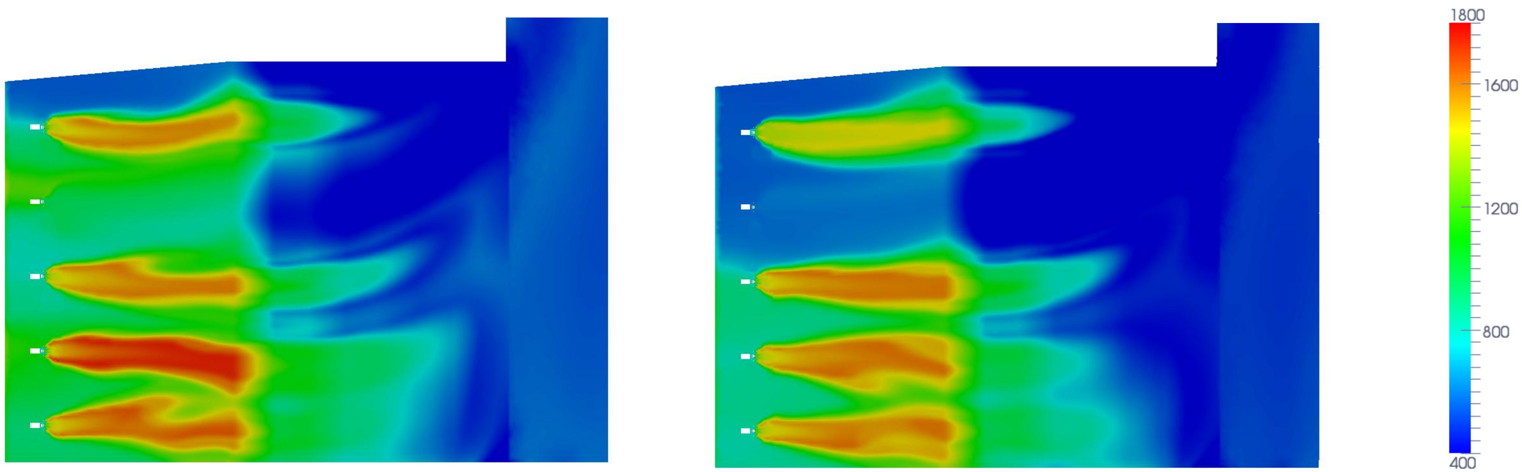
Industrial Furnace - Heat Recovery Steam Generator

Results

- 2nd stage



(a) Velocity [m/s]



(b) Temperature [K]

Industrial Furnace - Heat Recovery Steam Generator

Results

- **Comparison with the result for FLUENT**

Case		Units	Fluent	OpenFOAM	Measured / Performance	Ratio	
		Units	Outlet	Outlet	Outlet	Fluent	OpenFOAM
Temperature		K	385.95	453.275	401.85	**0.96**	**1.12**
Composition	**O2**	mass fraction	9.08E-02	8.98E-02	9.71E-02	**0.94**	**0.92**
	CO2	mass fraction	8.99E-02	9.75E-02	8.60E-02	**1.05**	**1.13**
	H2O	mass fraction	9.97E-02	9.28E-02	9.34E-02	**1.07**	**0.99**
	N2	mass fraction	7.07E-01	7.12E-01	7.09E-01	**1.00**	**1.00**
	AR	mass fraction	1.18E-02	1.16E-02	1.19E-02	**0.99**	**0.97**
	CO	ppm vd @actual O2	**21.9**	**33.2**	**44.32**	**0.49**	**0.75**
	NO	ppm vd @actual O2	**5.68**	**29.5**	**21.64**	**0.26**	**1.36**

Turbulent Partially Premixed Flames

Modified Weller(FSD) Model

Model description

- **XiFoam (basic solver)**
  - Reasonable combustion model for partially premixed flame using Weller wrinkling factor(Xi)
  - Steady solver(transient calculation takes 10 times longer than steady calculation)

- **XiFlameletsFoam (advanced solver)**
  - Steady solver newly implemented combining modified Weller and LFM
  - Premixed process by modified Weller, nonpremixed by LFM
  - CO and NO prediction method

Algebraic equation for flame wrinkling factor

$$\Xi_{eq}^{*} = 1 + 0.62\sqrt{\frac{u'}{S_L}}R_\eta$$

$$\Xi_{eq} = 1 + 2\tilde{c}(\Xi_{eq}^{*} - 1)$$

Transport equation of progress variable

$$\frac{\partial\langle\rho\rangle\tilde{c}}{\partial t} + \frac{\partial\langle\rho\rangle\tilde{U}_i\tilde{c}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\Gamma_c\frac{\partial\tilde{c}}{\partial x_i}\right) + \tilde{\omega}_c + 2\frac{\Gamma_c}{(\tilde{Y}_{fu}-\tilde{Y}_{fb})}\frac{\partial\tilde{c}}{\partial x_i}\frac{\partial(\tilde{Y}_{fu}-\tilde{Y}_{fb})}{\partial x_i}$$

Modified for partially premixed combustion

$$\tilde{c} = \frac{\tilde{Y}_{Fu} - \tilde{Y}_F}{\tilde{Y}_{Fu} - \tilde{Y}_{Fb}} \qquad \tilde{\omega}_c = \rho_u S_L \Xi|\nabla c|$$

Unburned state

$$\tilde{\Phi}_u(\tilde{f}; \underline{x}, t) = \Phi_O + \tilde{f}(\Phi_F - \Phi_O)$$

Burned state

$$\tilde{\Phi}_b(\tilde{f}, \tilde{\chi}; \underline{x}, t) = \iint \Phi(f,\chi)P(f,\chi)df d\chi$$

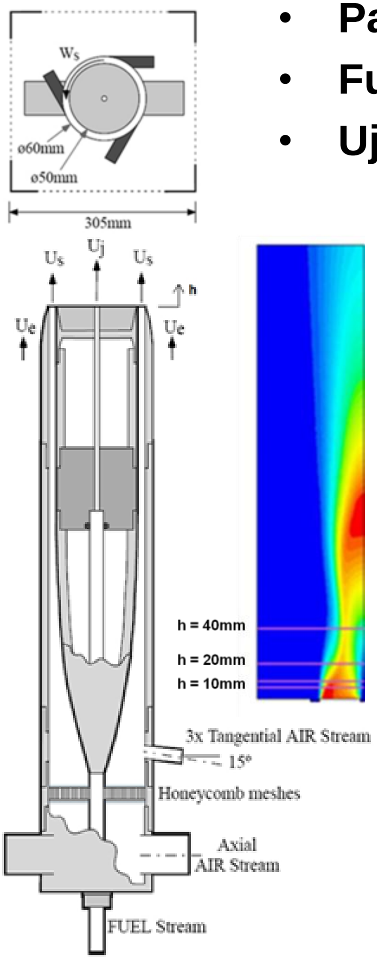
Mean conserved scalar

$$\tilde{\Phi}(\tilde{f}, \tilde{c}, \tilde{\chi}; \underline{x}, t) = (1 - \tilde{c})\tilde{\Phi}_u(\tilde{f}; \underline{x}, t) + \tilde{c}\tilde{\Phi}_b(\tilde{f}, \tilde{\chi}; \underline{x}, t)$$

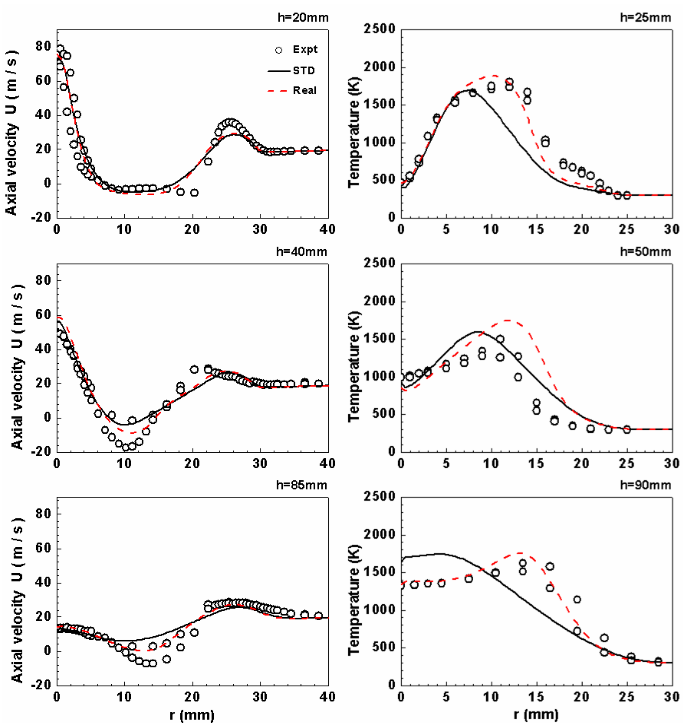
Basic Flame – Sydney Swirl Flame SMA1

Results

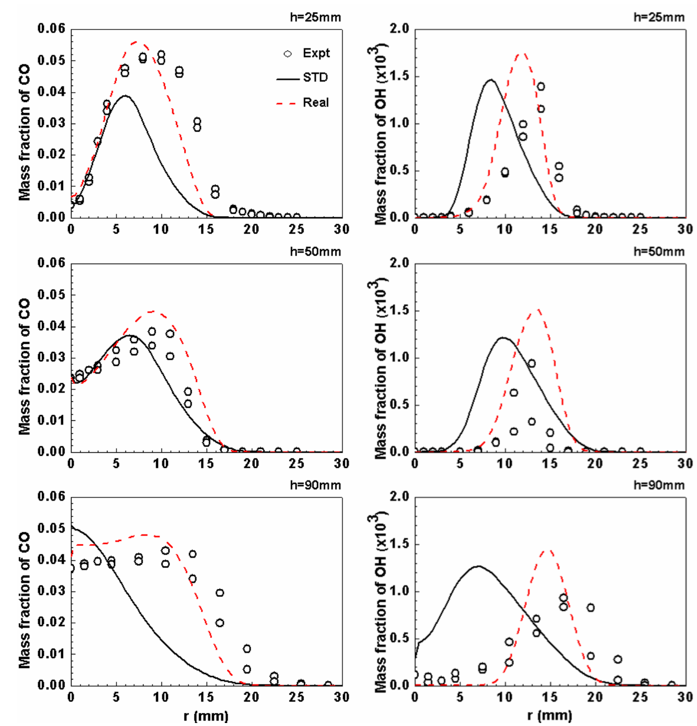
- **Partially premixed swirl flame SMA1 with XiFlameletsFoam**
- **Fuel = CH_4/air (1:2), Coflow = air**
- **Ujet = 66.3 m/s, Us = 32.9 m/s, Swirl ratio = 0.7**



Schematic of the burner



Axial velocity and temperature



Distributions of CO and OH

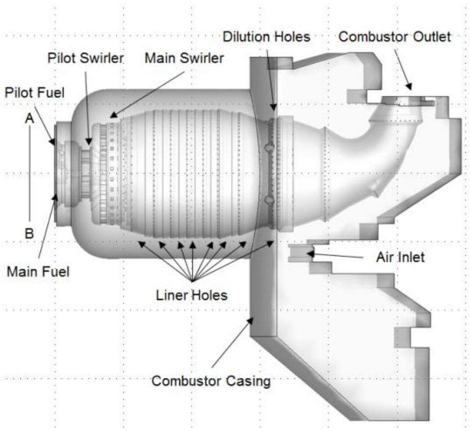
Industrial Furnace – 5MWe Micro Gas Turbine

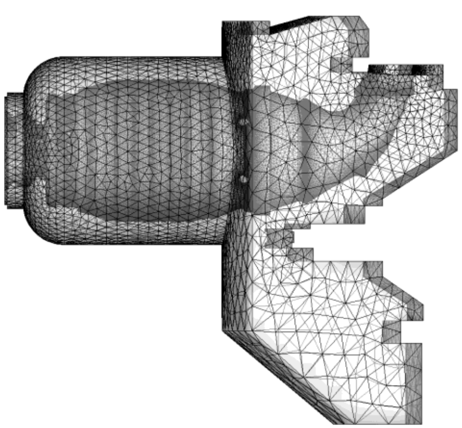
Case description

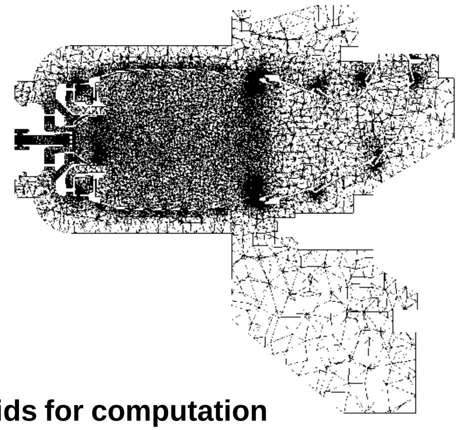
- Reverse-flow semi silo type with compressed air entering through pilot and main nozzles
- Two coaxial annular nozzles with radial swirlers
- Fuel is injected to be partially premixed with air in both nozzles

- **Numerical Method**
  - Pressure-velocity coupling based on SIMPLE algorithm
  - Gauss upwind scheme for spatial discretization of convection term
  - Mass flow inlet B.C with zero gradient pressure and fixed temperature
  - normalized residual of P < 10^{-3}, the other < 10^{-6} for convergence

- **Grid generation**
  - 14 MM tetrahedral cells converted by STAR_CCM+(5.04)



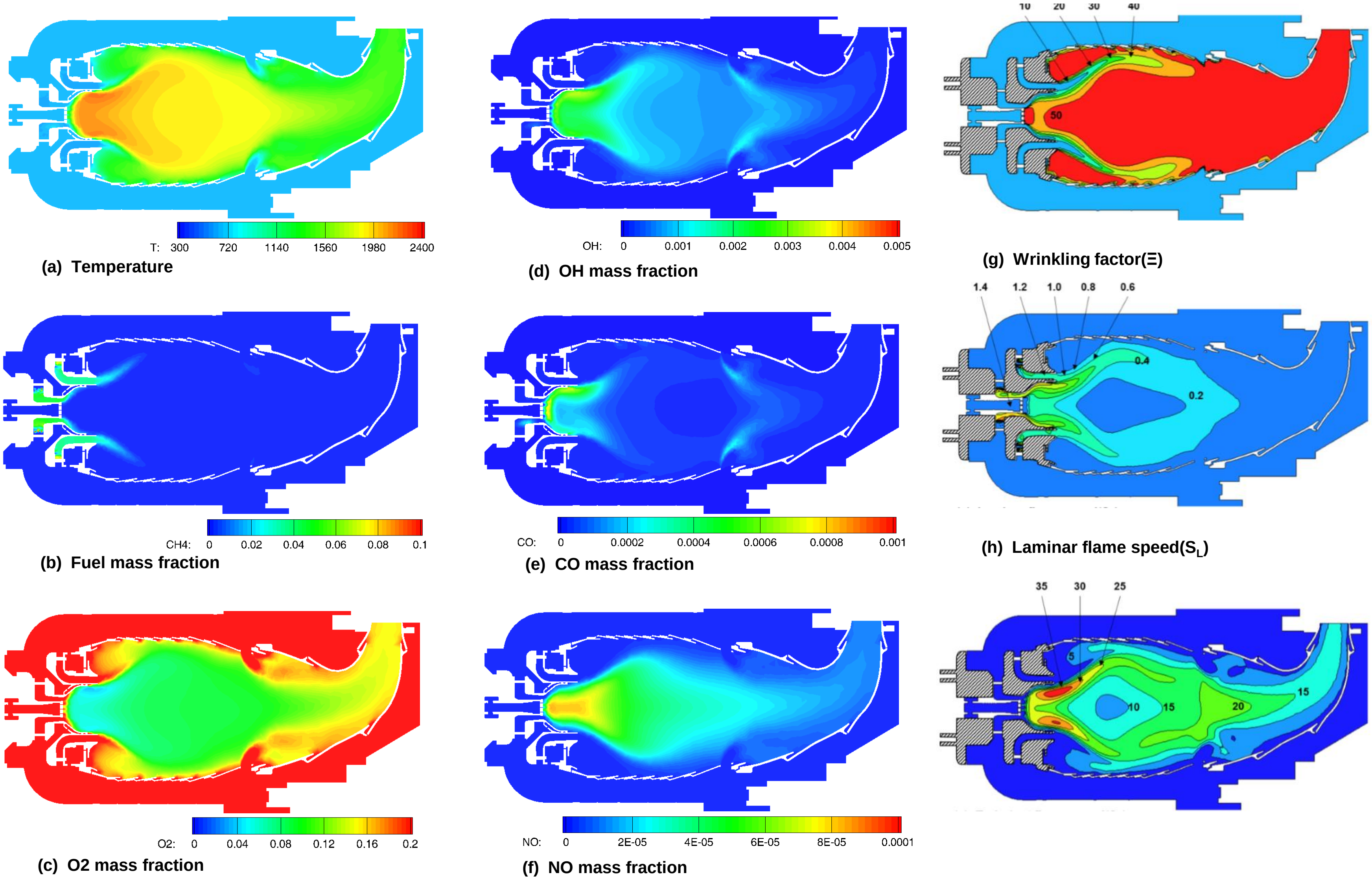




Grids for computation

Industrial Furnace – 5MWe Micro Gas Turbine

Results



(a) Temperature

(b) Fuel mass fraction

(c) O2 mass fraction

(d) OH mass fraction

(e) CO mass fraction

(f) NO mass fraction

(g) Wrinkling factor(Ξ)

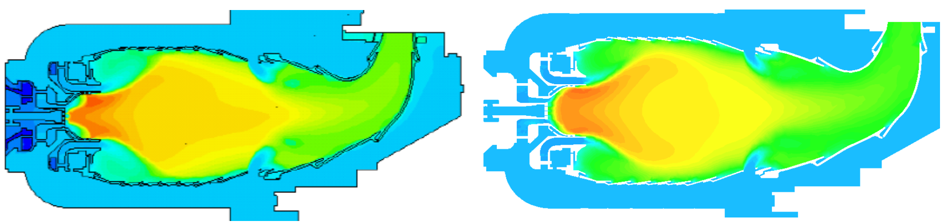
(h) Laminar flame speed(S_L)

Industrial Furnace – 5MWe Micro Gas Turbine

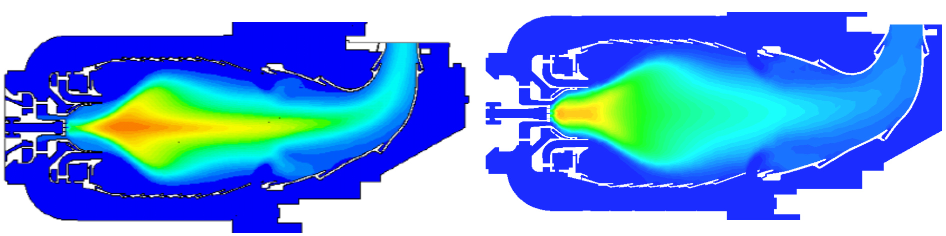
Results

- **PCFM(STAR-CCM+) provides insight for complex reacting flow fields but**
  - **Non-premixed combustion region is calculated by equilibrium PPDF (Over-prediction of CO)**
  - **Thermal NO only considered**

