Generic numerical test case to understand cryogenic methane combustion dynamics

3rd International Seminar on Non-Ideal Compressible Fluid Dynamics for Propulsion & Power

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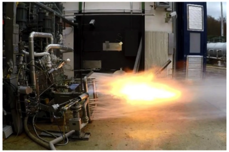
DLR

Motivation: Reusable methane rocket engines

NextGeneration reusable rocket engines
(e. g. Prometheus engine):

- Complex methane-oxygen combustion kinetics (reduced mechanisms and flamelet models)
- Cryogenic combustion chambers ($T_{O2} \in [100, 3500]$K, $T_{CH4} \in [200, 3500]$K)
- Cryogenic effects at injection and in cooling channels
- Transcritical effects (especially) at part-load conditions ($p_{CC} \approx 50$ bar)



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EOS choice(s)

Cryogenic EOS models

- Cubic EOS models: SRK, PR
- Helmholtz based EOS
- PCSAFT based models

⇒ focus on cubic EOS models due to:

- simplicity and fast evaluation for 3D CFD
- mixing efects can be represented
- VLE methods available

Main cubic species in methane combustion:

species	T_c [K]	p_c [MPa]
O_2	154.6	5.0
CH_4	190.54	4.6
CO_2	304.1	7.4
H_2O	647.1	22.1
⋮	⋮	⋮

⇒ close critical conditions of O_2 and CH_4

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New numerical test case
    Methane-Oxygen mixing test case
    Methane-Oxygen reacting test case

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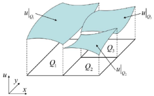
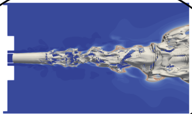
CFD methodology



Numerical method



Turbulence modeling

Compressible multi-phase flow

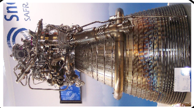
$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$(\rho \mathbf{u})_t + \nabla \cdot ((\rho \mathbf{u}) \circ u) + \nabla p = \nabla \tau$$

$$e_t + \nabla \cdot (\mathbf{u}\,(e + p)) = \nabla \cdot (\tau \mathbf{u}) - \nabla \cdot \mathbf{q}$$

$$+\text{Equation of State} \quad p = p\,(\rho, \epsilon)$$

Combustion model
(DC/Flamelet)



Coupled simulations

Numerical approach

Numerical approach for cryogenic, supercritical combustion chambers is based on DLR inhouse flow solver TAU:

- 2nd order hybrid finite-volume flow solver
- RANS & DES turbulence models
- Cryogenic flamelet combustion model
- EOS model: low T: cubic mixture model (Peng-Robinson EOS)
  high T: ideal gas mixture ($c_v = f(T)$)
- high-pressure transport properties (Chung mixture rules, Poling et al. [1])
- Homogenous-Equilibrium Model for subcritical states using VLE

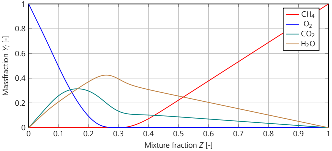
Cryogenic flamelet combustion framework

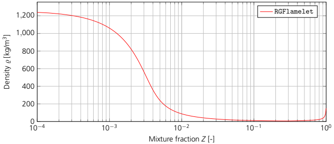
- Solves flamelet equations in enthalpy formulation

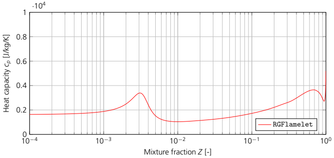
$$-\rho\frac{\chi}{2}\frac{\partial^2 Y_s}{\partial Z^2} = \dot{m}_s$$

$$-\rho\frac{\chi}{2c_p}\left(\frac{\partial^2 h}{\partial Z^2} - \sum_{s=1}^{N_s} h_s \frac{\partial^2 Y_s}{\partial Z^2}\right) = -\frac{1}{c_p}\sum_s h_s \dot{m}_s$$

- Uses the same gas model as the TAU solver
- 2nd order `PETSc`-based solution algorithm with preconditioning
- Tabulation of linearized cubic mixture coefficients and transport properties for solver acceleration







