An OpenFOAM-based framework for sCO_2 oxy-fuel combustion using real-fluid based three-feed stream steady laminar flamelet model

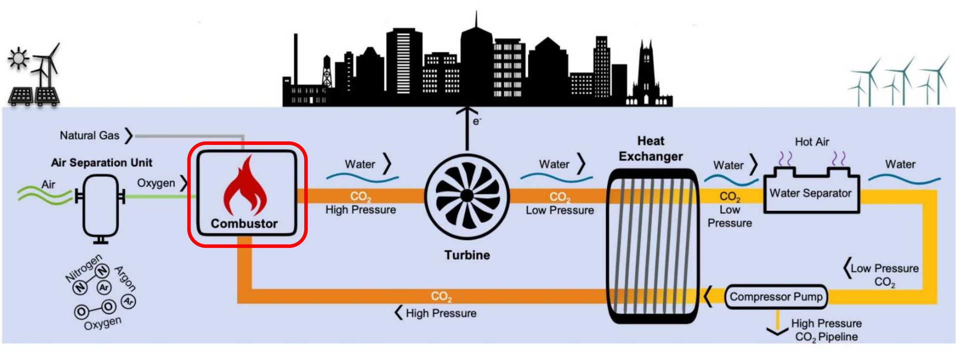
Danh Nam Nguyen[1], Jae Hun Lee[1], Chun Sang Yoo[1]

1. Department of Mechanical Engineering, Ulsan National Institute of Science and Technology (UNIST), Republic of Korea.

E-mail address : danhnam@unist.ac.kr, [1] csyoo @unist.ac.kr

Introduction

➢ Allam-Fetvedt power cycle (direct-fired supercritical CO_2 (sCO_2)):



Source: from https://netpower.com/technology

- Advantages such as high efficiency, zero emission, lower-cost power, and small land usage (> 40% less than similar output natural gas plant) [1].
- Challenging and complicated in its component designs due to extremely high pressure (200-300 atm), highly diluted CO_2 injecting at order of 1000 K, and no experimental data available.
- Lack of research on materials, chemical kinetics, combustion modeling, heat transfer, CO_2 effects, etc.,

➢ Previous studies:

- Banuti et al. [2] showed that the flame blow-out at high strain rate, and it is captured well with flamelet progress variable model (FPV). In addition, there is an unexpected deviation from ideal gas behavior for O_2/CH_4 combustion in CO_2 dilution despite the high temperatures, even at the hot reaction zone.
- Indelicato et al. [3] proved that the extension of standard flamelet by means of three-feed stream model can be an efficient approach for the simulation of diluted oxy-fuel non-premixed combustion.
- To the best of authors' knowledge, there exists no published an OpenFOAM-based framework including three-feed stream steady laminar flamelet model with consideration of real-fluid effects.

➢ Our objectives:

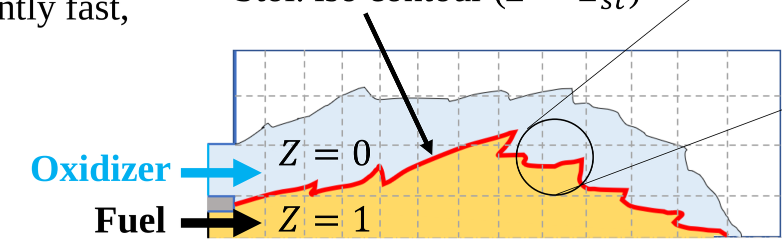
- Develop a new OpenFOAM-based framework including real-fluid based three-feed stream steady laminar flamelet model for sCO_2 combustion.