- **Margin of Errors of XiFlameletsFoam(OpenFOAM)**
  - **T < 0.8%, O2 < 6%**
  - **reasonable order of degree for CO**



(a) Temperature



(b) NO mass fraction

PCFM (STAR-CCM+) — **XiFlameletsFOAM (OpenFOAM)**

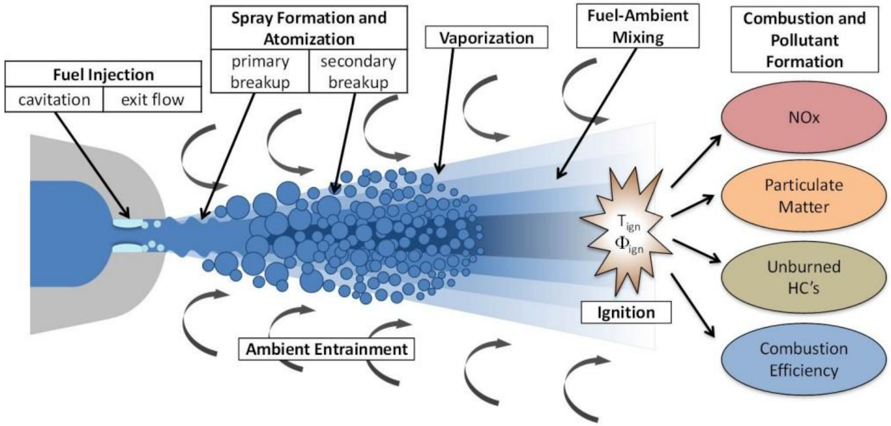
Specification	Measured	PCFM (STAR-CCM+)	XiFlamelet (OpenFOAM)
Temperature	1371.5 K	1382.2 K	1360.6 K
O_2	14.8 %	13.9 %	14.2 %
CO (@15%O_2)	12.6 ppm	350.7 ppm	5.33 ppm

Measured and calculated scalars at the outlet

Spray Combustion Modeling

Spray Combustion Modeling

CMC equation with spray



CMC $$\frac{\partial Q_\eta}{\partial t} = \langle N|\eta\rangle \frac{\partial^2 Q_\eta}{\partial \eta^2} + \langle \dot{w}_\eta|\eta\rangle$$

Mixture fraction $$\xi = \frac{Z_i - Z_{i,oxi}}{Z_{i,fuel} - Z_{i,oxi}}$$

Assumed beta-function PDF

$$\tilde{P}(\eta) = \frac{\zeta^{\alpha-1}(1-\zeta)^{\beta-1}}{\Gamma(\alpha)\Gamma(\beta)}\Gamma(\alpha+\beta)$$

$$where\ \alpha = \tilde{\zeta}\gamma,\ \ \beta = (1\text{-}\tilde{\zeta})\gamma,\ \ \gamma = \frac{\tilde{\zeta}(1-\tilde{\zeta})}{\zeta''^2}$$

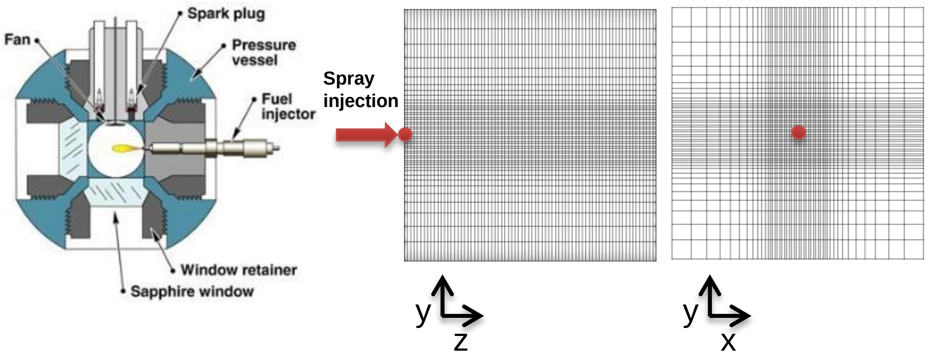
Mixture fraction $$\frac{\partial(\bar{\rho}\tilde{\xi})}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{\boldsymbol{u}}\tilde{\xi}) = \nabla\cdot\left[\frac{\mu_t}{Sc_{\tilde{\xi}}}\nabla\tilde{\xi}\right] + \bar{\rho}\tilde{\dot{s}}_\xi$$

Mixture fraction variance $$\frac{\partial(\bar{\rho}\widetilde{\xi''^2})}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{\boldsymbol{u}}\widetilde{\xi''^2}) = \nabla\cdot\left[\frac{\mu_t}{Sc_{\widetilde{\xi''^2}}}\nabla\widetilde{\xi''^2}\right] + \frac{2\mu_t}{Sc_{\widetilde{\xi''^2}}}(\nabla\tilde{\xi})^2$$

$$-2\rho\tilde{\xi}''\dot{s}_\xi(1-\tilde{\xi}) - \rho\tilde{\xi}''\dot{s}_\xi - \rho\tilde{\chi}$$

Case description

- **Library of recent well-documented spray experiments**
- **Includes parametric variation of oxygen concentration, ambient temperature, ambient density, fuel type, fuel temperature, injection duration, etc.**
- **Website : http://public.ca.sandia.gov/ECN/**



Constant volume combustion chamber (Experimental setup and computational grid)

- **Injector Specification**

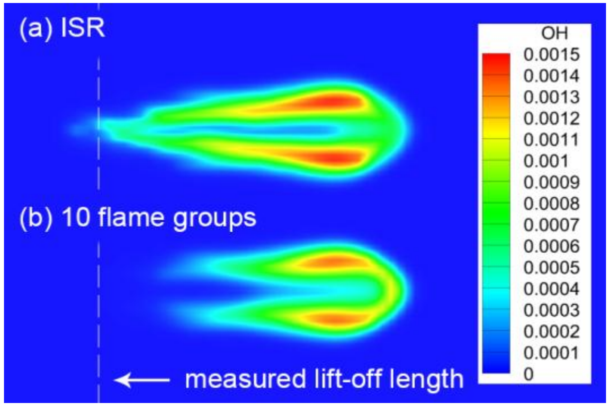
Parameters	Values
Injector type	Common-rail injector
Nozzle outlet diameter [mm]	0.1
Nozzle K factor	1.5
Nozzle shaping	Hydro-eroded
Discharge Coefficient	0.86
Fuel injection Pressure [MPa]	150

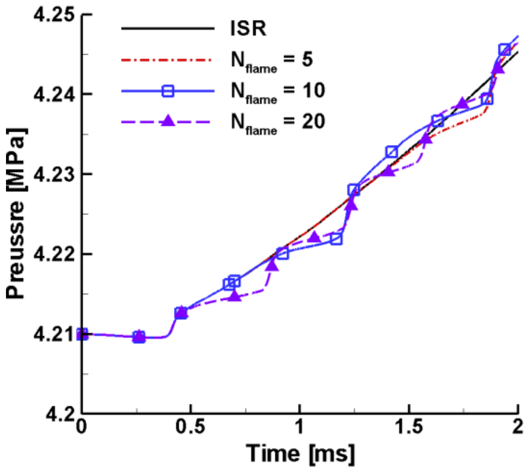
- **Simulation Cases (n-heptane spray)**

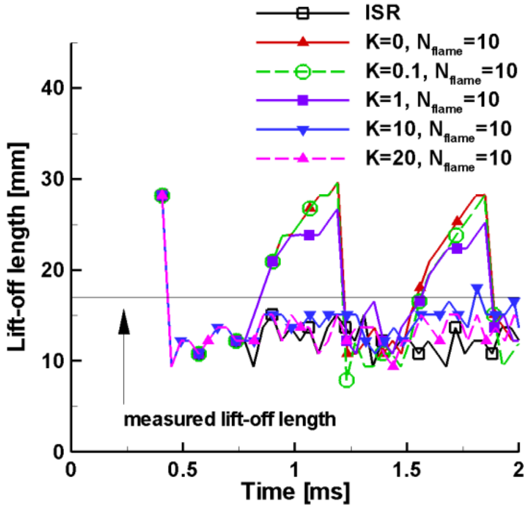
Case	O_2 [%]	Ambient Temperature [K]	Ambient Density [kg/m^3]	Measured Lift-off Length [mm]
1	21	1000	14.8	17.0
2	21	1100	14.8	13.0
3	21	1200	14.8	10.0
4	15	1000	14.8	23.4
5	12	1000	14.8	29.2

Results

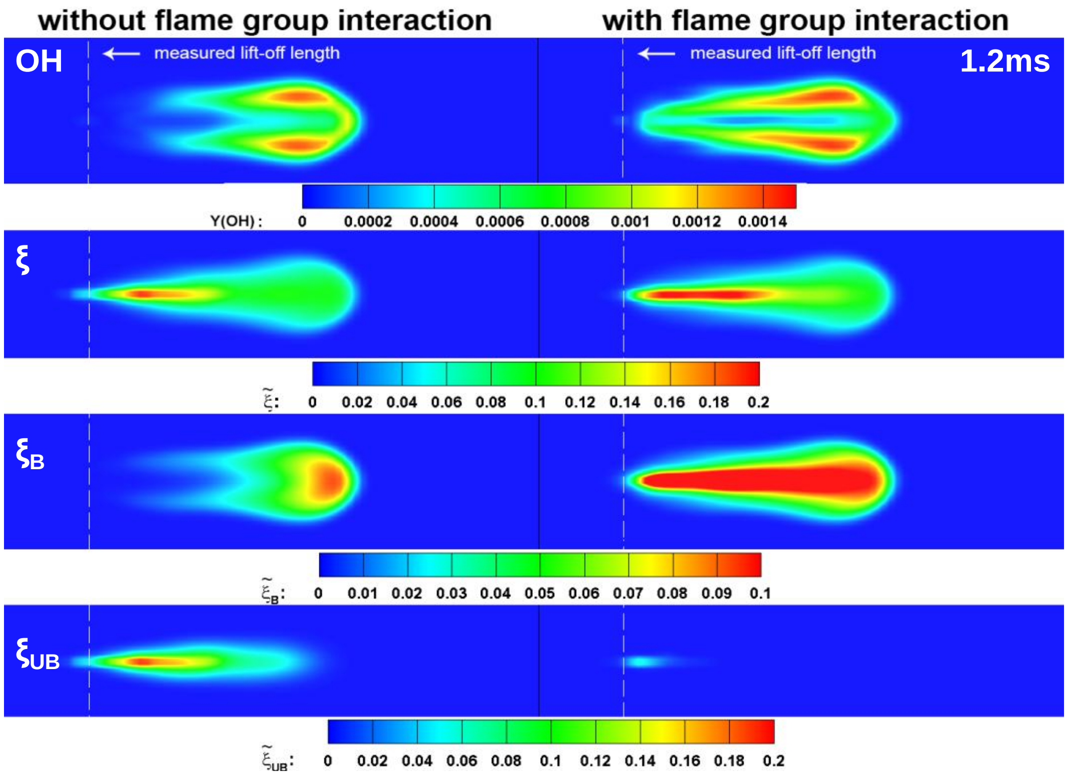
- Total fuel injected is divided into the given number of groups of equal mass according to evaporation sequence.
- The pressure shows a regular pattern of oscillation with abrupt rise at the moment of ignition of sequential flame groups.
- Without flame group interaction newly introduced flame groups undergo their own ignition delay period and sequential independent auto-ignition, even though there exist neighboring flame groups already ignited at the same location

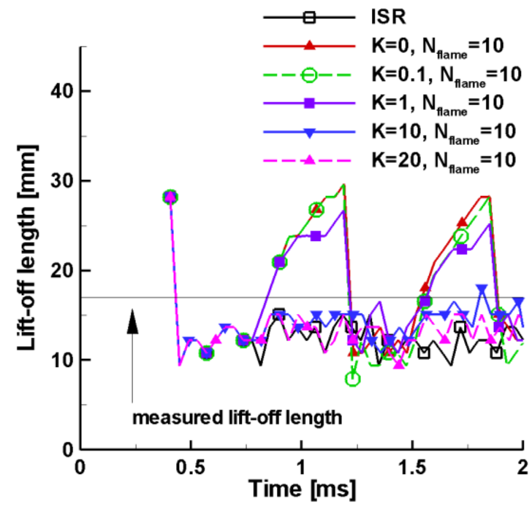






Results



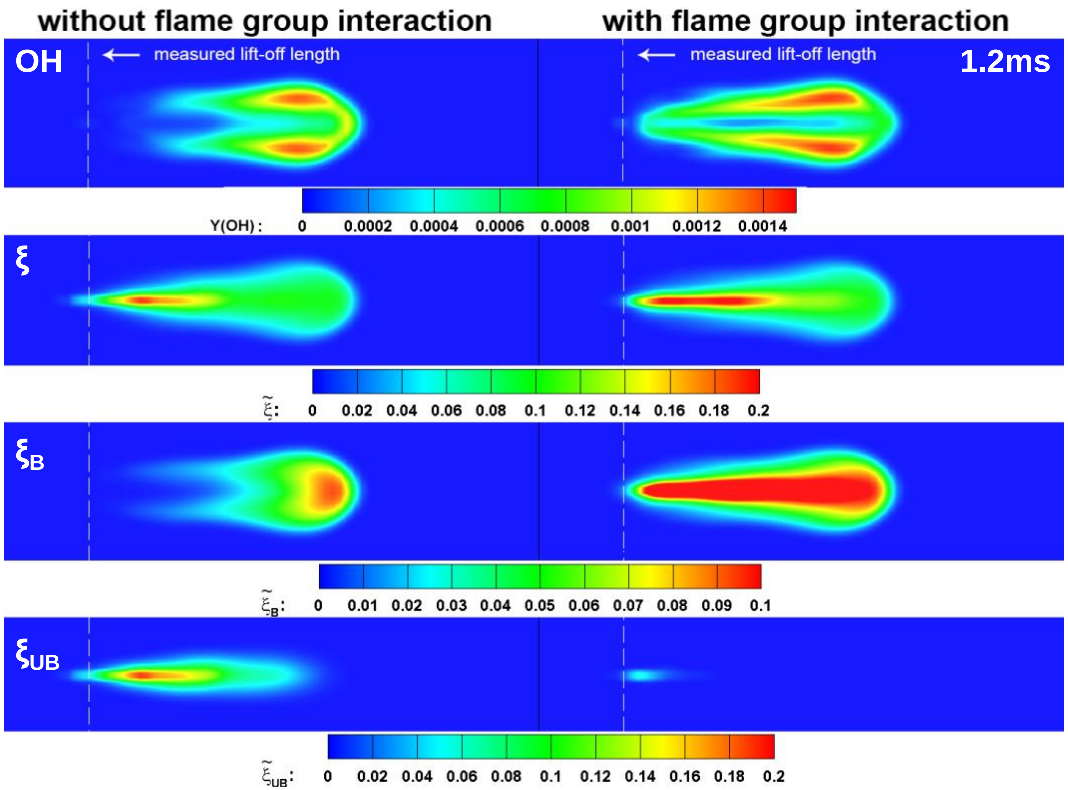


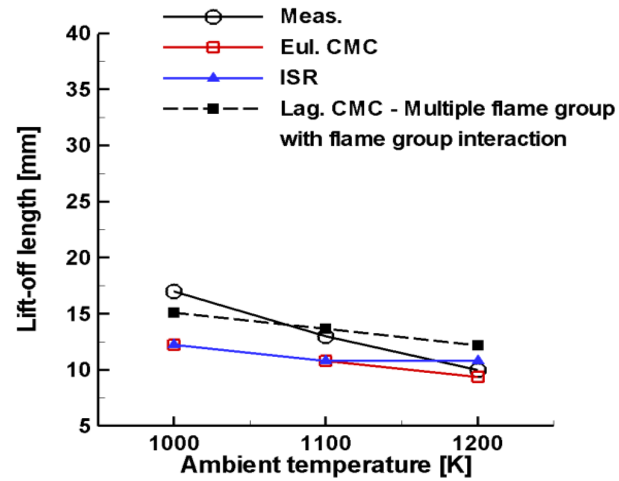
$$\frac{\partial\left(\bar{\rho}\tilde{\xi}_j\right)}{\partial t}+\nabla\cdot\left(\rho\mathbf{v}\tilde{\xi}_j\right)=\nabla\cdot\left[\frac{\mu_t}{Sc_{\xi_j}}\nabla\tilde{\xi}_j\right]+\bar{\rho}\tilde{s}_{\xi,j}+\bar{\rho}\tilde{\xi}_j K\frac{(1-\tilde{c})}{\tau_t}$$ for the burned state

$$\frac{\partial\left(\bar{\rho}\tilde{\xi}_j\right)}{\partial t}+\nabla\cdot\left(\rho\mathbf{v}\tilde{\xi}_j\right)=\nabla\cdot\left[\frac{\mu_t}{Sc_{\xi_j}}\nabla\tilde{\xi}_j\right]+\bar{\rho}\tilde{s}_{\xi,j}-\bar{\rho}\tilde{\xi}_j K\frac{\tilde{c}}{\tau_t}$$ for the unburned state

Case	Lift-off length [mm]
Measured	17.0
ISR	12.2
K=0 (without flame group interaction)	7.9 / 29.6
K=0.1	7.9 / 29.6
K=1	9.3 / 25.2
K=10	15.1
K=20	13.6