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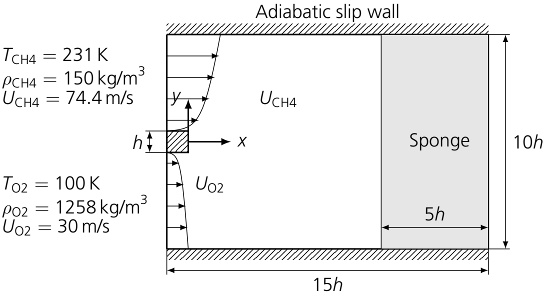
Methane-Oxygen mixing test case



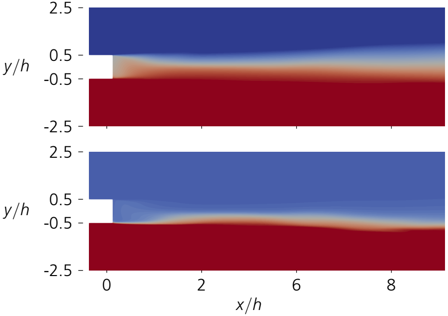
Geometry taken from [2]

- 100 bar pressure
- Velocity inflow profile
- Peng-Robinson EOS
- RANS: Menter SST model
  DDES: Spalart-Alamaras subgrid scale model
- Lip thickness: 0.5
- Mesh size: DDES: 0.56 Mio DOF
  RANS: 56 000 DOF

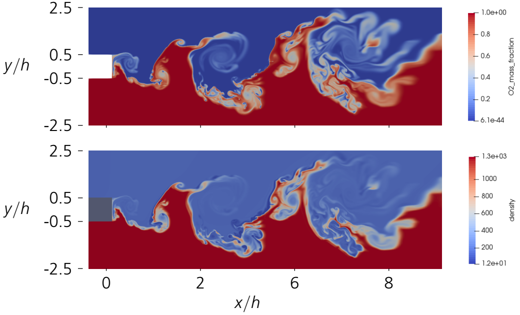
⇒ Aim: Simple and well documented test case for cryogenic methane mixtures!

Comparison of RANS and DES solution

RANS turbulence model:



DES:



Comparison of turbulence statistics

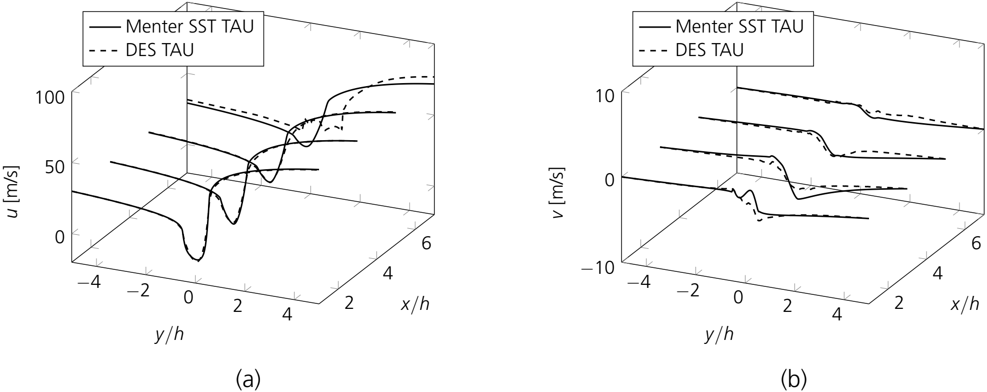


Figure: Transverse cuts of (a) mean axial and (b) mean transverse velocity of the two-dimensional LOX/GCH4 mixing case.

Comparison of turbulence statistics

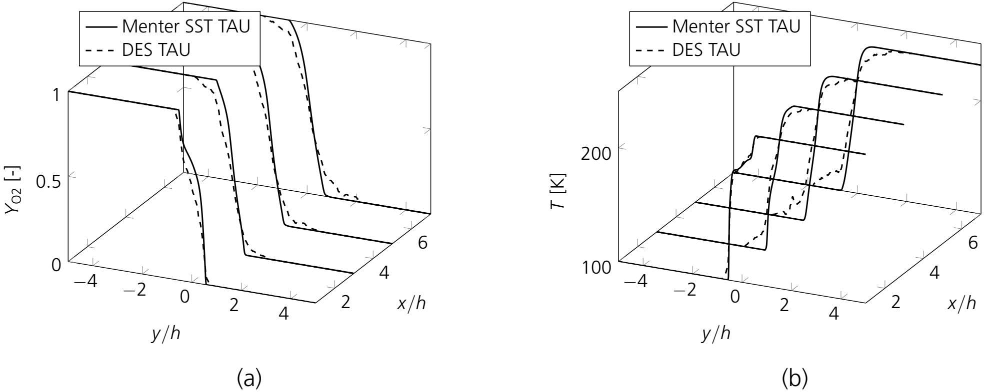
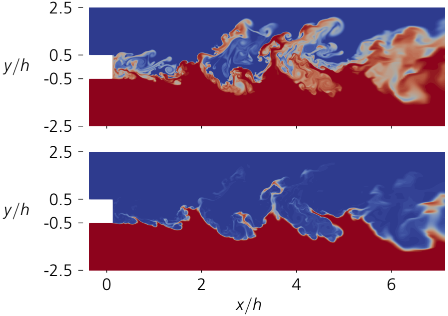