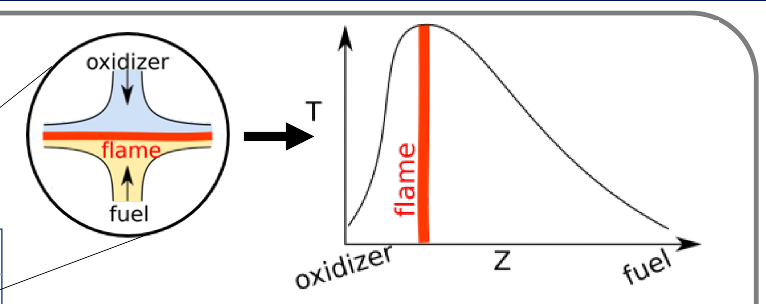
Combustion Modeling

➢ Two-feed stream steady laminar flamelet model:

- Assumptions:
  - Chemistry is sufficiently fast,
  - Le = 1 ($\rho D \equiv \frac{\lambda}{c_p}$),
  - Sc = 1 ($\rho D \equiv \mu$).
- Procedure:
  1. Solving continuity
  2. Solving momentum
  3. ~~Solving species~~
  4. ~~Solving energy~~

Stoi. iso contour ($Z = Z_{st}$)





- Counterflow diffusion flame (flamelet):

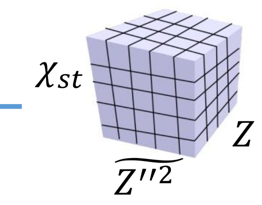
$$\rho \frac{\partial Y_k}{\partial \tau} = \frac{1}{2}\rho \chi \frac{\partial^2 Y_k}{\partial Z^2} + \dot{\omega}_k; \quad \chi = 2D\left(\frac{\partial Z}{\partial x_j}\right)^2;$$

$\boxed{Y_k(Z, \chi_{st});}$ $\boxed{T(Z, \chi_{st});}$

- Solve only for controlling parameters:

$(\tilde{Z}, \tilde{\chi}, \widetilde{Z''^2})$ → Interpolate → Y_k, h_s (or T)

Library (3D)



Tabulate

- Turbulent fluctuations can be represented by a PDF distribution:

$$\tilde{\phi} = \int_0^{\infty}\int_0^{1} \phi(Z, \chi_{st}) P(Z, \chi_{st})\, dZ\, d\chi_{st}$$

Assume independently

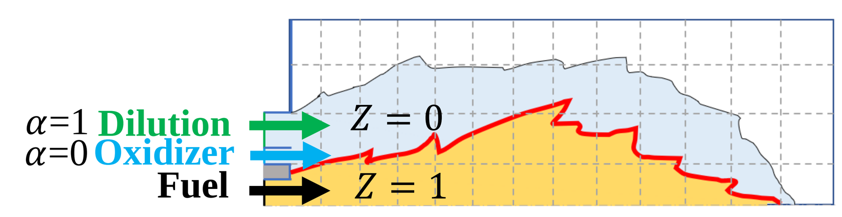
$P(Z)P(\chi_{st})$

β-PDF δ-function

➢ Three-feed stream steady laminar flamelet model:

- By introducing a new conserved scalar variable α to account for different mixture compositions in the oxidizer stream [3]:

$$\alpha = \frac{Y_k|_{Z=0} - Y_k^{(0)}}{Y_k^{(1)} - Y_k^{(0)}};$$



where $Y_k^{(0)}$ and $Y_k^{(1)}$ are nominal mass fraction of oxidizer and diluent stream.

- Solve for controlling parameters:

$(\tilde{Z}, \tilde{\chi}, \widetilde{Z''^2}, \tilde{\alpha})$ → Interpolate → Y_k, h_s (or T)

Library (4D) ← Tabulate

- PDF: $\tilde{P}(Z, \chi_{st}, \alpha) = \tilde{P}(Z)\, \tilde{P}(\chi_{st}) \tilde{P}(\alpha)$