Results



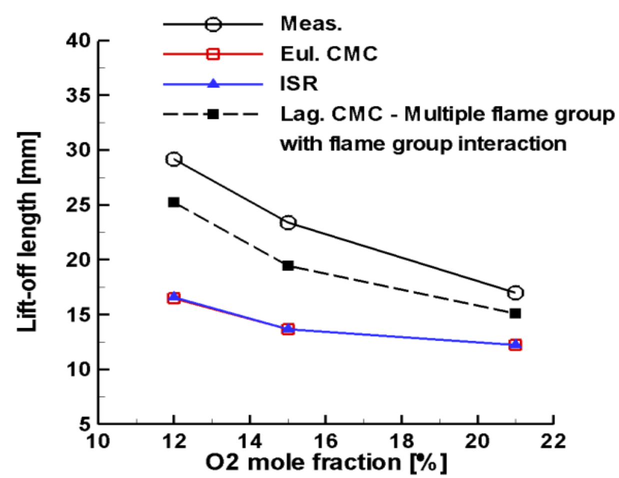


$$\frac{\partial\left(\bar{\rho}\tilde{\xi}_j\right)}{\partial t}+\nabla\cdot\left(\rho\mathbf{v}\tilde{\xi}_j\right)=\nabla\cdot\left[\frac{\mu_t}{Sc_{\xi_j}}\nabla\tilde{\xi}_j\right]+\bar{\rho}\tilde{s}_{\xi,j}+\bar{\rho}\tilde{\xi}_j K\frac{(1-\tilde{c})}{\tau_t}$$

for the burned state

$$\frac{\partial\left(\bar{\rho}\tilde{\xi}_j\right)}{\partial t}+\nabla\cdot\left(\rho\mathbf{v}\tilde{\xi}_j\right)=\nabla\cdot\left[\frac{\mu_t}{Sc_{\xi_j}}\nabla\tilde{\xi}_j\right]+\bar{\rho}\tilde{s}_{\xi,j}-\bar{\rho}\tilde{\xi}_j K\frac{\tilde{c}}{\tau_t}$$

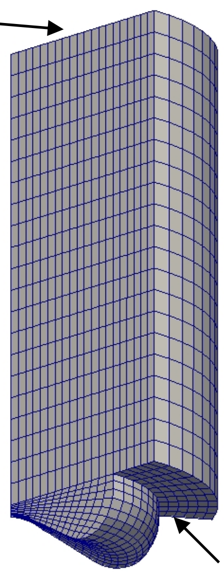
for the unburned state



Diesel Engine – ERC

Case description

- **Geometry**



✓ **Fuel spray**
Initial droplet size is determined by Rosin-Rammler distribution function with the SMD of 14 micron

✓ **Injected fuel temp : 311K**

✓ **Skeletal mechanism for n-heptane 44 species and 114 elementary steps**

- **Engine specification**

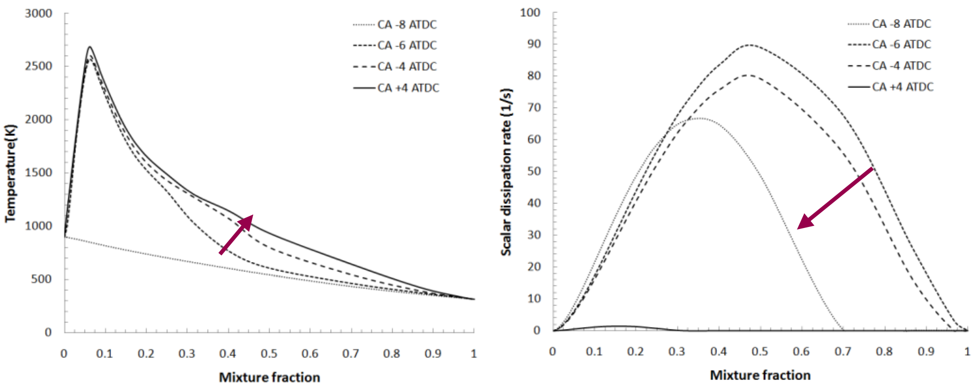
Description	Specification
Engine	Caterpillar 3401E
Engine speed (rpm)	821
Bore (mm) x Stroke (mm)	137.2 x 165.1
Compression ratio	16.1
Displacement (Liters)	2.44
Combustion chamber geometry	In-piston Mexican Hat with sharp edged crater
Max injection pressure (MPa)	190
Number of nozzle	6
Nozzle hole diameter (mm)	0.214
Spray angle (deg)	125

- **Operating condition**

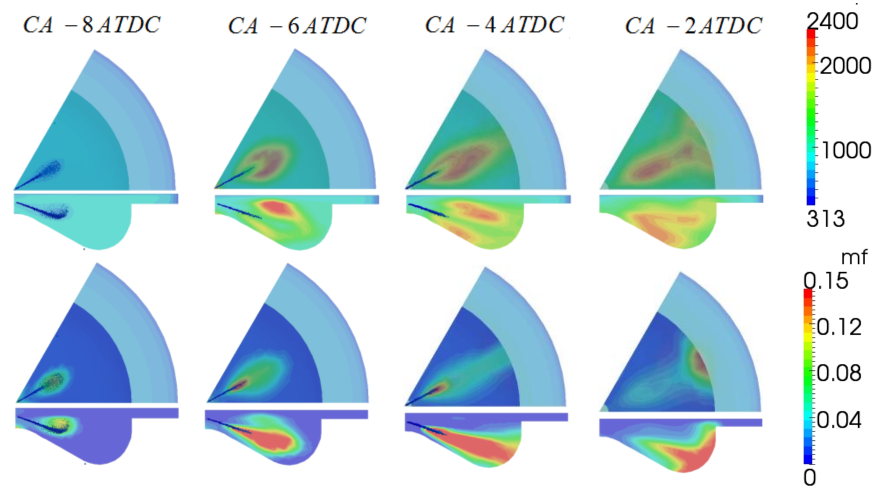
Operating conditions	
EGR level (%)	7, 27, 40
SOI timings (ATDC)	-20, -15, -10, -5 , 0, 5
Injection duration (deg)	6.5

Diesel Engine – ERC

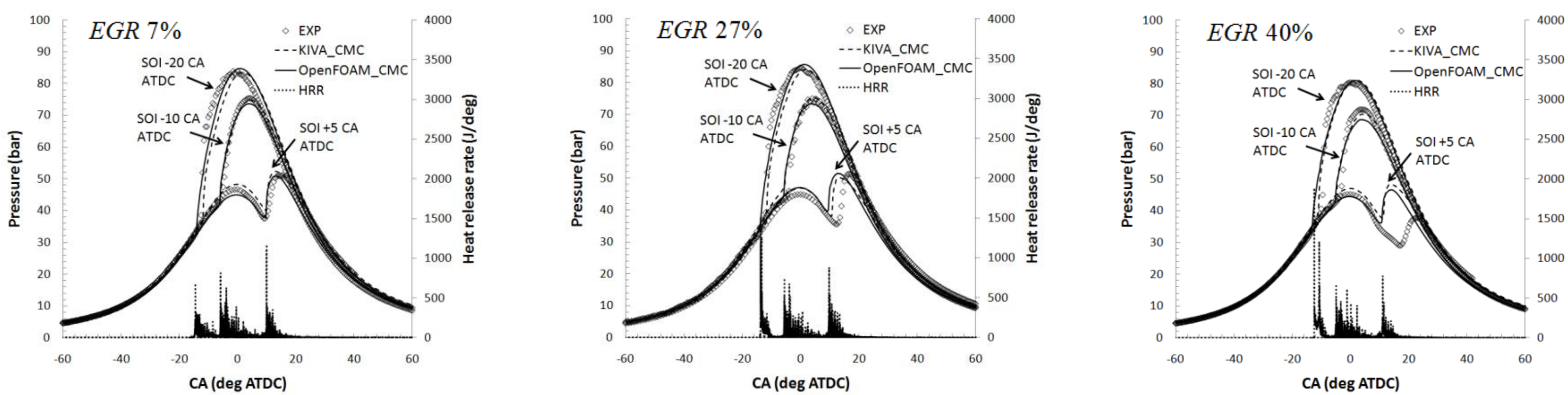
Results



Conditional mean temperature and scalar dissipation rate with respect to the mixture fraction



Spatial distributions of the temperature and mean mixture fraction

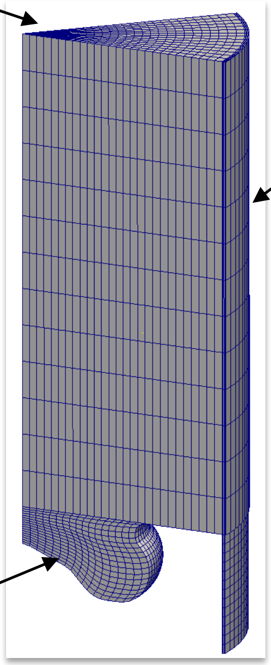


Pressure trace w.r.t different EGR (%)

Diesel Engine – D1

Case description

- **Geometry**



3-D sector mesh of 45° with periodic boundary condition

✓ **D1 diesel engine**

✓ **Multiple fuel injection**

- **Engine specification**

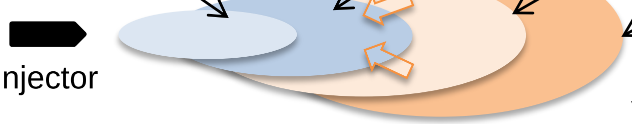
Description	Specification
Engine	D1
Engine speed (rpm)	1500
Bore (mm) x Stroke (mm)	85.4 x 96
Compression ratio	~ 16
Displacement (cm^3)	549.9
Max injection pressure (MPa)	190
Number of nozzle	8
Nozzle hole diameter (mm)	0.135

- **Operating condition**

Operating conditions	
SOI timings (ATDC)	-18 / -7.8 / 0.8
Injection duration (deg)	2.6 / 2.7 / 9.4

Diesel Engine - D1

Case description



- **Flame group interaction is modeled as propagating premixed combustion by the EBU model**
- **The mean reaction progress variable is defined as**

$$\tilde{c} \equiv \xi_B / \xi \quad \text{where} \quad \xi_B + \xi_{UB} = \xi \quad \text{and} \quad (1-\tilde{c})\xi = \sum_{all\ j\ unburned} \tilde{\xi}_j$$

- **The source term for $\tilde{c}$ is given by the EBU model for premixed combustion as**

$$\dot{w}_c = K \frac{\tilde{c}(1-\tilde{c})}{\tau_t} \quad \text{where integral time scale} \quad \tau_t = \tilde{k}/\tilde{\varepsilon}$$

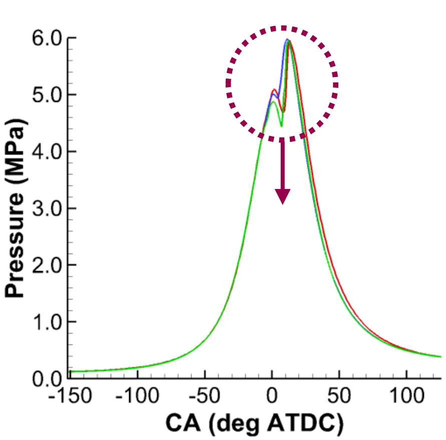
- **Transport equation for fuel fraction of the j-th fuel group**

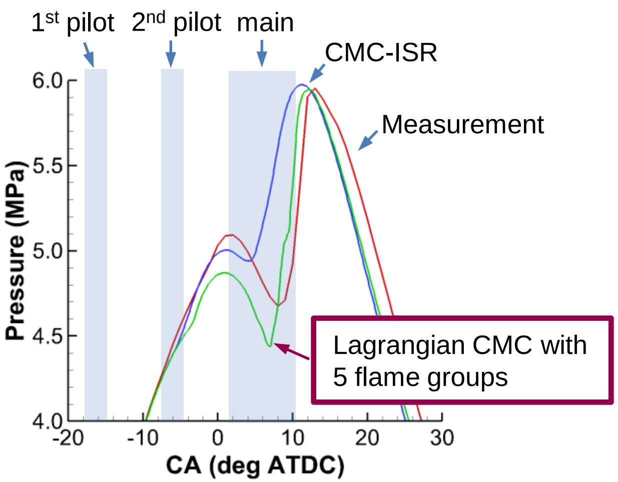
$$\frac{\partial(\bar{\rho}\tilde{\xi}_j)}{\partial t} + \nabla \cdot (\rho \mathbf{v} \tilde{\xi}_j) = \nabla \cdot \left[\frac{\mu_t}{Sc_{\xi_j}} \nabla \tilde{\xi}_j \right] + \bar{\rho}\tilde{s}_{\xi,j} + \bar{\rho}\tilde{\xi}_j K \frac{(1-\tilde{c})}{\tau_t} \quad \text{for flame groups in the burned state}$$

$$\frac{\partial(\bar{\rho}\tilde{\xi}_j)}{\partial t} + \nabla \cdot (\rho \mathbf{v} \tilde{\xi}_j) = \nabla \cdot \left[\frac{\mu_t}{Sc_{\xi_j}} \nabla \tilde{\xi}_j \right] + \bar{\rho}\tilde{s}_{\xi,j} - \bar{\rho}\tilde{\xi}_j K \frac{\tilde{c}}{\tau_t} \quad \text{for flame groups in the unburned state}$$

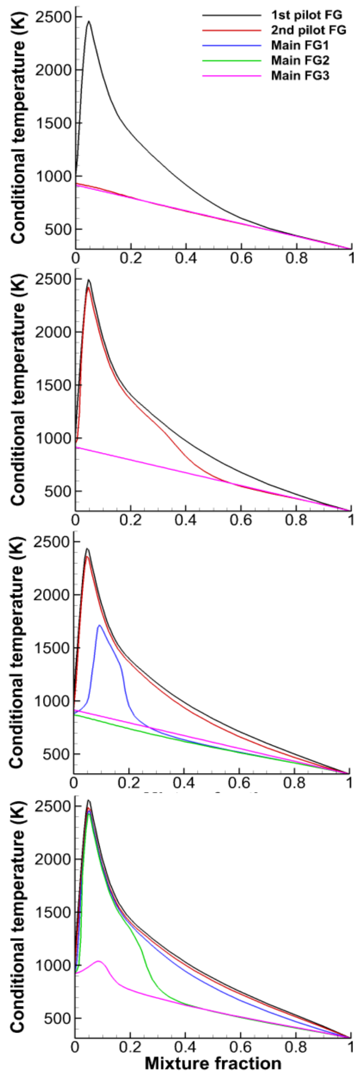
Diesel Engine - D1

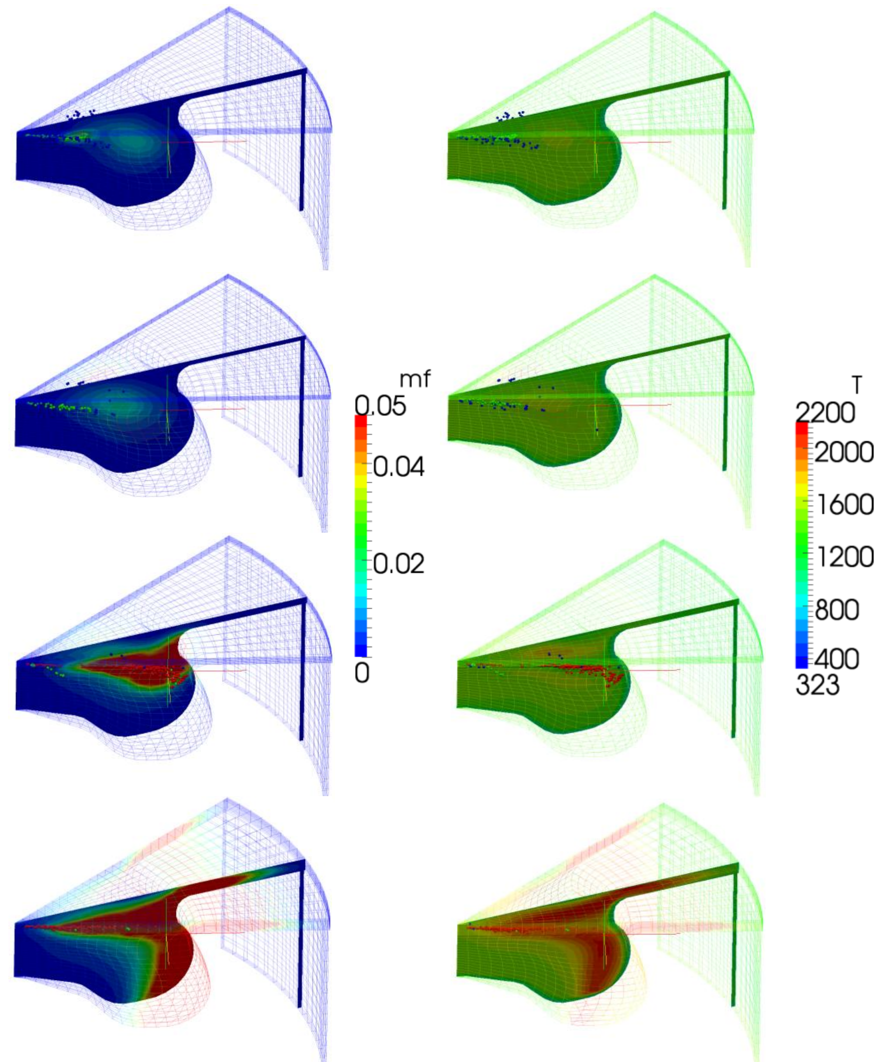
Results





Pressure trace

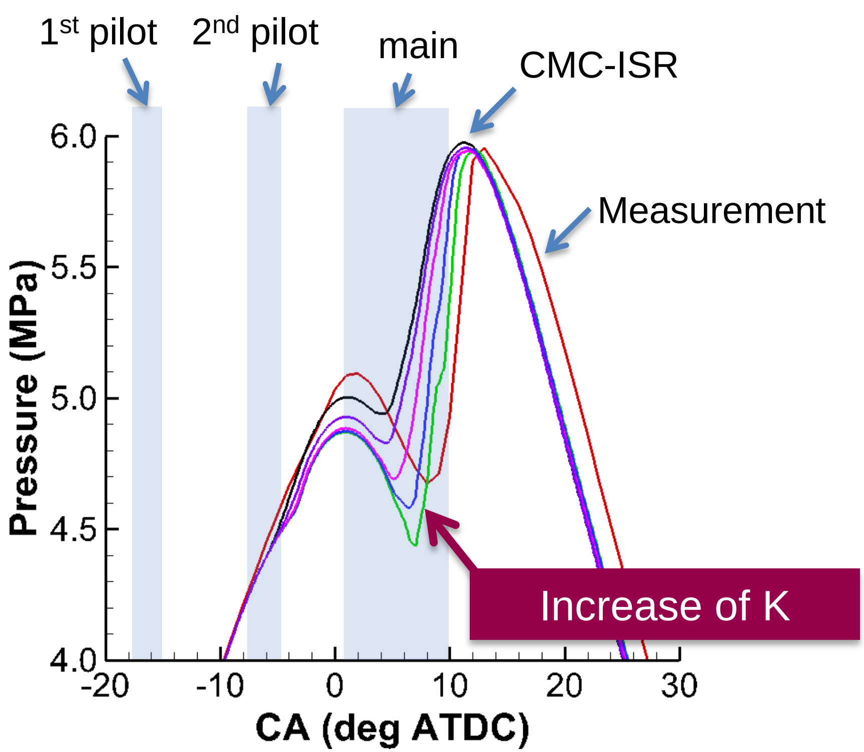




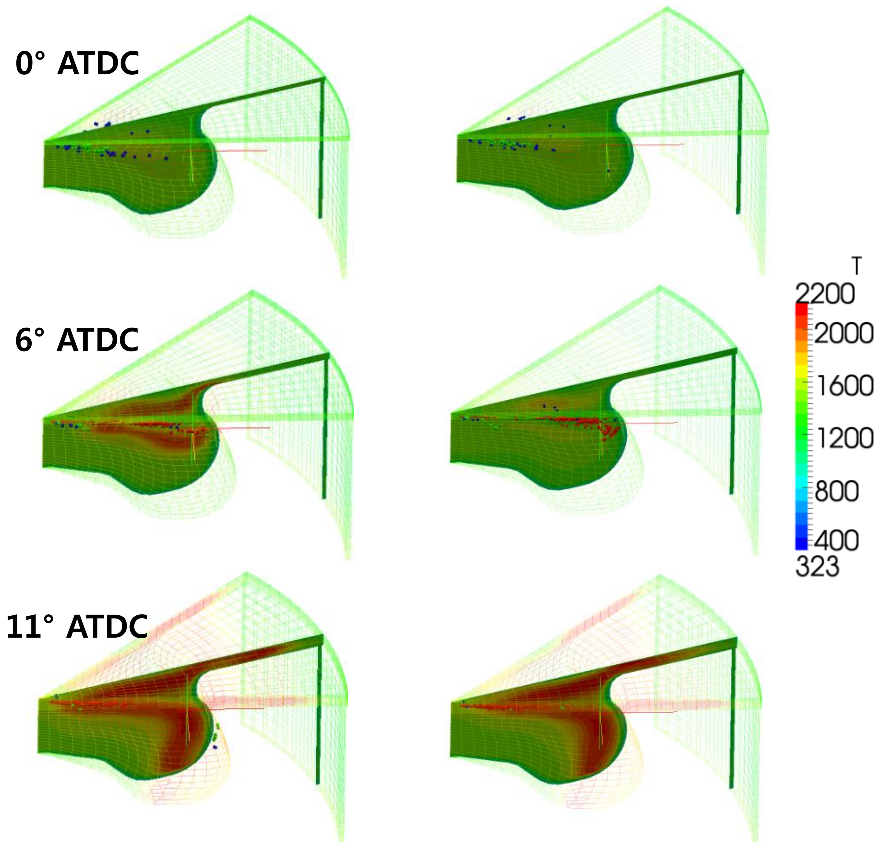
Diesel Engine - D1

Results

- **The first peak pressure is increased by higher constant K which is corresponding to intensive flame propagation between flame groups**