Figure: Transverse cuts of (a) mean oxygen mass fraction and (b) mean temperature of the two-dimensional LOX/GCH4 mixing case.

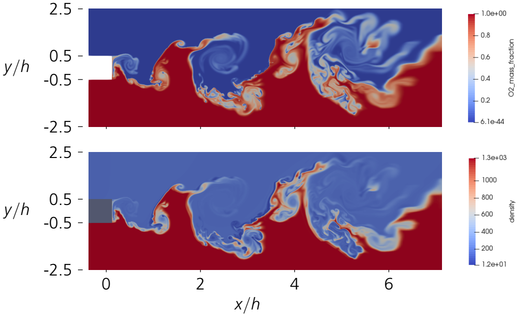
Comparison to original Ruiz test case

Hydrogen-Oxygen mixing:



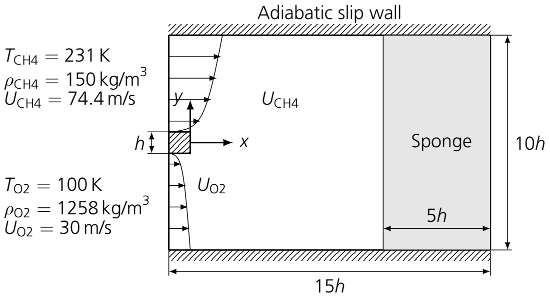
$$Re_{O_2H_2} = \frac{\rho v h}{\nu} = 164 \cdot 10^6$$

Methane-Oxygen mixing:



$$Re_{O_2CH_4} = 344 \cdot 10^6$$

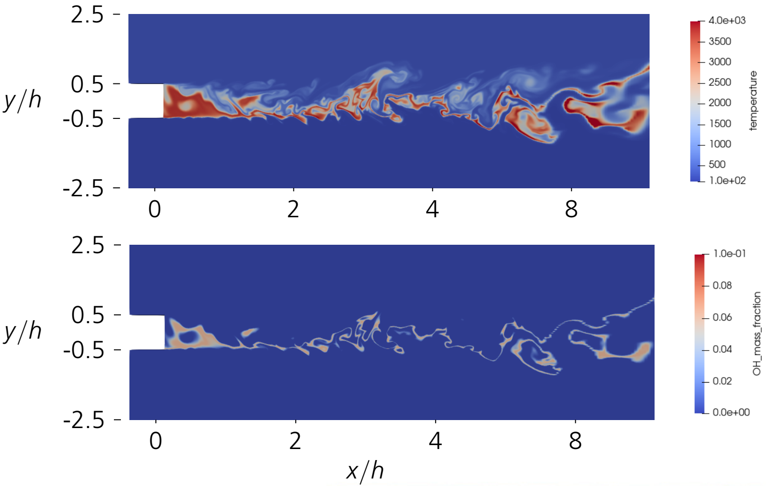
Methane-Oxygen reacting test case



Geometry and inlet conditions

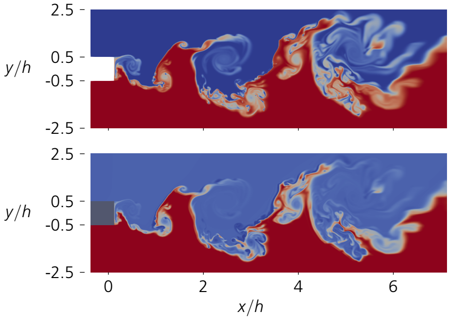
- 100 bar pressure
- Velocity inflow profile
- Peng-Robinson EOS
- DDES: Spalart-Alamaras subgrid scale model
- Flamelet combustion model Zhukov-Kong reaction mechanism [3]
- Lip thickness: 0.5
- Mesh size: DDES: 0.56 Mio DOF