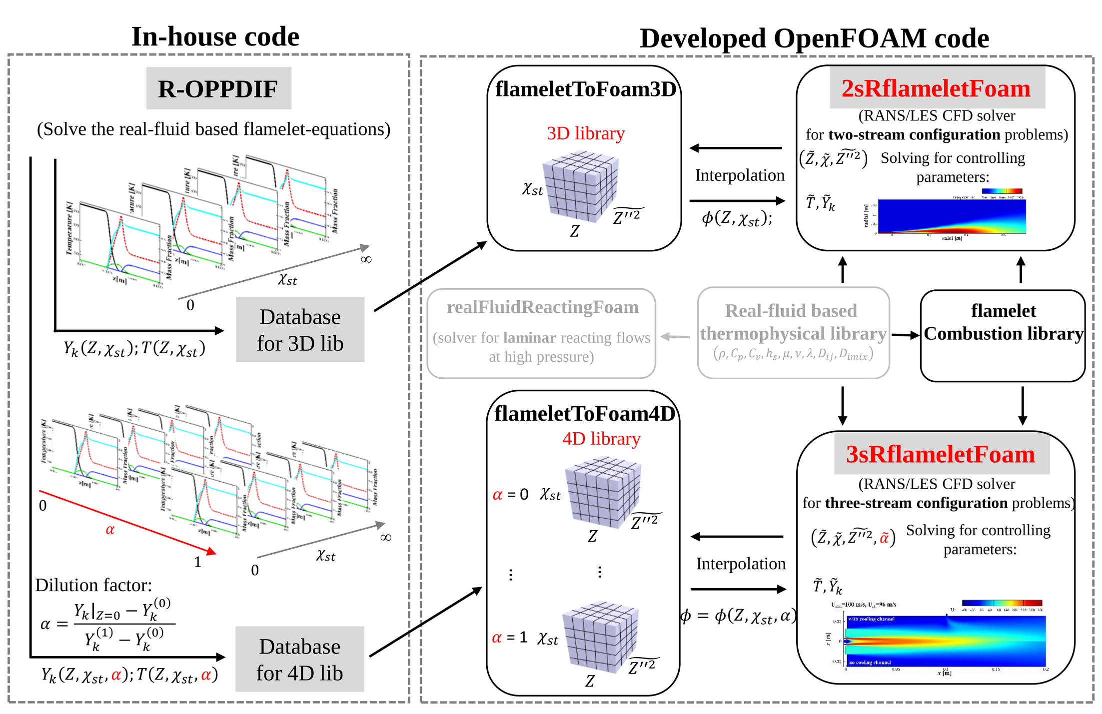
β-PDF δ-function

- Flamelets: $\phi = \phi(Z, \chi_{st}, \alpha)$

Results & Discussion

➢ The OpenFOAM-based developed framework:

- The schematic of the framework:



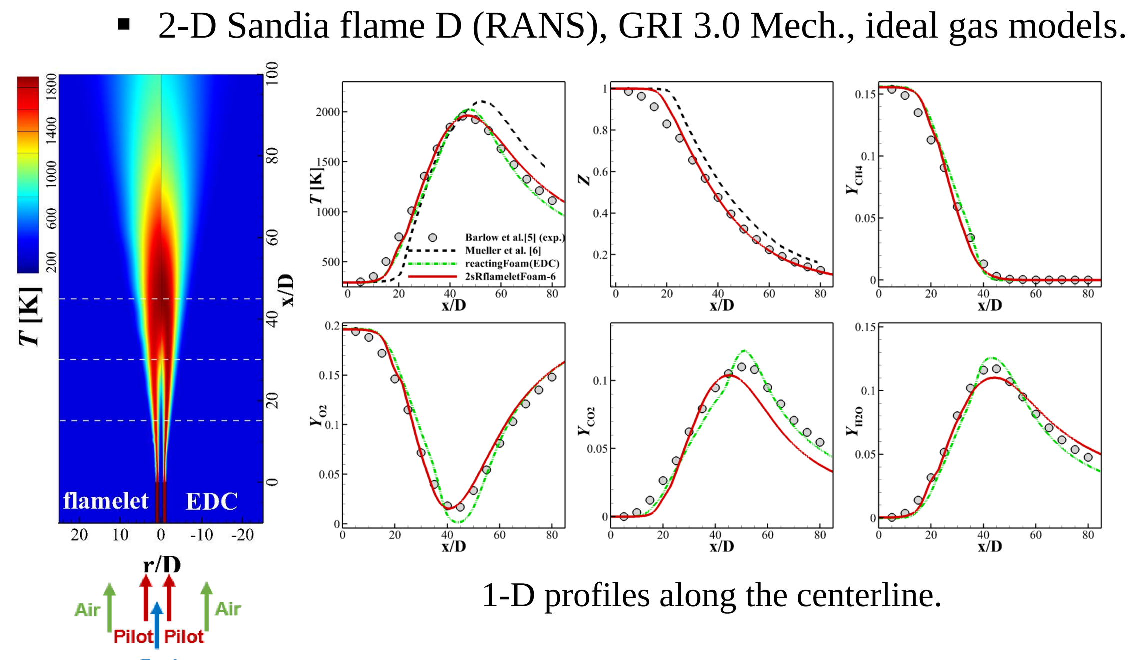
- List of real-fluid models implemented [4]:

EoS	Thermodynamic	Transport
- Modified SRK. - PR.	- Basic thermodynamic theory (JANAF-based).	- Chung (1998) for μ, λ. - Fuller and Takahashi for binary diffusion coefficients. - Standard Kinetic Theory for binary diffusion coefficients.

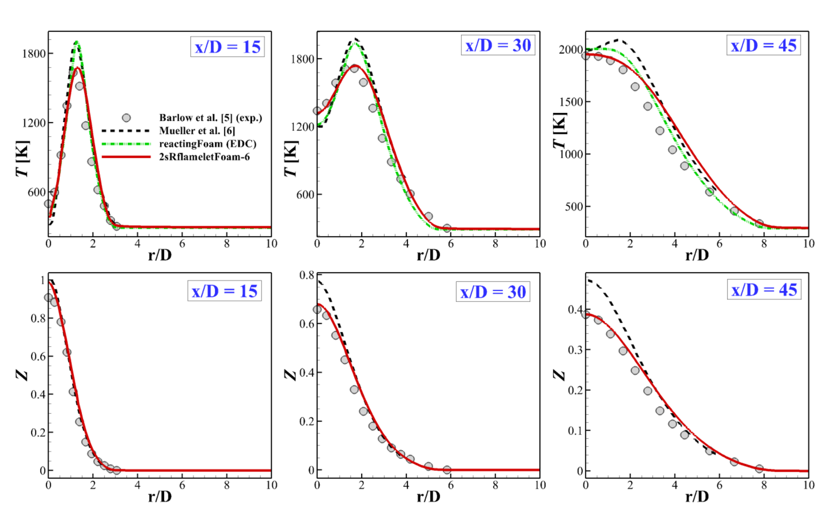
- List of real-fluid based flamelet solvers:
  - *2sRflameletFoam*: a solver for two-feed stream configurations.
  - *3sRflameletFoam*: a solver for three-feed stream configurations.

➢ Validation of *2sRflameletFoam* at low pressure (1atm):

- 2-D Sandia flame D (RANS), GRI 3.0 Mech., ideal gas models.



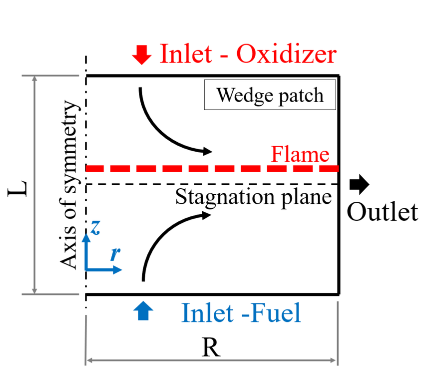
1-D profiles along the centerline.



1-D radial profiles at different x/D.

➢ Validation of *2sRflameletFoam* at high pressure:

- 2-D laminar counterflow CH_4/sCO_2-O_2 flame at 200 atm [4]: GRI 3.0 Mech., modified SRK, Chung (1998).



BCs:

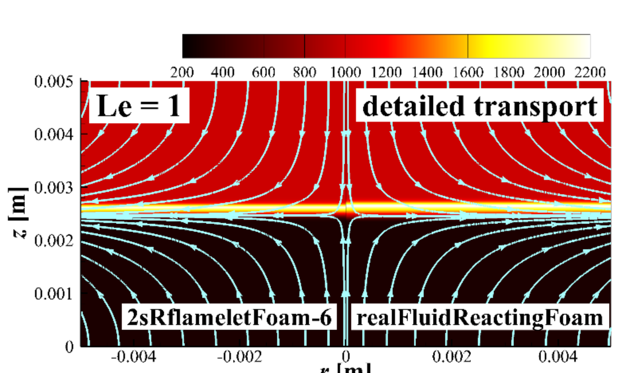
Oxidizer	Fuel
$X_{O2} = 0.21$ $X_{CO2} = 0.79$	$X_{CH4} = 1$
T = 1000 K	T = 300 K