Pressure trace w.r.t different EBU constant K (K = 0.1 / 1 / 2 / 5 / 20)



Spatial distributions of temperature w.r.t different K (left K = 5, right K = 0.1)

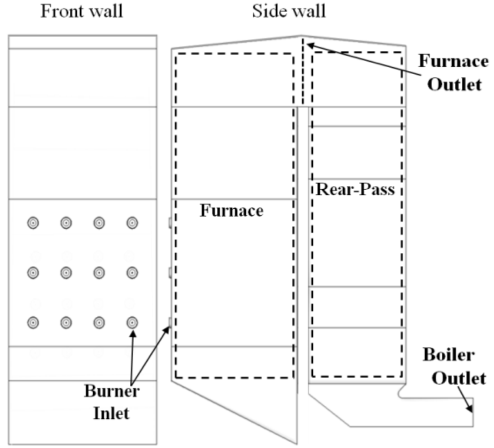
Heavy Oil Furnace - Full Scale

Case description

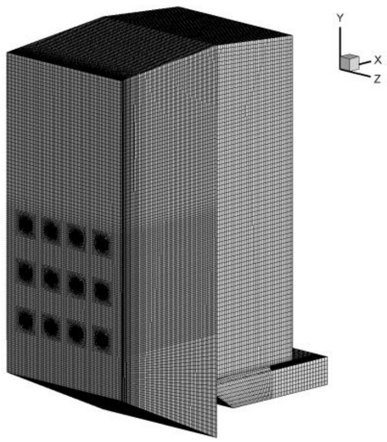
- Fuel (Heavy fuel oil) is injected from 12 burners into a furnace
- Computational domain covers from downstream of burner swirlers to the boiler outlet
- Incoming flow at each burner inlet has the swirl number

- Numerical Method and Models
  - Pressure-velocity coupling based on SIMPLE algorithm
  - Gauss upwind scheme for spatial discretization of convection term
  - k-ε model is employed with the wall function method
  - Fuel burning rate is given by the EDM (Eddy-dissipation Model)

- Grid generation
  - Hexahedral structured mesh with about 4 million elements for RANS simulation



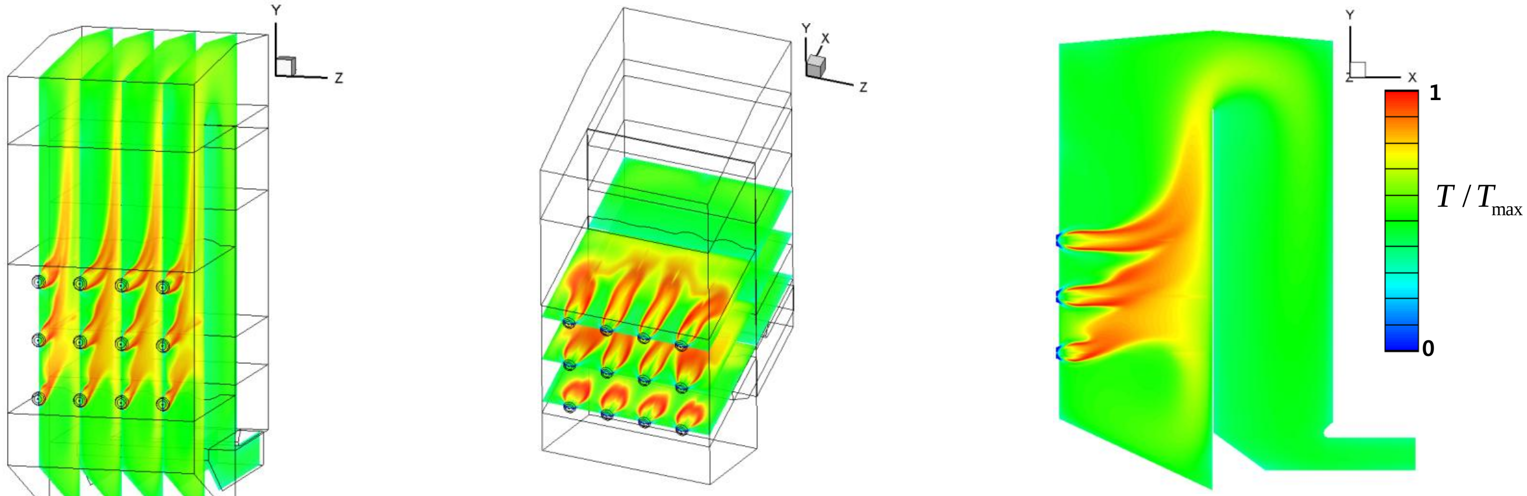
Schematic of the oil boiler



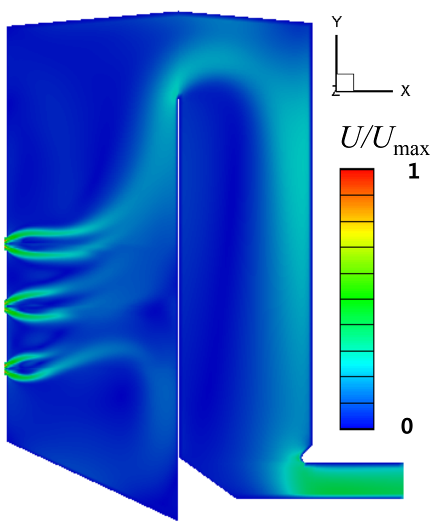
Grids for computation

Heavy Oil Furnace - Full Scale

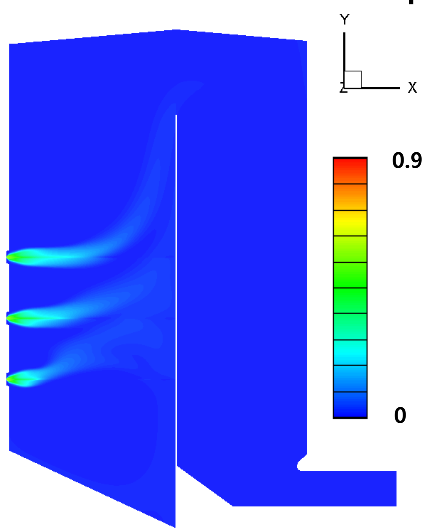
Results



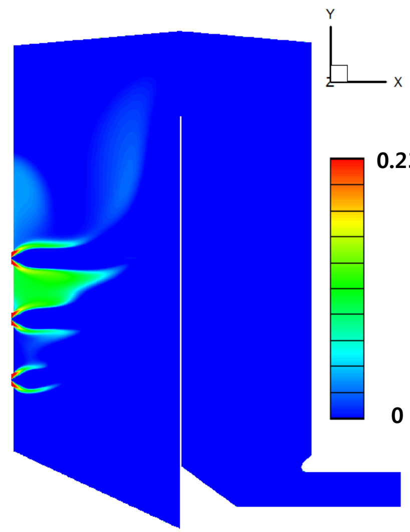
Temperature



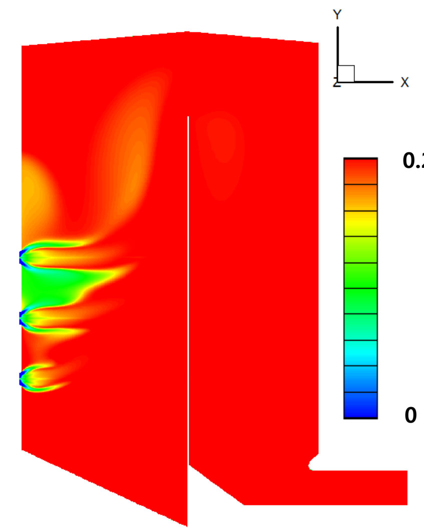
Velocity magnitude



Fuel mass fraction



O_2 mass fraction



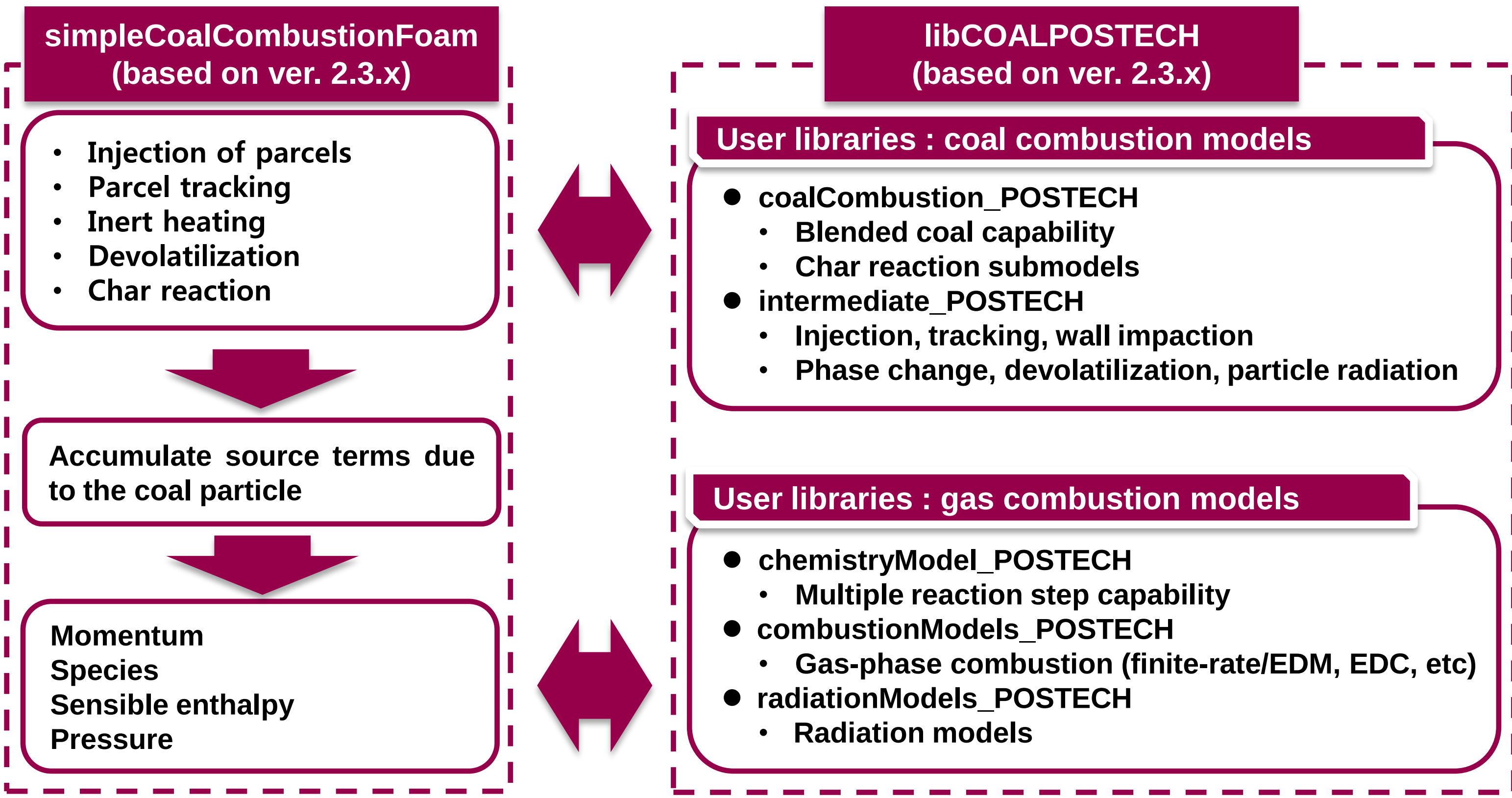
CO_2 mass fraction

Solid Combustion Modeling

Solid Combustion Modeling

simpleCoalCombustionFoam

- **Steady state blended or single coal combustion solver**
- **Developed based on OpenFOAM ver. 2.3.x**
- **Includes various improved devolatilization, char surface reaction and gas combustion models**

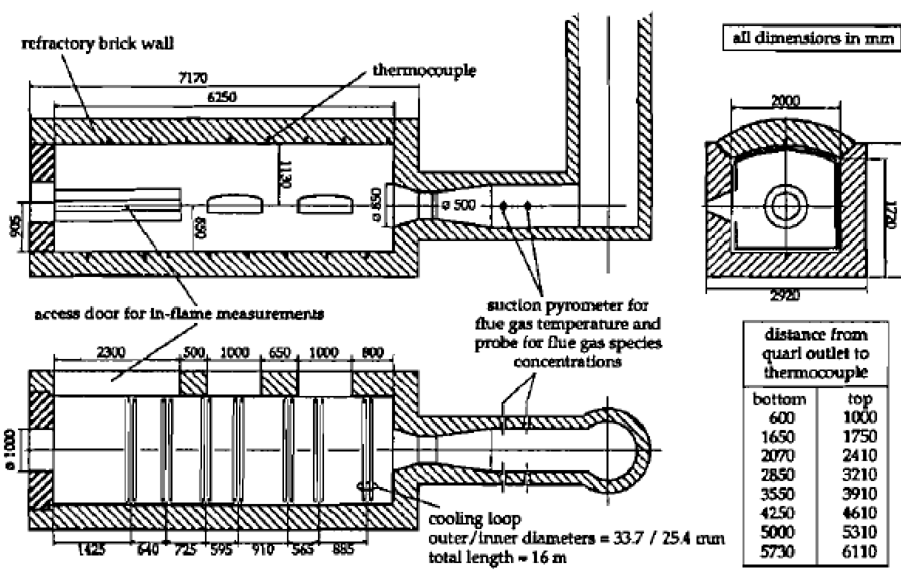


The schematic diagram of the simpleCoalCombustionFoam

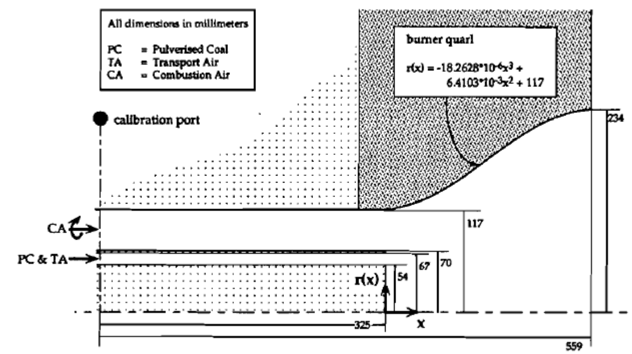
IFRF MMF 5-2 Flame

Case description

- Square cross section 2 m x 2 m, 6.25 m long with 7 cooling loops
- Measurement location(250, 500, 850, 1250, 1950 mm – V, T, O2, CO2, CO, NO)
- Air-staged burner(coal+transport air, combustion air)
- Saar hvBb coal
- Operating pressure : 1 atm
- Coal mass flow rate : 263 kg/h for 2.165 MW
- 22% Excess air
- Swirl number of combustion air(momentum ratio) : 0.923



R. Webber et al., IFRF Doc. No.F36/y/20.

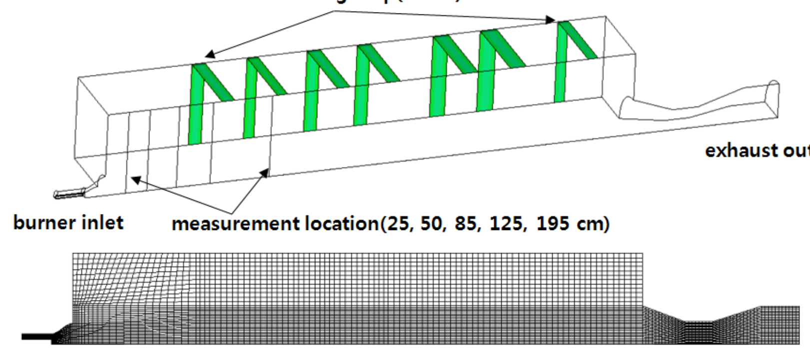


	Mass flow rate(kg/h)	V(m/s)		T(℃)
Pulverized Coal	263	23		70
Transport Air	421	23		70
		Axial	Tan	
Combustion Air	2670	43.9	49.4	300

