High fidelity simulations of turbulent combustion applications using the parallel multiphysics code Alya

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BIOMASS FOR ENERGY – Motivation

Simulations of turbulent combustion, which involves complex coupled multi-physic phenomena, can play an important role in the development of combustors

- **Optimization of combustor designs** towards systems with:
    - Increased thermal efficiency
    - Low emissions level
    - Fuel flexibility
    - High acoustic stability
- Minimize the **cost**:
    - Reduce the amount of experimental testing
    - Better insight of the flow field and flame dynamics

BIOMASS FOR ENERGY – Outline

1. Computational framework
   - Alya
2. Modelling approach
   - Governing equations
   - Thermochemical database
3. Test cases
   - Sandia flame
   - PRECCINSTA
4. Conclusions and future work
5. Acknowledgements

BIOMASS FOR ENERGY – Alya

Alya is in the PRACE benchmark suite

a final list of 12 codes to form the initial version of UEABS, w

Particle Physics:	QCD
Classical MD:	NAMD, GROMACS
Quantum MD:	Quantum Espresso, CP2K, GPAW
CFD:	Code_Saturne, ALYA
Earth Sciences:	NEMO, SPECFEM3D
Plasma Physics:	GENE
Astrophysics:	GADGET

Available online at www.prace-ri.eu

PRACE

Partnership for Advanced Computing in Europe

Selection of a Unified European Application Benchmark Suite

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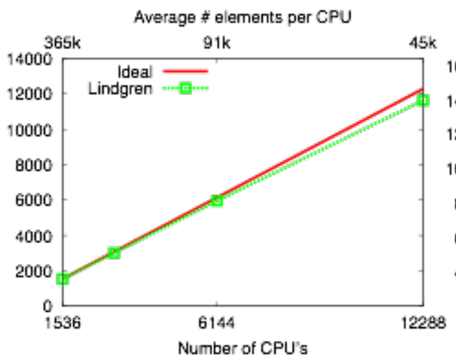
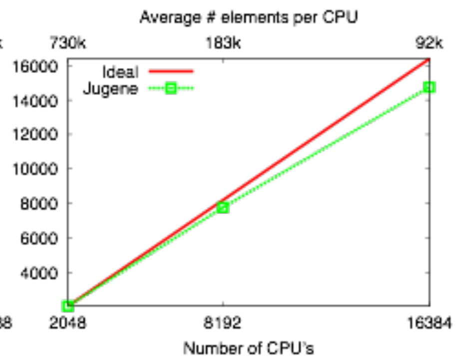
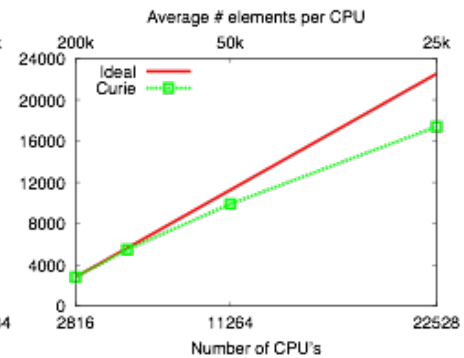
Lindgren - Cray XE6 Sweden



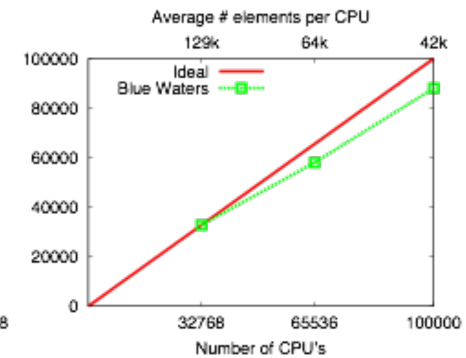
Jugene - Blue Gene/P Germany



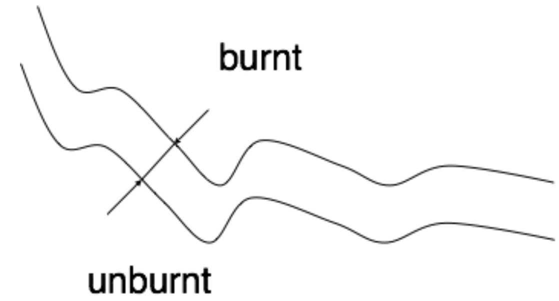
Curie - BullX France



Blue Waters - Cray XE6 USA



BIOMASS FOR ENERGY – Governing equations



Continuity:

$$\frac{\partial\bar{\rho}}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{u})=0$$

Momentum:

$$\frac{\partial(\bar{\rho}\tilde{u})}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{u}\tilde{u})= -\nabla\bar{p} + \nabla\cdot\tau$$

Energy:

$$\frac{\partial(\bar{\rho}\tilde{h})}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{u}\tilde{h})=\nabla\cdot\left[\left(\frac{\bar{\lambda}}{\bar{c_p}}+\frac{\mu_t}{Sc_t}\right)\nabla\tilde{h}\right]$$

Progress variable:

$$\frac{\partial(\bar{\rho}\tilde{c})}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{u}\tilde{c})=\nabla\cdot\left[\left(\frac{\bar{\lambda}}{\bar{c_p}}+\frac{\mu_t}{Sc_t}\right)\nabla\tilde{c}\right] + \tilde{\dot{\omega}}_c$$

Progress variable variance:

$$\frac{\partial(\bar{\rho}\widetilde{c_v^2})}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{u}\widetilde{c_v^2})=\nabla\cdot\left[\left(\frac{\bar{\lambda}}{\bar{c_p}}+\frac{\mu_t}{Sc_t}\right)\nabla\widetilde{c_v^2}\right] + 2\left(\widetilde{c\,\dot{\omega}_c} - \tilde{\dot{\omega}}_c\,\tilde{c}\right) + 2\bar{\rho}\frac{\mu_t}{Sc_t}\left(|\nabla\tilde{c}|^2 - \frac{\widetilde{c_v^2}}{\Delta^2}\right)$$