$a = 2(|U_F| + |U_O|)/L$

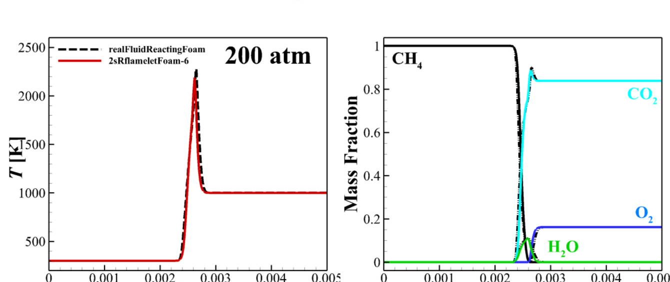
Global strain rate: a = 100 s^{-1}

Computational domain and grid sizes:

	RxL[mm]	Δr [μm]	Δz [μm]
realFluidReactingFoam [4]	5x5	5	5-10
2sRflameletFoam	5x5	**20**	**50**



2-D temperature contour.

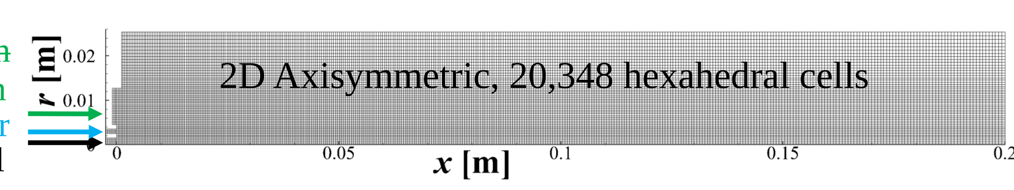


1-D profiles along the centerline.

➢ *3sRflameletFoam* vs. *2sRflameletFoam* at high pressure (RANS):

- 2-D CH_4/sCO_2-O_2 flame at 200 atm: GRI 3.0 Mech., modified SRK, Chung (1998).

~~(pure sCO_2) Dilution~~
(sCO_2 +O_2) Dilution
(sCO_2+O_2) Oxidizer
(pure CH_4) Fuel



BCs

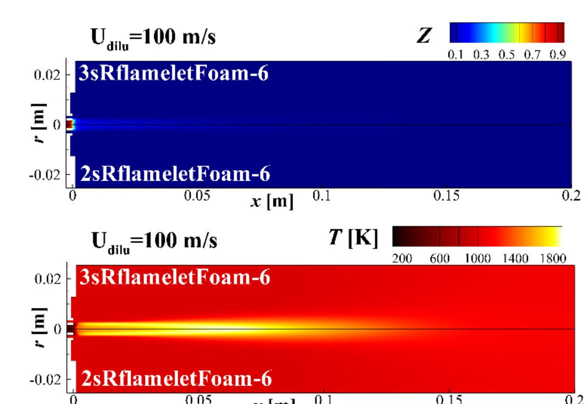
Stream	Composition	T [K]
Fuel	$X_{CH4} = 1.0$	300
Oxidizer	$X_{O2} = 0.21$ $X_{CO2} = 0.79$	1000
Dilution	$X_{CO2} = 1.0$	1000

(α = 0 at dilution stream)

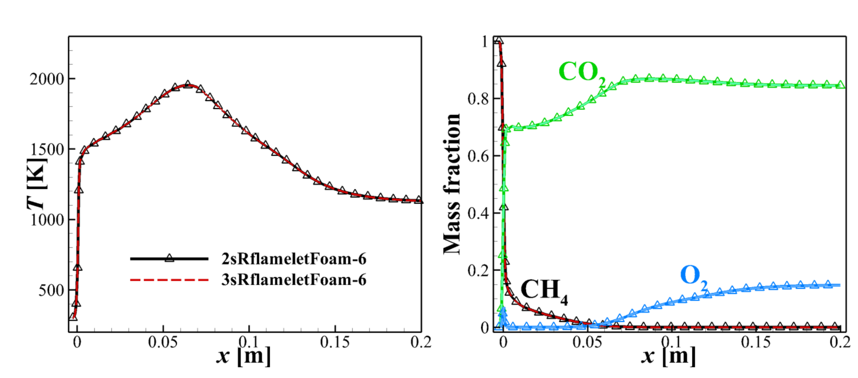
Nominal mass fraction

α	CO_2	O_2
0	0.7900	0.2100
0.25	0.8425	0.1575
0.50	0.8950	0.1050
0.75	0.9475	0.0525
1	1.0	0