IFRF MMF 5-2 Flame

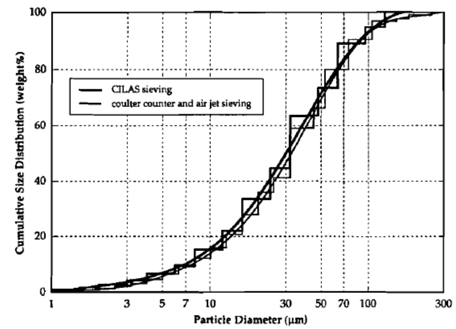
Case description

- Coal HCV(J/kg) = 2.79e+07 (AR)
- Vaporization T(K) = 773
- VM molecular weight(kg/kmol) = 45.6
- P1 radiation (α : 0.1, $E_{particle}$ = 0.8, $S_{particle}$ = 0.5)
- Standard k-e model with 1st order upwind
- Stochastic particle dispersion
- 2-step eddy dissipation
- ¼ sector periodic B.C, 50,000 structured cells



Proximate analysis (weight %)	
VM	37
Fixed Carbon	52.5
Ash	8.5
Moisture	2
Ultimate analysis (weight %, daf)	
C	79.3
H	4.7
O	13.7
N	2.3

Coal particle property	
Density(kg/m^3)	1101
Cp(J/kg·K)	1990
Min size(μm)	10
Max size(μm)	150
Mean size(μm)	60
Spread parameter	1.13
Swelling Index	1
Vaporization T(℃)	500
Kinetics limited, A	6.7
Kinetics limited, Ea(MJ/kmol)	113.82
Single rate, A	2e+05
Single rate, Ea(J/kmol)	7.4e+07



Rosin-Rammler Distribution

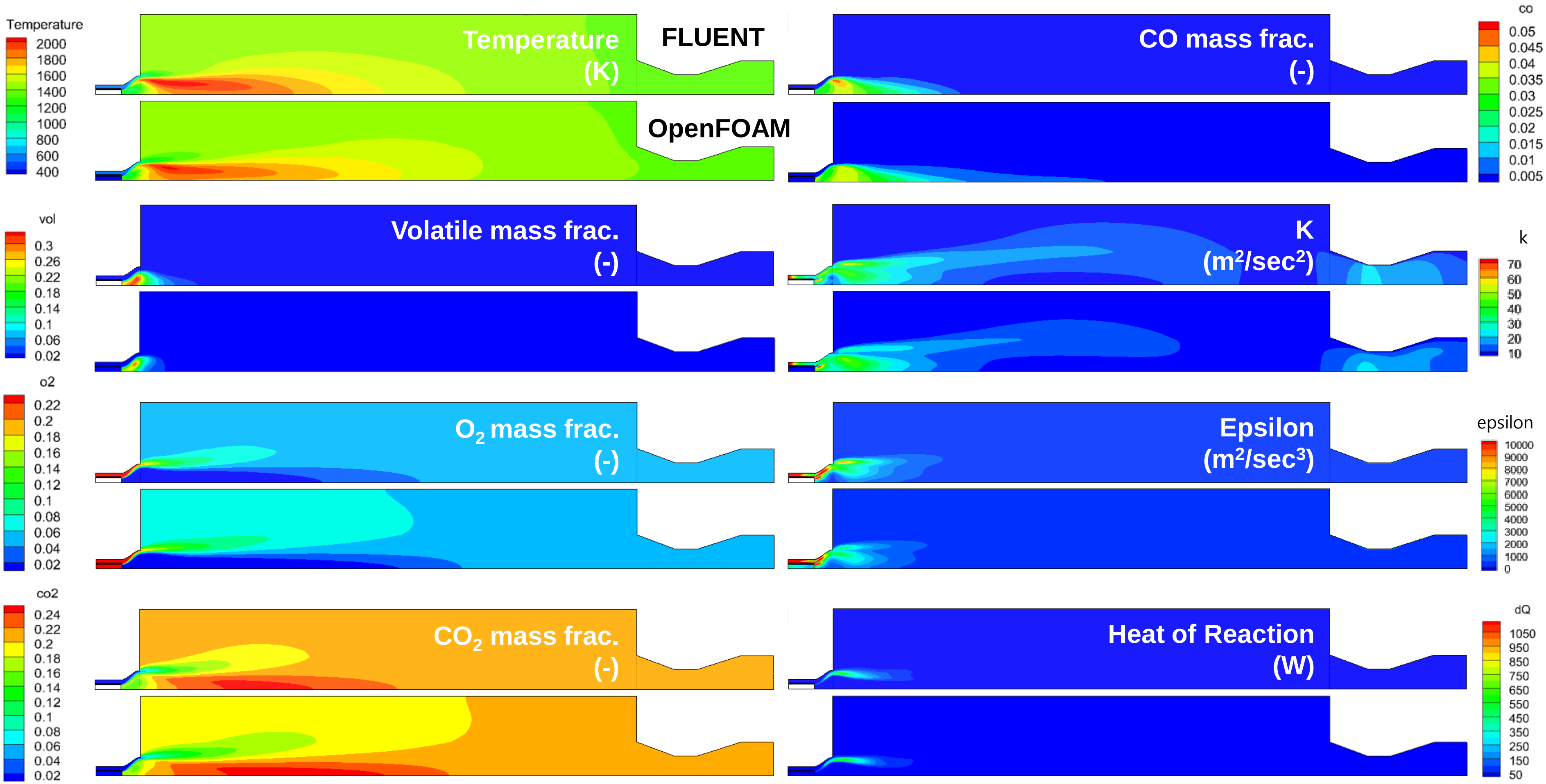
kinetic/diffusion limited char oxidation (product is assumed as CO)

single rate devolatilization

IFRF MMF 5-2 Flame

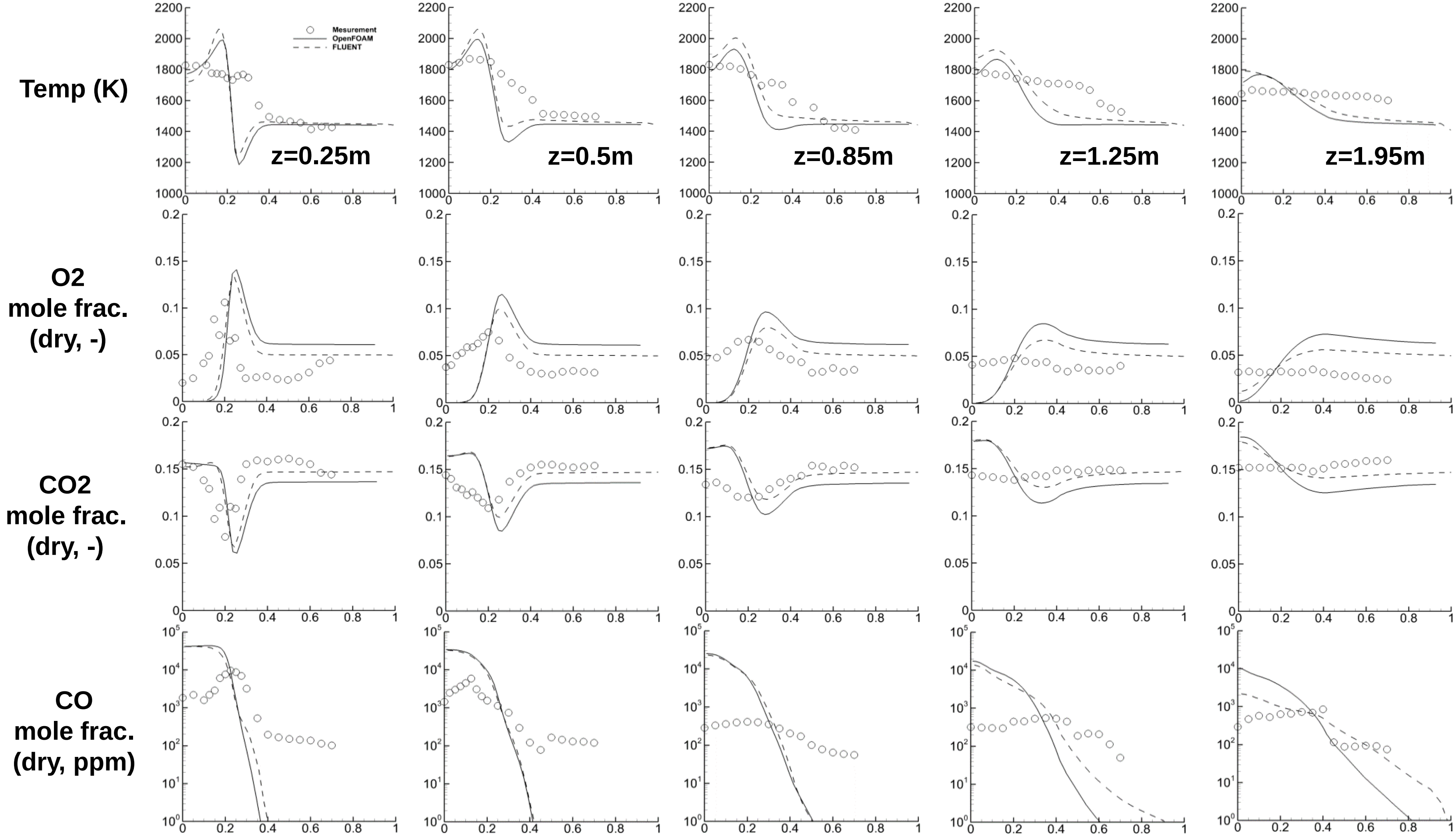
Results

- Single step kinetics devolatilization with 2-step EDM
- Kinetic diffusion limited model (also called Field's model)
- Radiation is considered by P1 model



IFRF MMF 5-2 Flame

Results

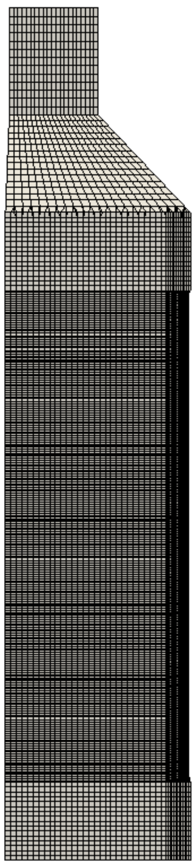


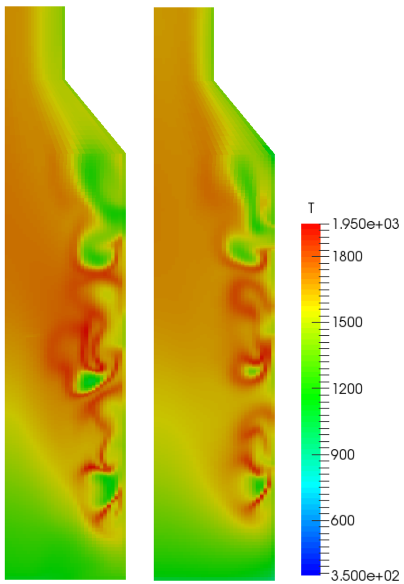
500MWe Tangentially fired pulverized-coal boiler

Results

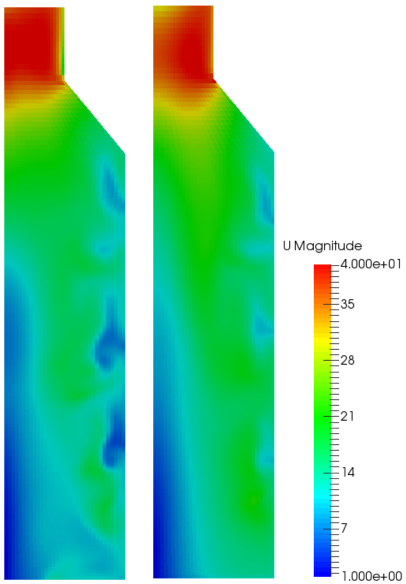
OpenFOAM - Left

FLUENT - Right

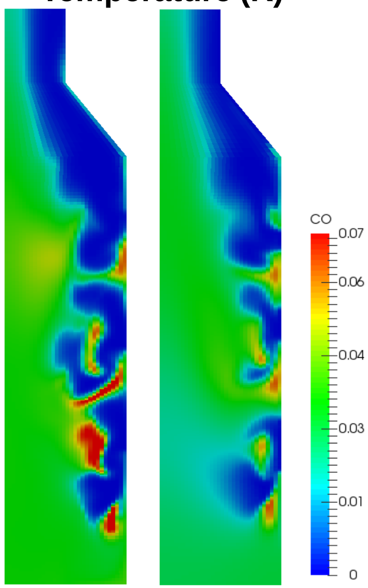




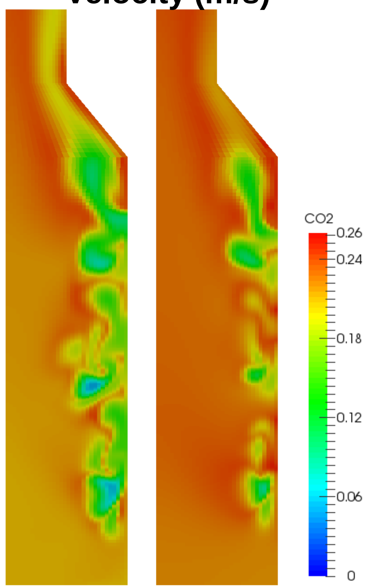
Temperature (K)



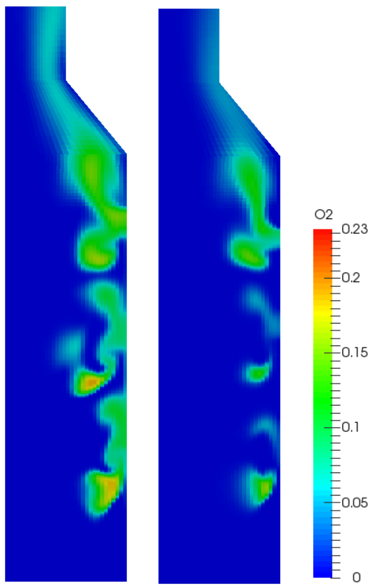
Velocity (m/s)



CO mass fraction



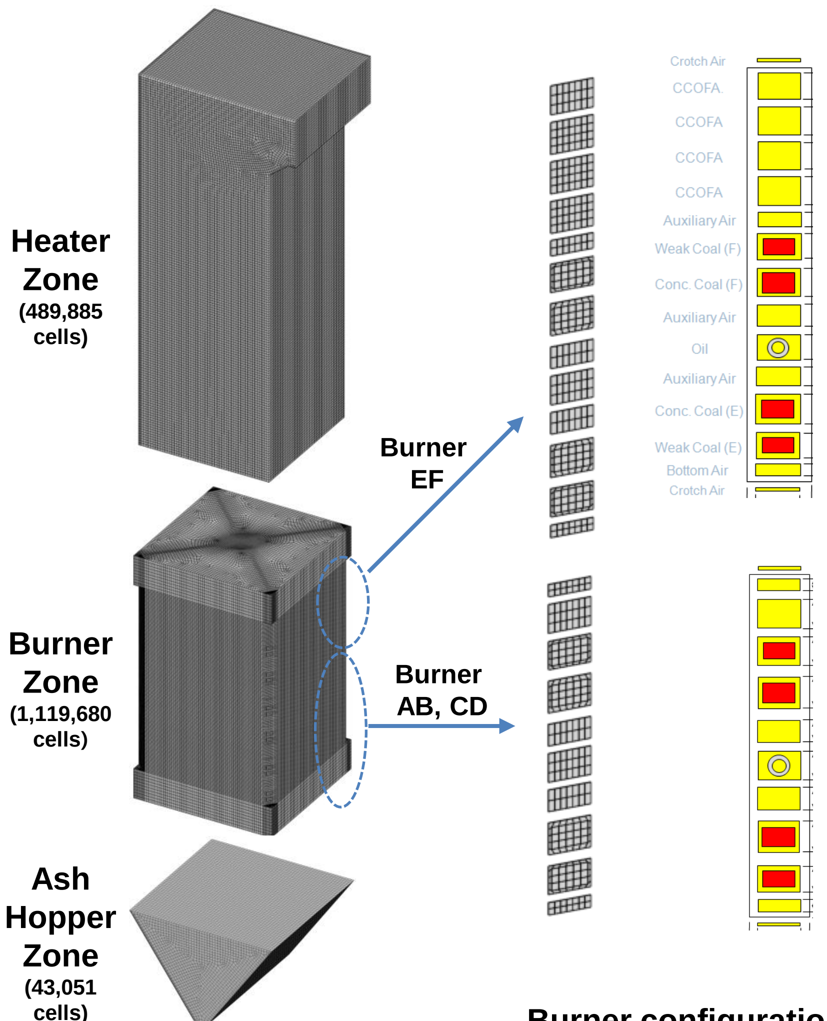
CO_2 mass fraction



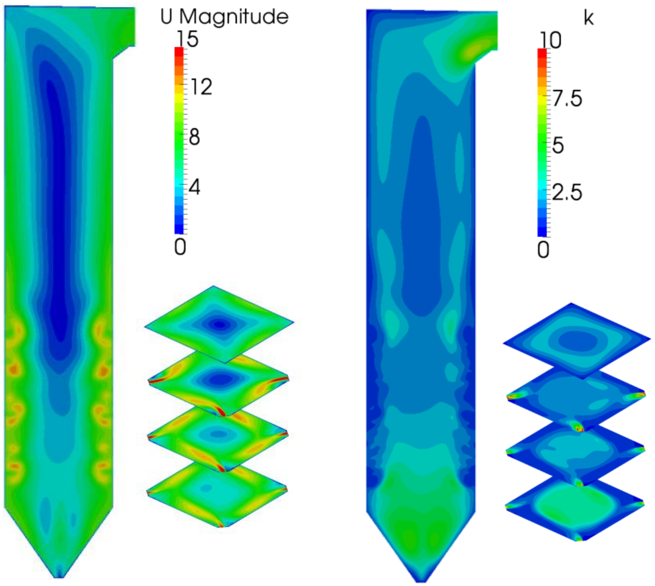
O2 mass fraction

500MWe Tangentially fired pulverized-coal boiler

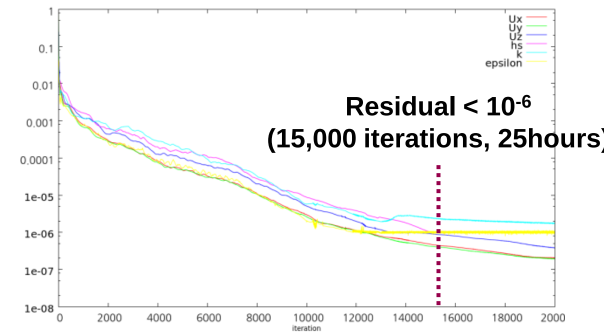
Results



Burner configurations



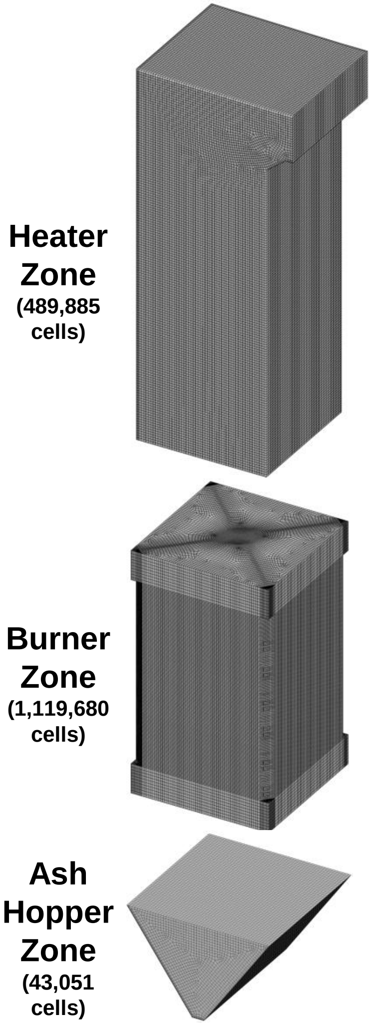
Distributions of velocity magnitude and turbulent kinetic energy