Instantaneous DES snapshots

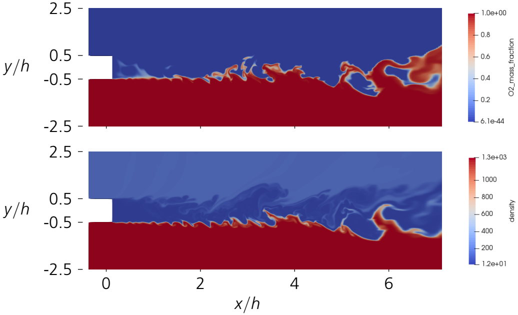


Comparison mixing/reacting test case

Mixing:



Reacting:



- large-scale vortex structures

- small vortex structures
- large temperature gradient

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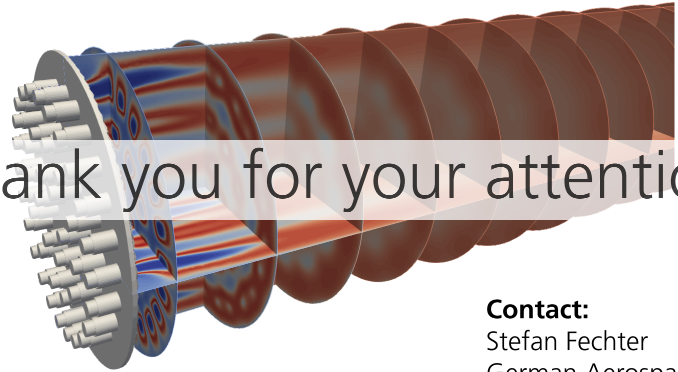
Conclusion and Outlook

- Provided simple numerical test case for methane-oxygen mixing and combustion at purely supercritical conditions
- Generic 2D test case allows for code-code comparison
- Compared to hydrogen-oxygen mixing less turbulent structures resolved in DES due to higher Reynolds number
- In reacting test case smaller turbulent structures due to large temperature gradients

What to come?

- Decrease pressure to part-load conditions ($\approx 50\,\text{bar}$)
- Detailed combustion statistics



Thank you for your attention!

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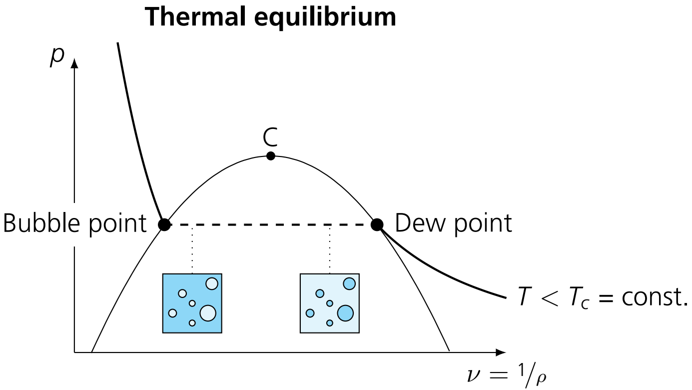
References I

Poling, B. E., Prausnitz, J. M., and O'Connel, J. P., *The properties of gases and liquids*, McGraw Hill Book Co., New York, NY, 5th ed., 2007.

Ruiz, A. M., Lacaze, G., Oefelein, J. C., Mari, R. H., Cuenot, B., Sell e, L., and Poinsot, T., "Numerical benchmark for high-Reynolds-number supercritical flows with large density gradients," *AIAA Journal*, 2015.

Zhukov, V. P. and Kong, A. F., "A compact reaction mechanism of methane oxidation at high pressures," *Progress in reaction kinetics and mechanism*, Vol. 43, No. 1, 2018, pp. 62–78.