If dilution = Oxidizer, this configuration is valid for both **three-feed** stream with inlet dilution α = 0 and **two-feed** stream model.



2-D mixture fraction and temperature contours.



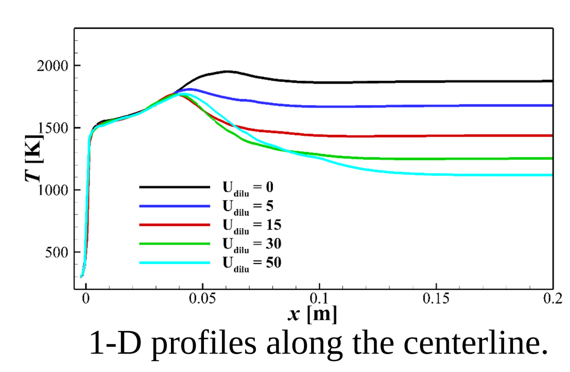
1-D profiles along the centerline.

➢ Dilution effect in sCO_2 combustion (RANS) using *3sRflameletFoam*:

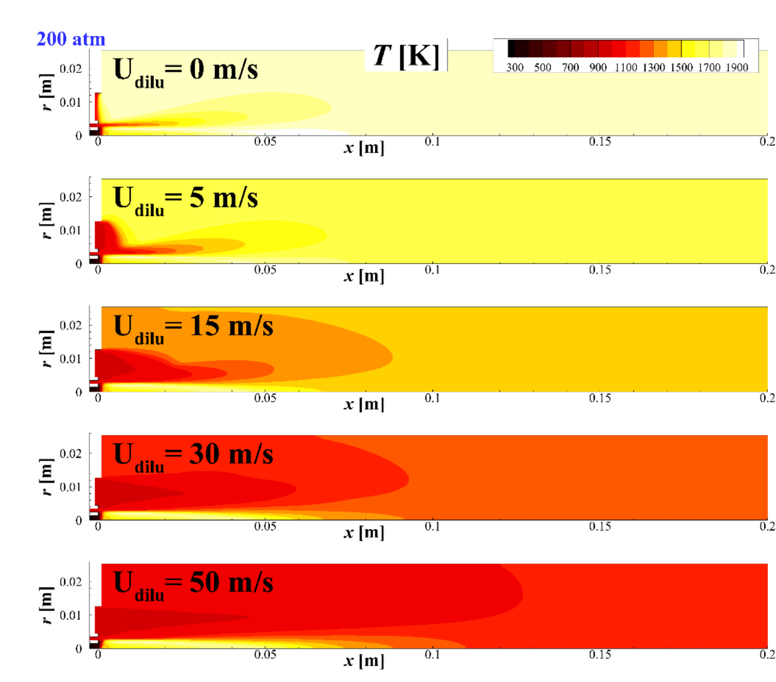
- 2-D CH_4/sCO_2-O_2 flame at 200 atm: GRI 3.0 Mech., modified SRK, Chung (1998).

BCs:

Fuel	Oxidizer	Dilution
$X_{CH4} = 1.0$	$X_{O2} = 0.21$ $X_{CO2} = 0.79$	$X_{O2} = 0$ $X_{CO2} = 1.0$
T = 300 K	T = 1000 K	T = 1000 K
U_{fuel} = 15 m/s	U_{oxid} = 313 m/s	U_{dilu} = 0 – 50 m/s
Z = 1	Z = 0	Z = 0
α = zeroGradient	α = 0	α = 1



1-D profiles along the centerline.



2-D temperature contour.

✓ **Acknowledgement**

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✓ **References**

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