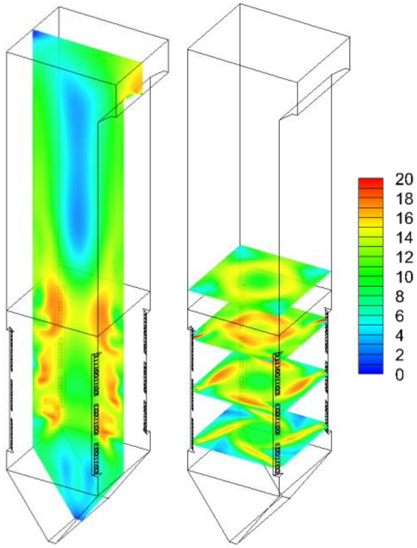


Convergence history in terms of residuals

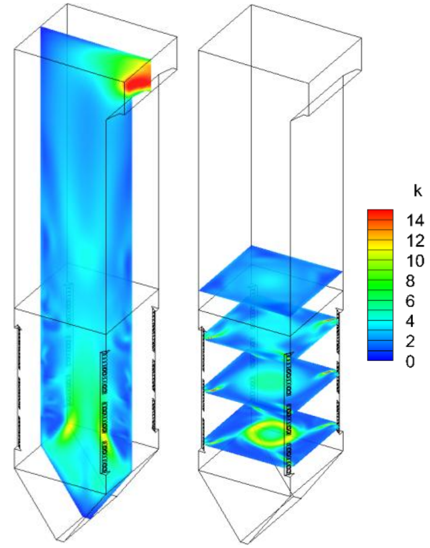
500MWe Tangentially fired pulverized-coal boiler

Results

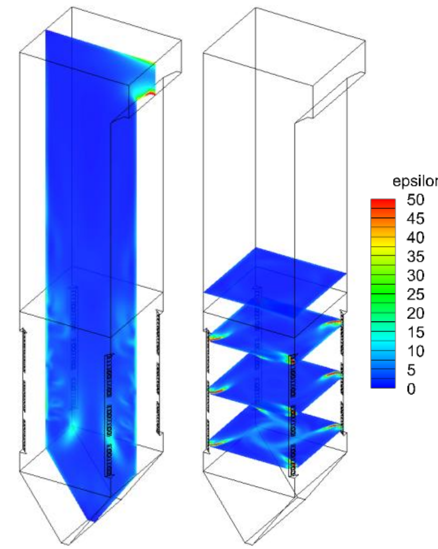




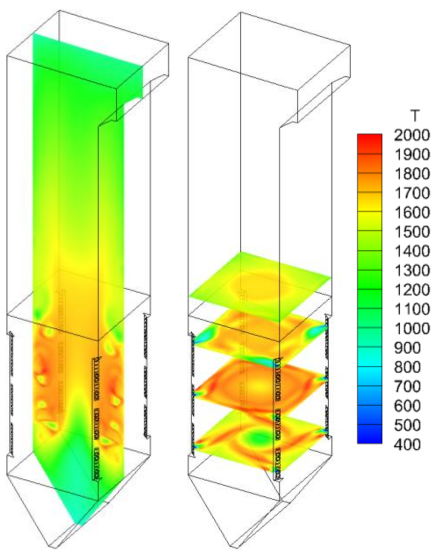
Velocity magnitude



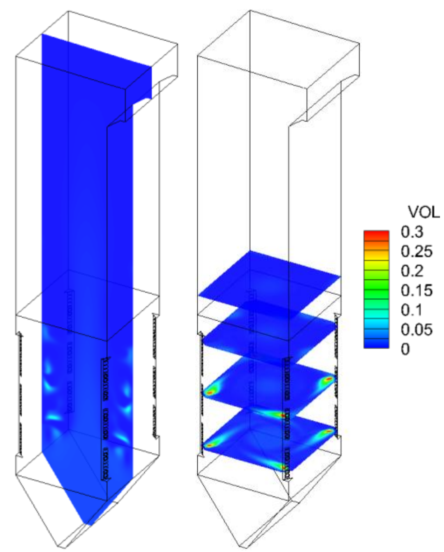
Turbulent kinetic energy



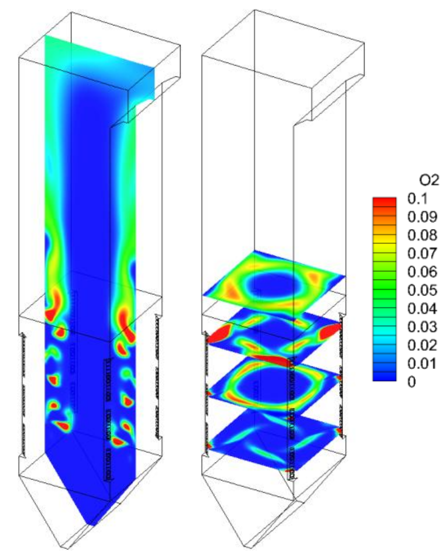
Turbulent dissipation rate



Temperature



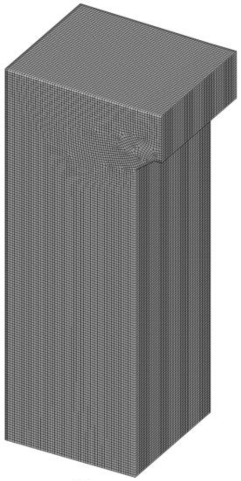
Volatile mass fraction



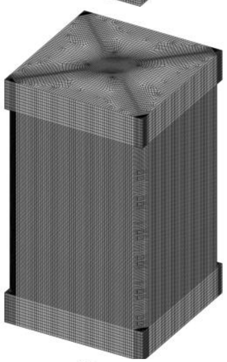
O_2 mass fraction

500MWe Tangentially fired pulverized-coal boiler

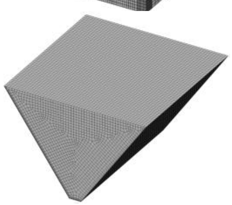
Results



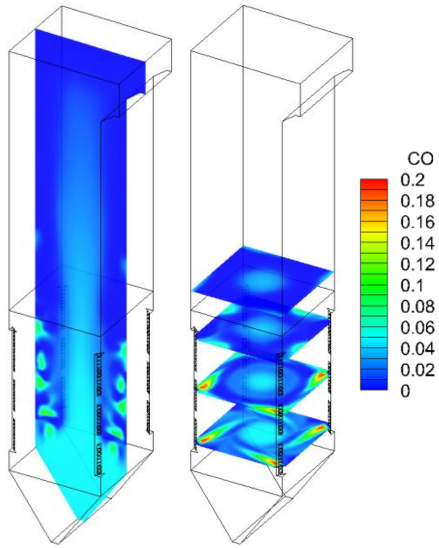
Heater Zone
(489,885 cells)



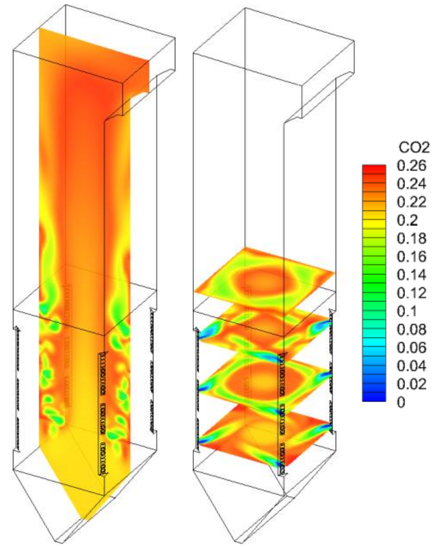
Burner Zone
(1,119,680 cells)



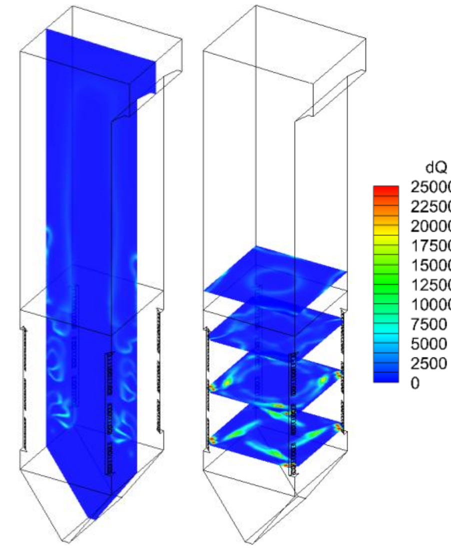
Ash Hopper Zone
(43,051 cells)



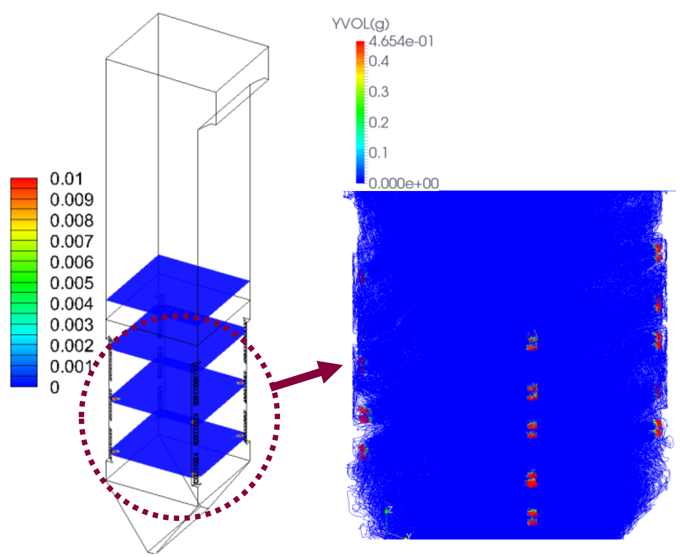
CO mass fraction



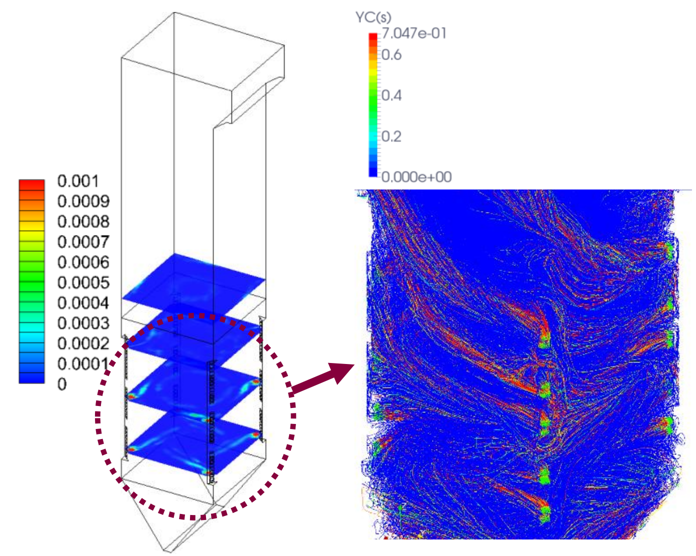
CO2 mass fraction



Heat release rate



Devolatilization rate **Particle volatile mass frac.**



Char burning rate **Particle char mass frac.**

Material Processing Furnace

ReactingMPPICFoam

MPPIC Cloud

- MPPIC motions of particles can be analyzed
- **Surface reactions of particles can not be analyzed**

ReactingMultiphase Cloud

- Surface reactions of particles can be analyzed
- **MPPIC motions of particles can not be analyzed**

ReactingMultiphaseMPPIC Cloud

- **MPPIC motions and surface reactions of particles can be analyzed together**

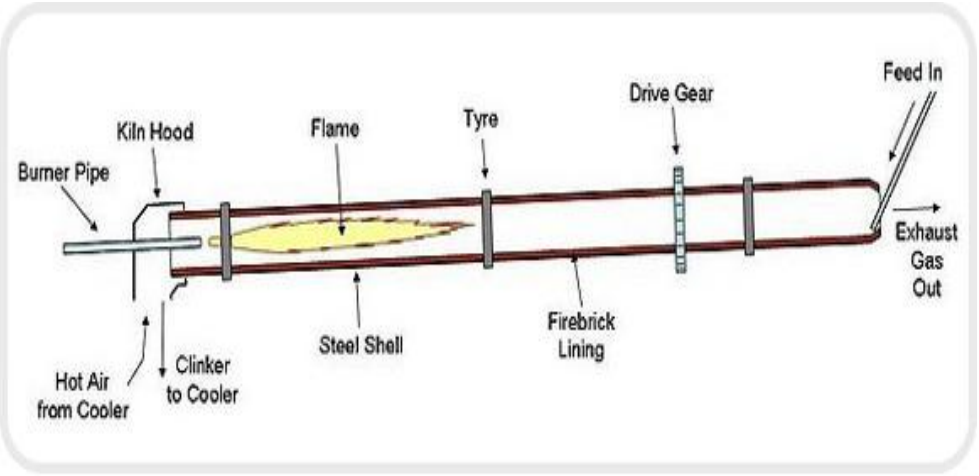
ReactingParcelFoam (based on ver. 2.3.x) → **ReactingMPPICFoam (based on ver. 2.3.x)**

Rotary Klin

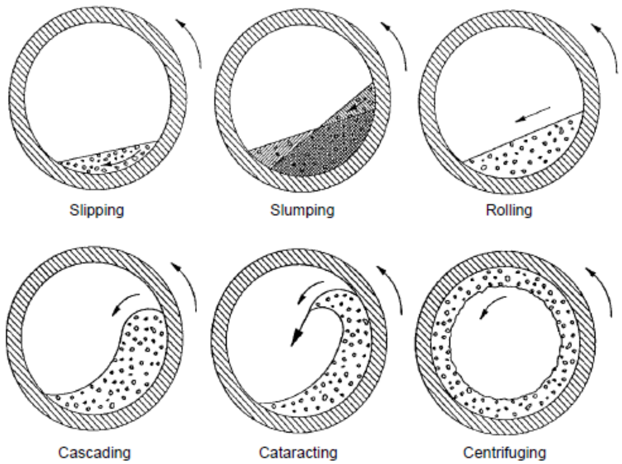
Case description

- A rotary kiln is fundamentally a heat exchanger from which energy from a hot gas phase is transferred to the bed material
- Carry out a wide range of operations such as reduction of oxide ore, reclamation of hydrated lime, calcination of petroleum coke and reclamation of hazardous waste
- Material within the kiln is heated to high temperature so that chemical reactions can take place

- Major Features
  - Material motion through the cylindrical workspace
  - Mass transfer between gas and solid phase
  - Heat transfer and chemical reaction



A Schematic diagram of direct heated rotary kiln



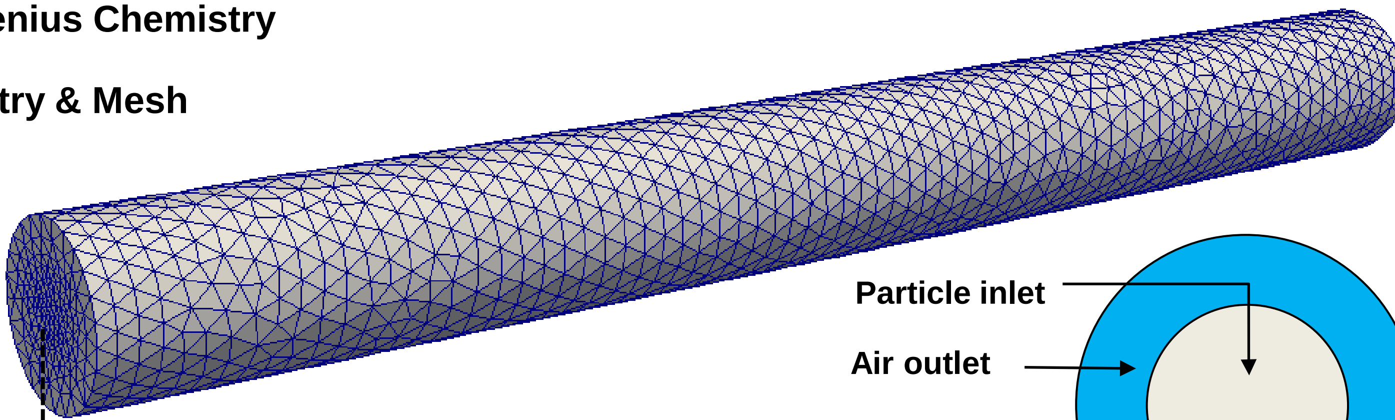
Different modes of operation in the transversal mixing plane

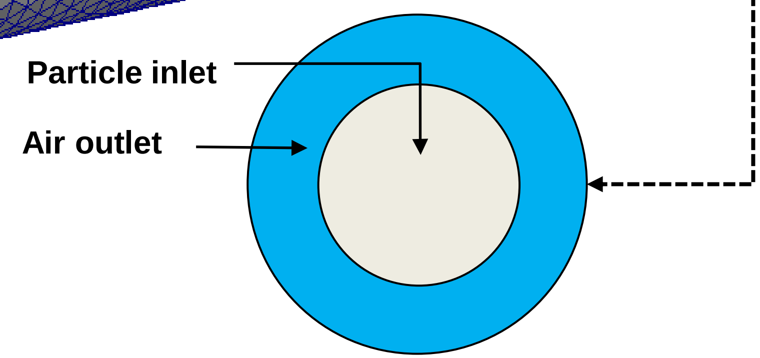
Rotary Klin

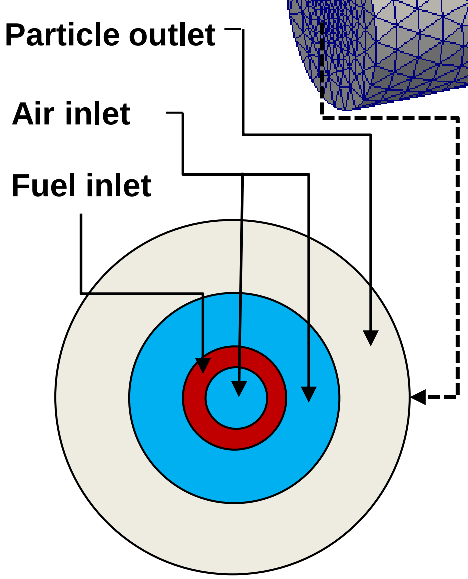
Test Case

- **Numerical Method**
  - Eulerian(gas phase) - Lagrangian(solid phase) approach
  - MP-PIC (Multi Phase – Particle in Cell) method for particle motion
  - Arrhenius Chemistry