Vaper-Liquid Equilibria (VLE)



$\Rightarrow$ integral model for the vapor-liquid mixture within one cell

$\Rightarrow$ consistent thermodynamic state is given by VLE calculation

Reduced Kong methane mechanism [3]

					Rate Constants		
No.	Reaction				A	n	E
1[a]	$H + CH_2O(+M)$	$\rightleftharpoons$	$CH_3O(+M)$	k_∞	5.4000e+11	0.45	2.6000e+00
				k_0	2.2000e+30	-4.80	5.5600e+00
					A = 0.758, T_3 = 94.0, T_1 = 1555.0, T_2 = 4200.0		
2	$OH + CH_4$	$\rightleftharpoons$	$CH_3 + H_2O$		1.0000e+08	1.60	3.1200e+00
3	$CH_3 + O_2$	$\rightleftharpoons$	$O + CH_3O$		2.6750e+13	0.00	2.8800e+01
4	$CH_3 + O_2$	$\rightleftharpoons$	$OH + CH_2O$		3.6000e+10	0.00	8.9400e+00
5	$CH_3 + CH_2O$	$\rightleftharpoons$	$HCO + CH_4$		3.3200e+03	2.81	5.8600e+00
6	$CH_3O_2 + CH_3$	$\rightleftharpoons$	$CH_3O + CH_3O$		3.0000e+13	0.00	-1.2000e+00
7	$CH_3 + O_2$	$\rightleftharpoons$	CH_3O_2		1.7000e+60	-15.10	1.8785e+01
8	$CH_3O + CH_3$	$\rightleftharpoons$	$CH_2O + CH_4$		2.4100e+13	0.00	0.0000e+00
9	$O + CH_4$	$\rightleftharpoons$	$OH + CH_3$		1.0200e+09	1.50	8.6000e+00
10	$H + O_2$	$\rightleftharpoons$	$O + OH$		8.3000e+13	0.00	1.4413e+01
11	$O + CH_3$	$\rightleftharpoons$	$H + CH_2O$		8.4300e+13	0.00	0.0000e+00
12[b]	$H + OH + M$	$\rightleftharpoons$	$H_2O + M$		2.2000e+22	-2.00	0.0000e+00
13[c]	$H + CH_3(+M)$	$\rightleftharpoons$	$CH_4(+M)$	k_∞	1.2700e+16	-0.63	3.8300e-01
				k_0	2.4770e+33	-4.76	2.4400e+00
					A = 0.783, T_3 = 74.0, T_1 = 2941.0, T_2 = 6964.0		
14[d]	$H + HCO(+M)$	$\rightleftharpoons$	$CH_2O(+M)$	k_∞	1.0900e+12	0.48	-2.6000e-01
				k_0	1.3500e+24	-2.57	1.4250e+00
					A = 0.7824, T_3 = 271.0, T_1 = 2755.0, T_2 = 6570.0		
15[e]	$H + C_2H_4(+M)$	$\rightleftharpoons$	$C_2H_5(+M)$	k_∞	1.0800e+12	0.45	1.8200e+00
				k_0	1.2000e+42	-7.62	6.9700e+00
					A = 0.9753, T_3 = 210.0, T_1 = 984.0, T_2 = 4374.0		
16	$OH + CH_2$	$\rightleftharpoons$	$H + CH_2O$		2.0000e+13	0.00	0.0000e+00
17[f]	$HCO + M$	$\rightleftharpoons$	$H + CO + M$		1.8700e+17	-1.00	1.7000e+01
18	$CH_2 + CH_3$	$\rightleftharpoons$	$H + C_2H_4$		4.0000e+13	0.00	0.0000e+00
19	$OH + CH_2O$	$\rightleftharpoons$	$HCO + H_2O$		3.4300e+09	1.18	-4.4700e-01

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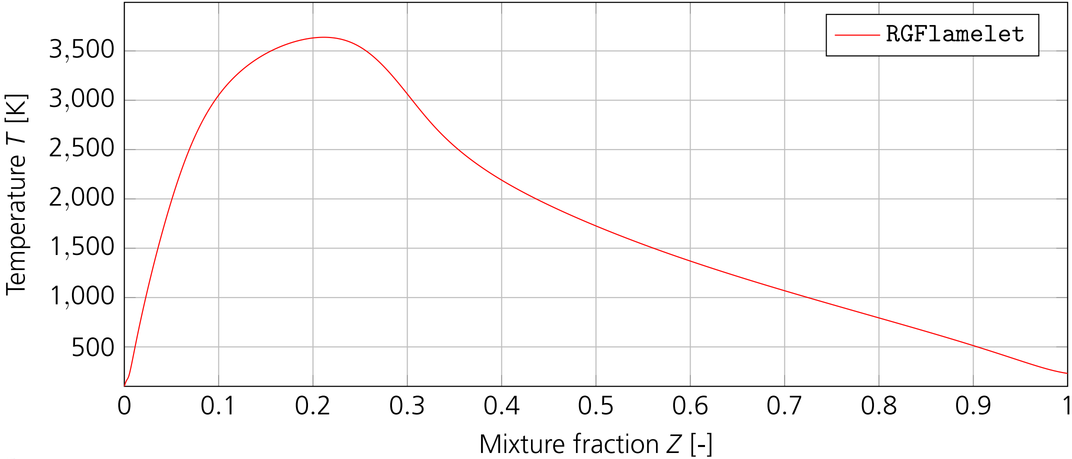
[a] $CH_4 = 2.0$, $CO = 1.5$, $H_2O = 6.0$