- **Geometry & Mesh**





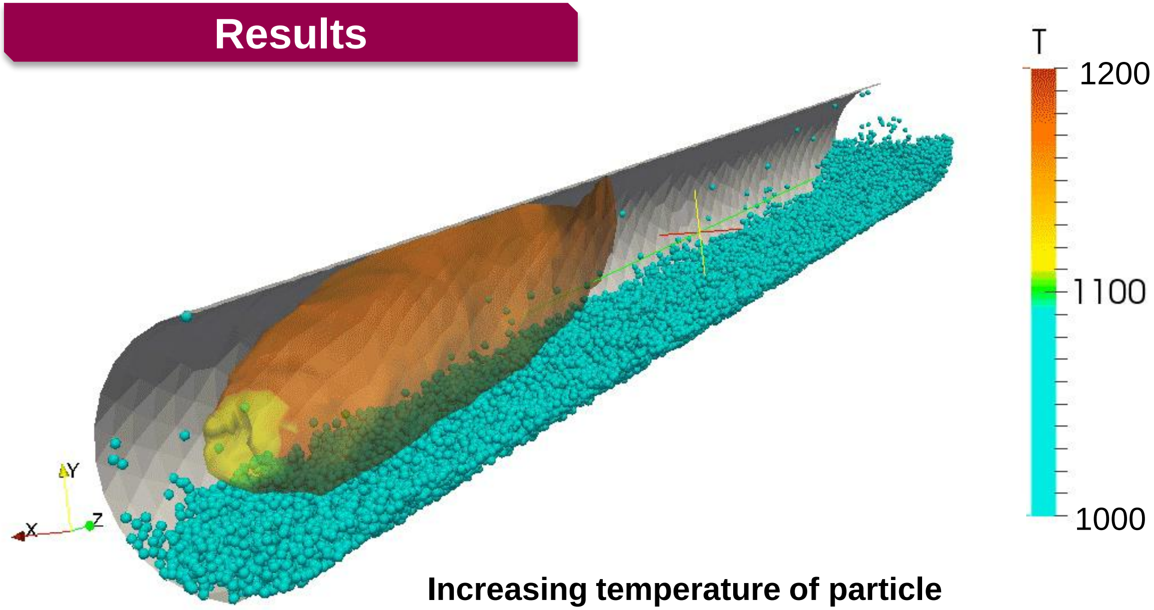


- **Particle characteristics**
  - Type : Iron ore
  - Diameter : 6mm
  - Initial mass : 1500kg
  - Mass input : 30kg/s
  - Initial Temperature : 1000K

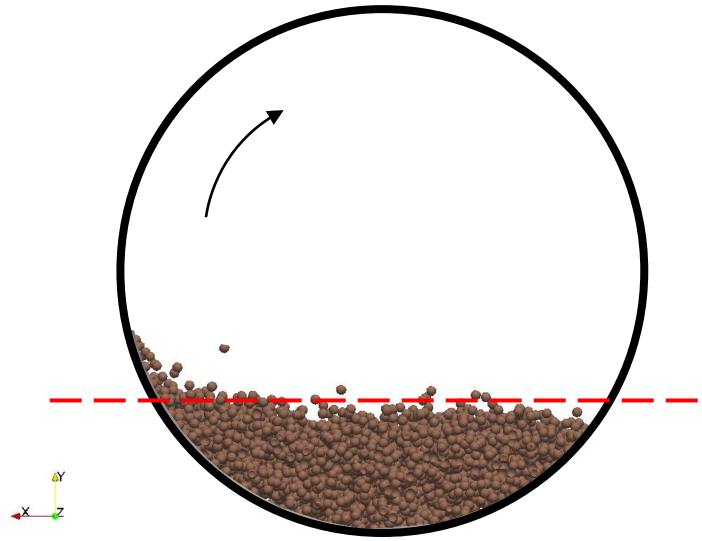
- **Operating conditions**
  - Fuel : CH_4
  - Rotational speed: 9.6rpm
  - Fuel & Air Injection Velocity : 10m/s

Rotary Klin

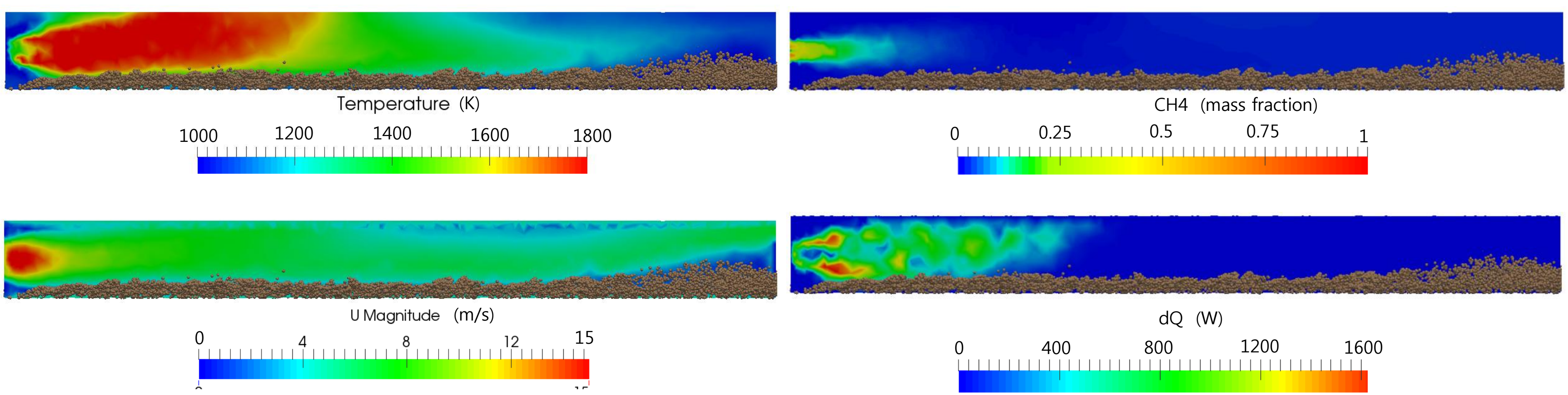
Results



Increasing temperature of particle



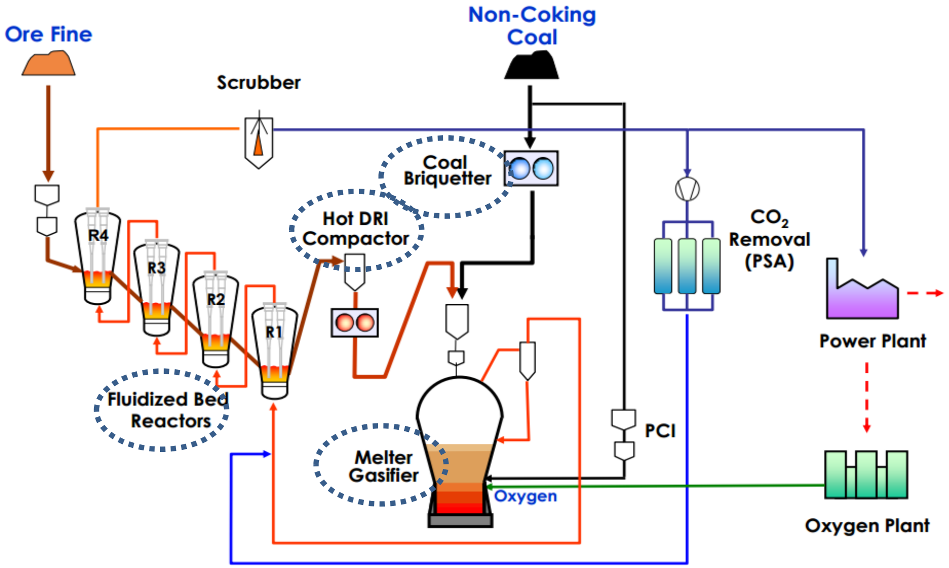
Rotating wall effect



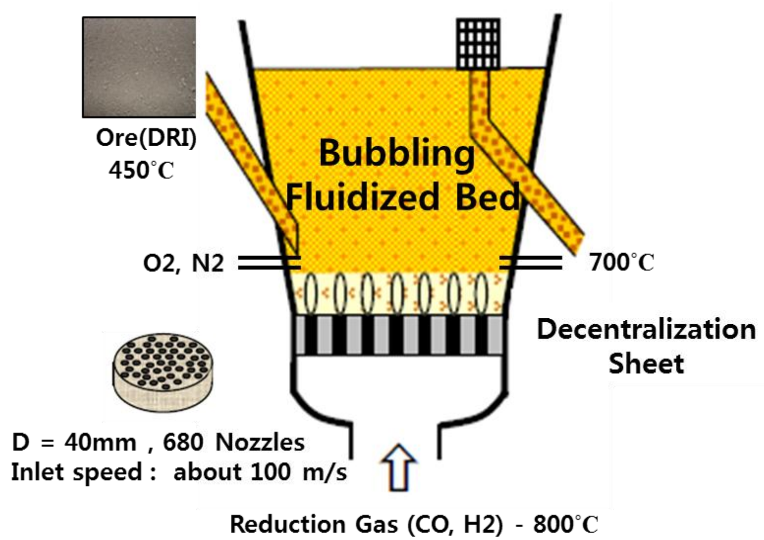
FINEX: R2

Case description

- A part of the iron-making process
- The biggest fluidized bed reactor in the world (12m toll)
- Multiphase flow: Gases(CO, H_2, N_2 ···) – Particles (HCI) flow
- Chemical reaction: reducing process, non-premixed combustion
  Both homogeneous and heterogeneous reactions are included
- Some tricky phenomenon such as sticking around O_2 nozzle
- Wide size distribution of particles



Whole process flow of the FINEX



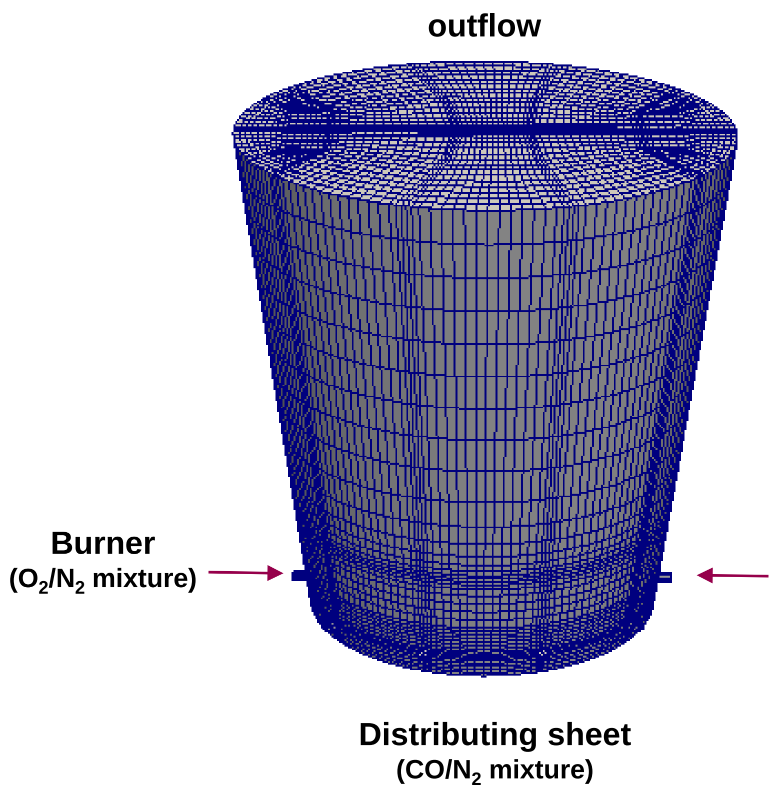
The second reactor

FINEX: R2

Test Case

- Numerical Method
  - Eulerian(gas phase) - Lagrangian(solid phase) approach
  - MP-PIC (Multi Phase – Particle in Cell) method for particle motion
  - EDM combustion model

- Geometry & Mesh



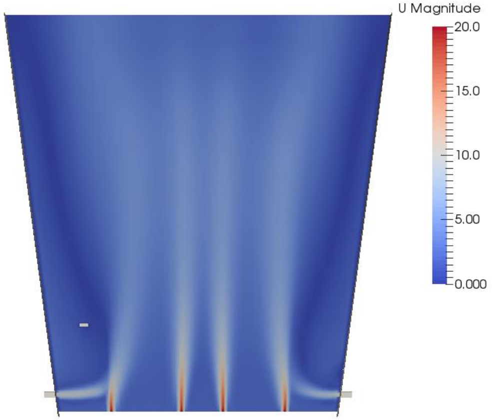
- Domain description
  - Fluidized bed reactor (particle I/O included)
  - Combustion (O_2 burner 10 pcs)
  - Distributing sheet
  - Height : 3m

- Particle characteristics
  - Type : Iron ore
  - Diameter : 1 mm (expectation)
  - Parcel Number : ~ 30000
  - Initial Temperature : 300K

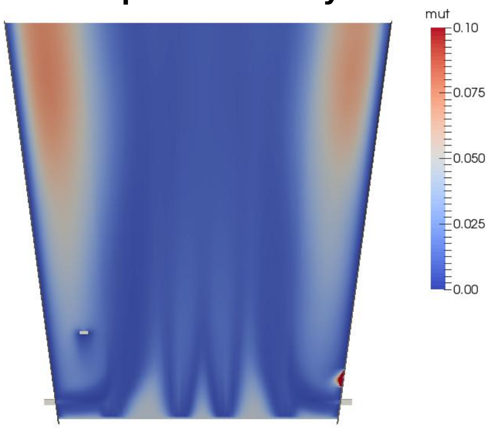
- Operating conditions
  - CO/N_2 : 20 m/s through distributing sheet
  - O_2/N_2 : 10 m/s at burner nozzle

FINEX: R2

Results



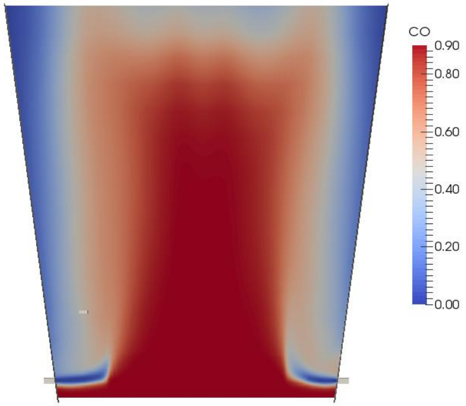
Gas phase velocity



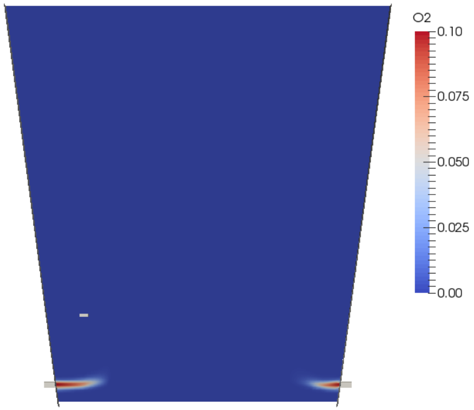
Turbulent viscosity

FINEX: R2

Results



CO mass fraction



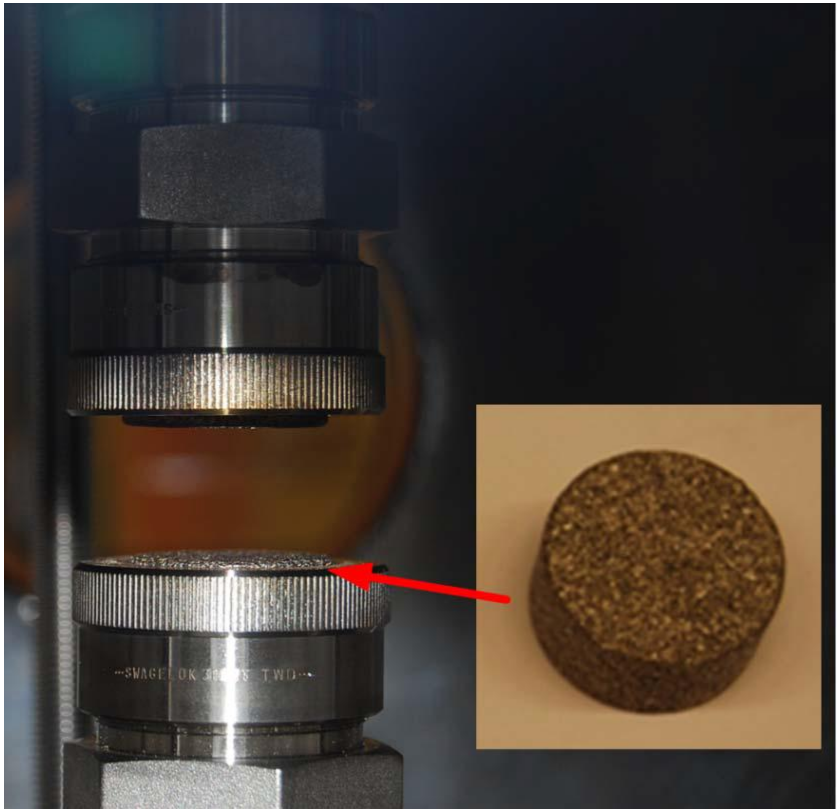
O_2 mass fraction

Plasma Assisted Combustion

Case description

- **Counterflow Burner with Stainless Steel Porous Electrodes**
  - **Diffusion flame between fuel stream and oxidizer stream**
  - **Fuel stream and oxidizer stream are CH_4 and O_2 diluted with He.**
  - **Pressure: 72 Torr**
  - **Inlet Temperature: 650 K and 600 K at oxidizer side and fuel side respectively.**
  - **Strain Rate: 400 1/s**

- **ns Pulsed Discharge**
  - **Polarity: +(oxidizer side), - (fuel side)**
  - **Pulse Duration : 12 ns (FWHM)**
  - **Pulse Voltage : 7.6 kV**
  - **Pulse Energy : 0.73 mJ/pulse**
  - **Frequency : 24 kHz**
  - **Power : 17.5 W**

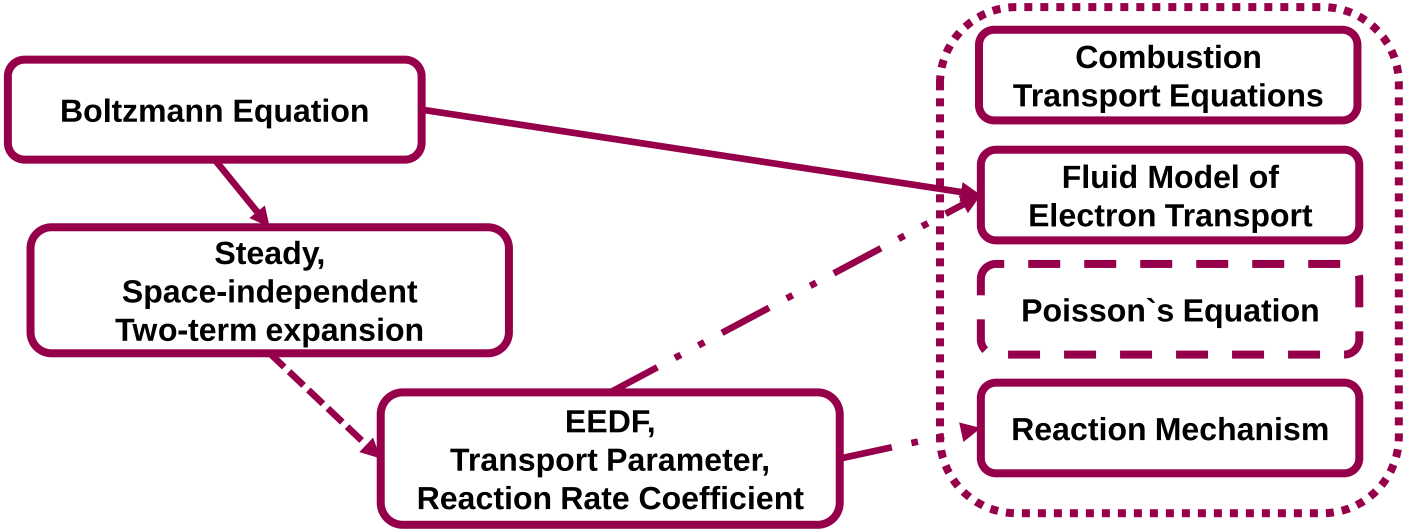


Counter flow burner with stainless steel porous electrodes (photograph)

W. Sun. (2013). *Non-equilibrium plasma-assisted combustion* (Doctoral dissertation)

Case description

- Opposed flow diffusion flame
- Transport of Electron and Electron Energy
  - Transport parameters of electron are calculated in-time with steady two-expansion Boltzmann equation solver (Instead of tabulation)
- Kinetic Model
  - Air-plasma model(M. Uddi, PROCI, 2009) (~ 450 reactions)
    + USC Mech II (111 species, 784 reactions)
    + Additional reactions involving excited particles and electrons (~ 50 reactions)
- Do not solve the Poisson equation for electric field. Rather, electric field is given as a parameter

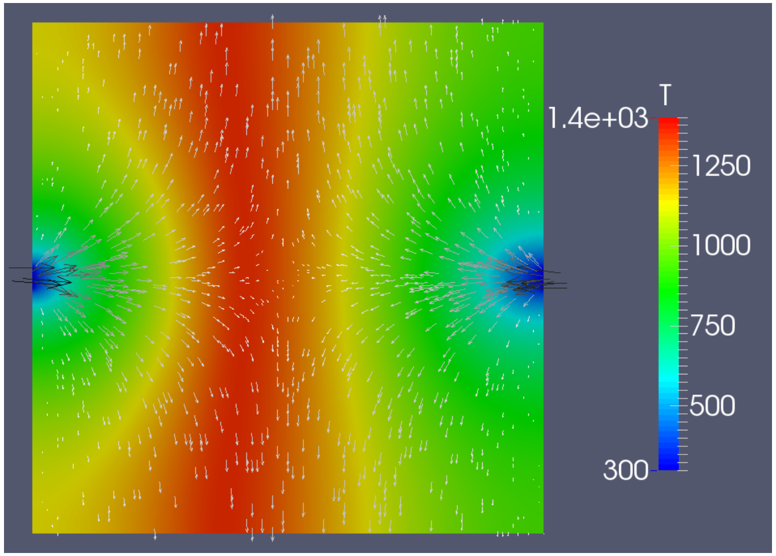


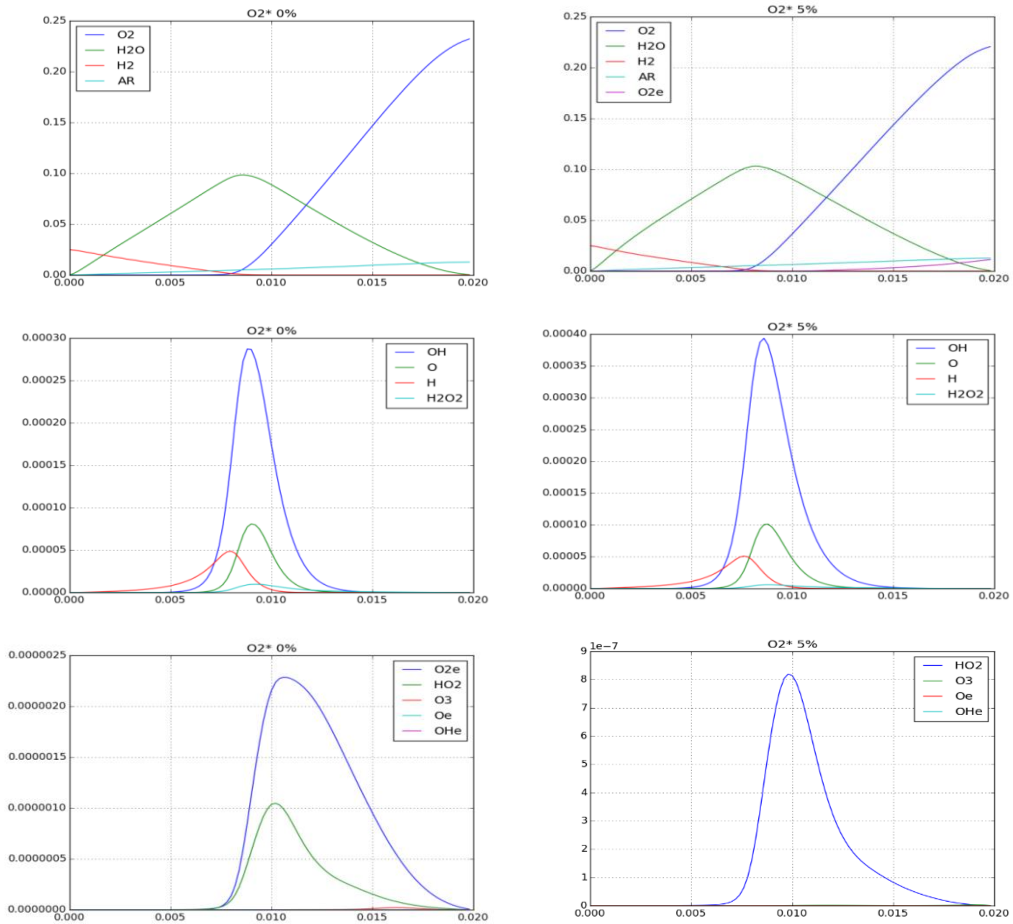
A Schematic diagram of plasma assisted combustion

Plasma Assisted Combustion

Results

- H_2 is diluted with N_2 ($Y_{H_2} = 2.5\%$)
- Oxidizer is air
- Discharge is applied before oxidizer nozzle
- 5% O_2 is electronically excited.
- Nozzle geometry is 1mm x 38mm slit
- Simulation flow rate is 0.1 m/s





Mass fractions along center line

BOURIG, A., THÉVENIN, D., MARTIN, J.-., JANIGA, G. and ZÄHRINGER, K., 2009. Numerical modeling of H2-O2 flames involving electronically-excited species O2(a1Δg), O(1D) and OH(2Σ+). Proceedings of the Combustion Institute, 32 II, pp. 3171-3179

Conjugate heat transfer analysis

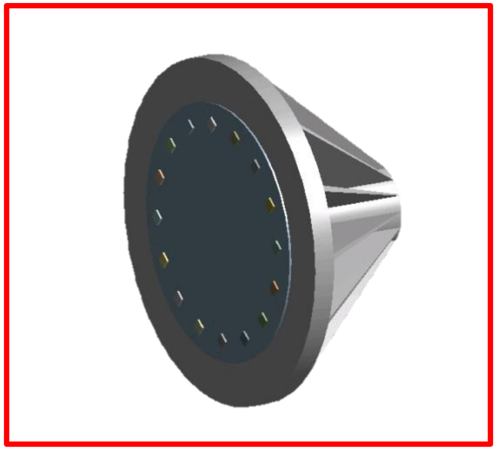
Case description

Geometry

Outer

- **Properties**

Part	Phase	Properties
LED (Sapphire)		$\rho = 1250 kg/m^3$ $C_p = 710 J/kgK$ $K = 1 W/mK$
PCB (Aluminum)	**Solid**	$\rho = 2680 kg/m^3$ $C_p = 880 J/kgK$ $K = 137 W/mK$
HeatSink (Composite)		$\rho = 3980 kg/m^3$ $C_p = 761 J/kgK$ $K = 23.1 W/mK$
Outer	**Fluid**	$\rho = 1.18415 kg/m^3$ $C_p = 1003.62 J/kgK$



LED

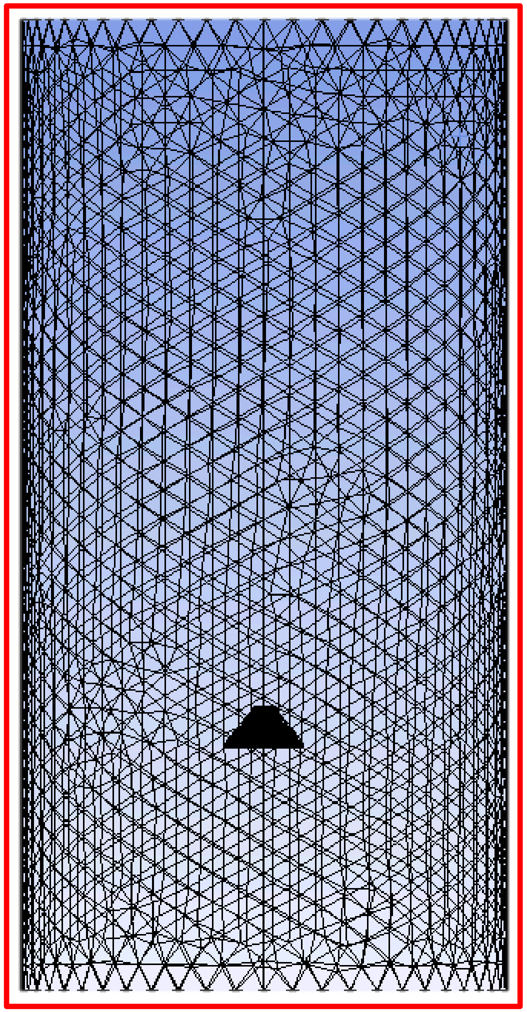
PCB

HeatSink

Conjugate heat transfer analysis

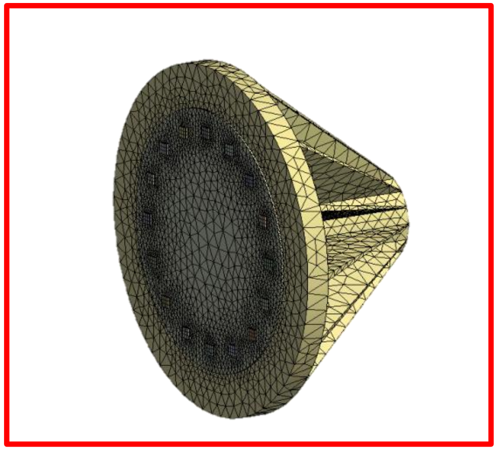
Case description

Computational mesh



Outer

- **Numerical Method and Model**
  - **OpenFOAM 2.3.x**
  - **chtMultiRegionSimpleFoam (Steady state conjugate heat transfer)**
  - **About 700,000 unstructured cells**
  - **Radiation model – View Factor**
- **Boundary condition**
  - **Heat Source - LED 18W**
  - **Initial temperature - 300K**
  - **Pressure - 1atm**
  - **Air is stationary**



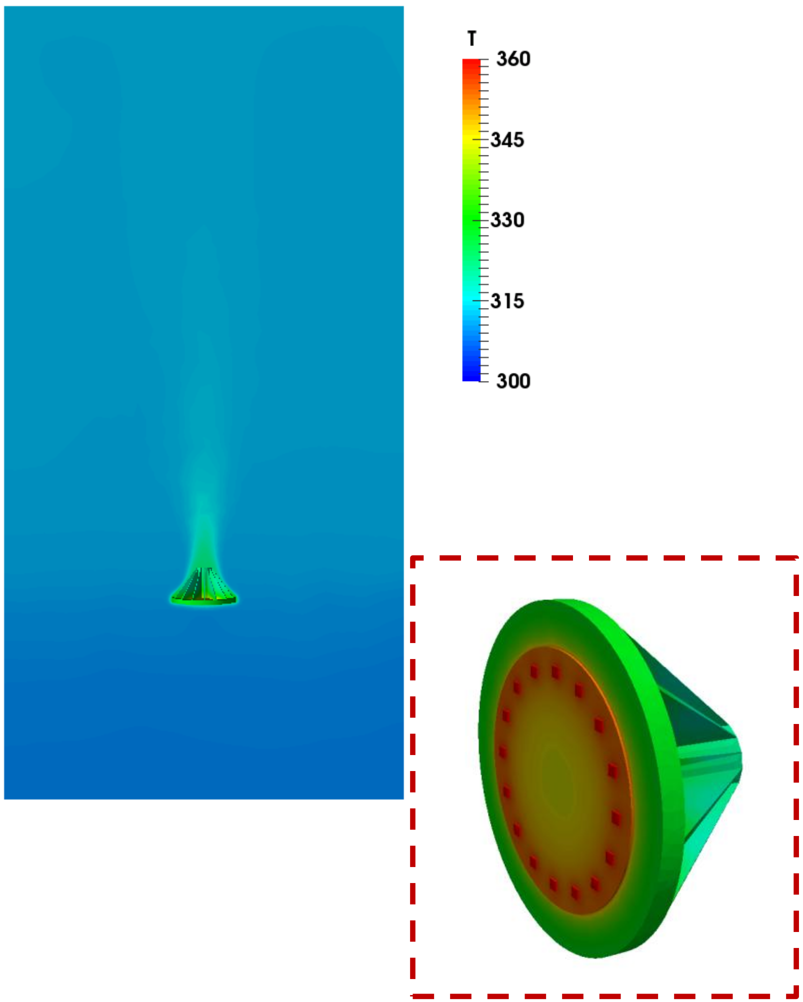
LED

PCB

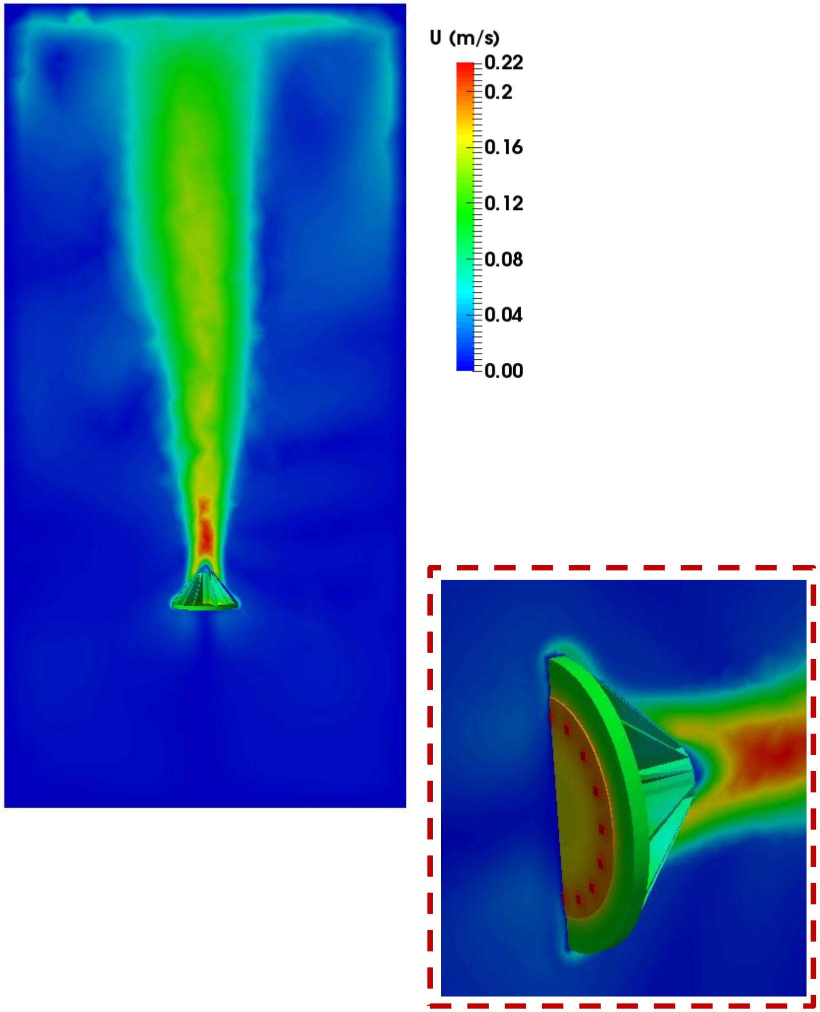
HeatSink

Conjugate heat transfer analysis

Result



Temperature (K)



Velocity (m/s)

Conclusion

(1) OpenFOAM is an open source program package useful for simulation of various industrial combustion devices involving complicated multiphase physics.

(2) Turbulent combustion models are reviewed in the perspective of practical CFD application for gaseous fuel (Premixed / Non-premixed), liquid fuel (Spray) and solid fuel (Fixed, Fludized and Entrained Bed).

(3) CFD simulation is now established as a useful design and analysis tool for complicated industrial combustion devices. Extensive industrial interests shown.

(4) Further work is required for validation and implementation of more advanced and reliable turbulent combustion models to improve accuracy of the simulation results.