[b] $CH_4 = 2.0$ $H_2O = 3.65$

Ruiz Methane Flamelet



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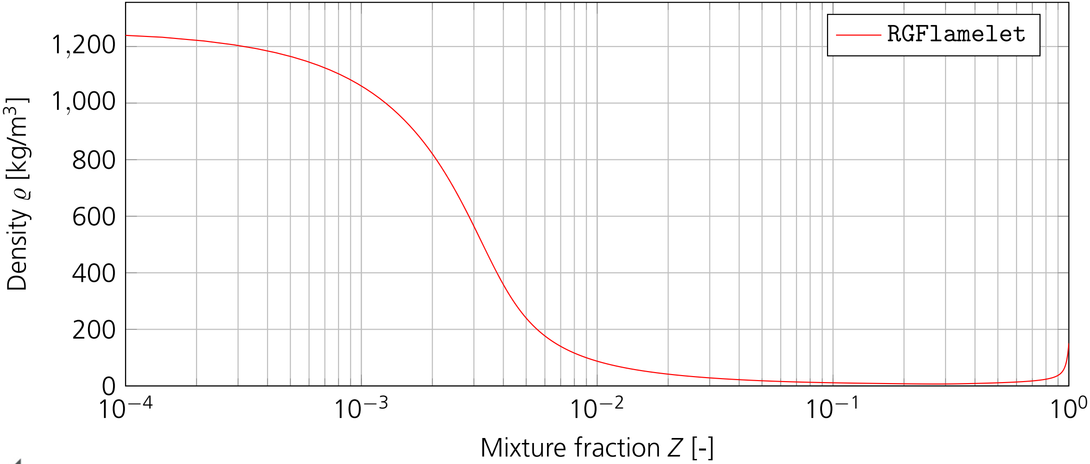

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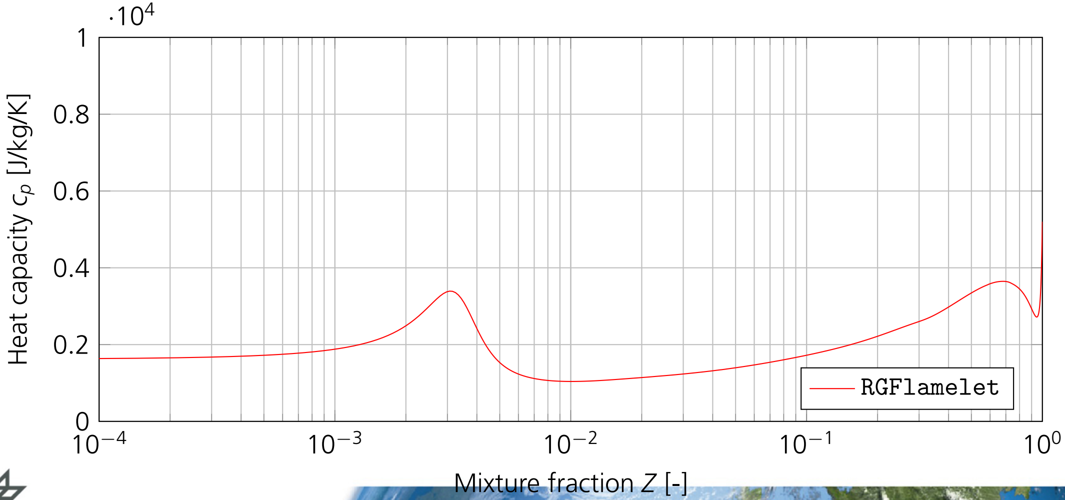

Ruiz Methane Flamelet