Mixture fraction:

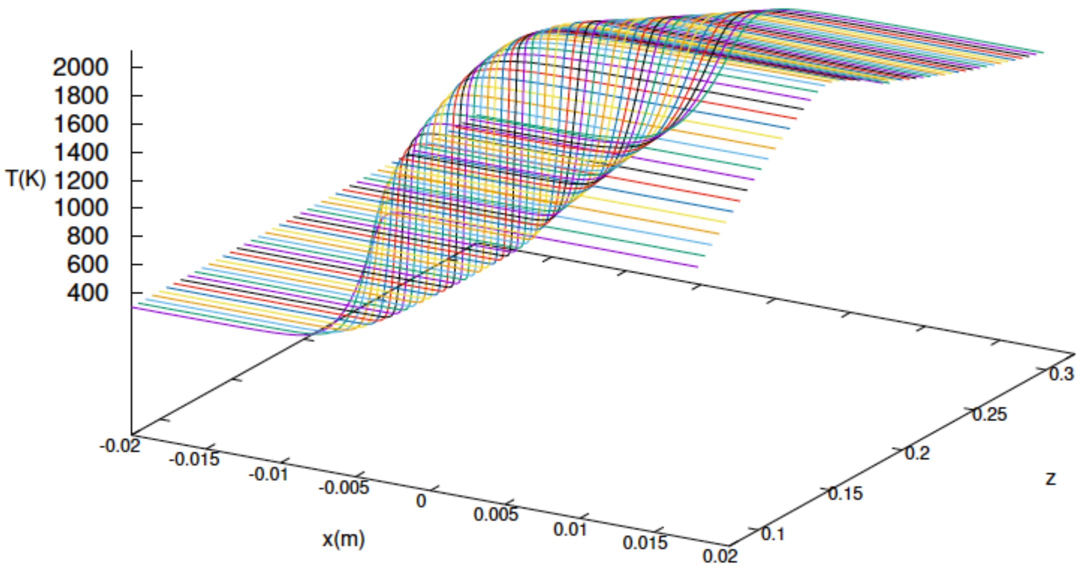
$$\frac{\partial(\bar{\rho}\tilde{Z})}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{u}\tilde{Z})=\nabla\cdot\left[\left(\frac{\bar{\lambda}}{\bar{c_p}}+\frac{\mu_t}{Sc_t}\right)\nabla\tilde{Z}\right]$$

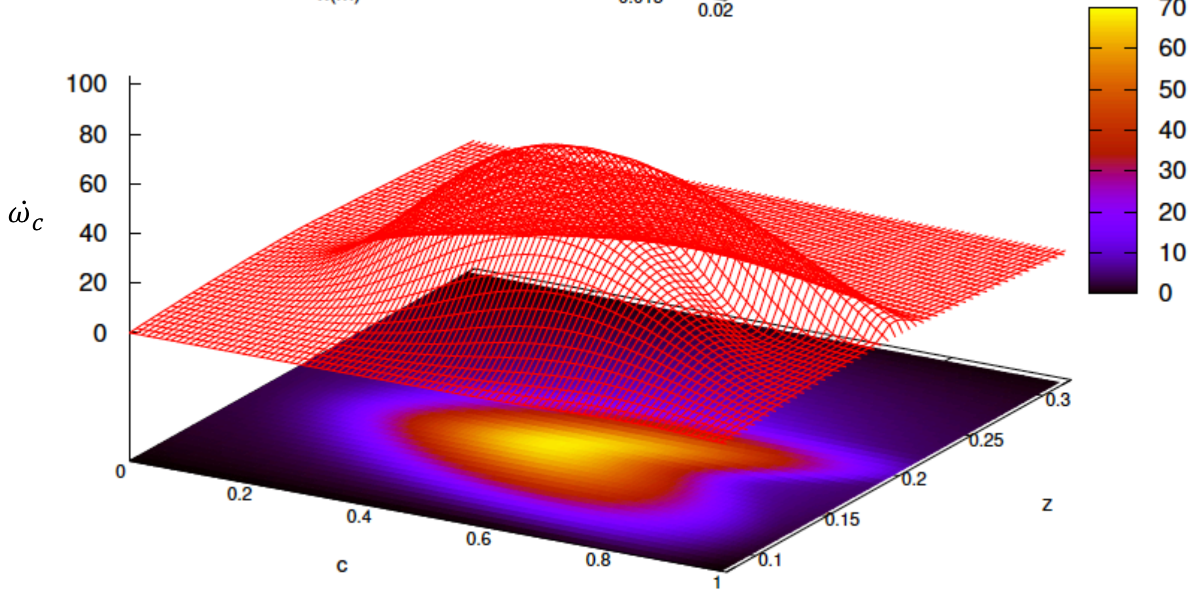
Mixture fraction variance:

$$\frac{\partial(\bar{\rho}\widetilde{Z_v})}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{u}\widetilde{Z_v})=\nabla\cdot\left[\left(\frac{\bar{\lambda}}{\bar{c_p}}+\frac{\mu_t}{Sc_t}\right)\nabla\widetilde{Z_v}\right] + 2\frac{\mu_t}{Sc_t}\left(\left|\nabla\tilde{Z}\right|^2 - \frac{\widetilde{Z_v^2}}{\Delta^2}\right)$$

WP5 BIOMASS FOR ENERGY – Premixed flamelets

Flamelets generated for CH_4-H_2-N_2 fuel





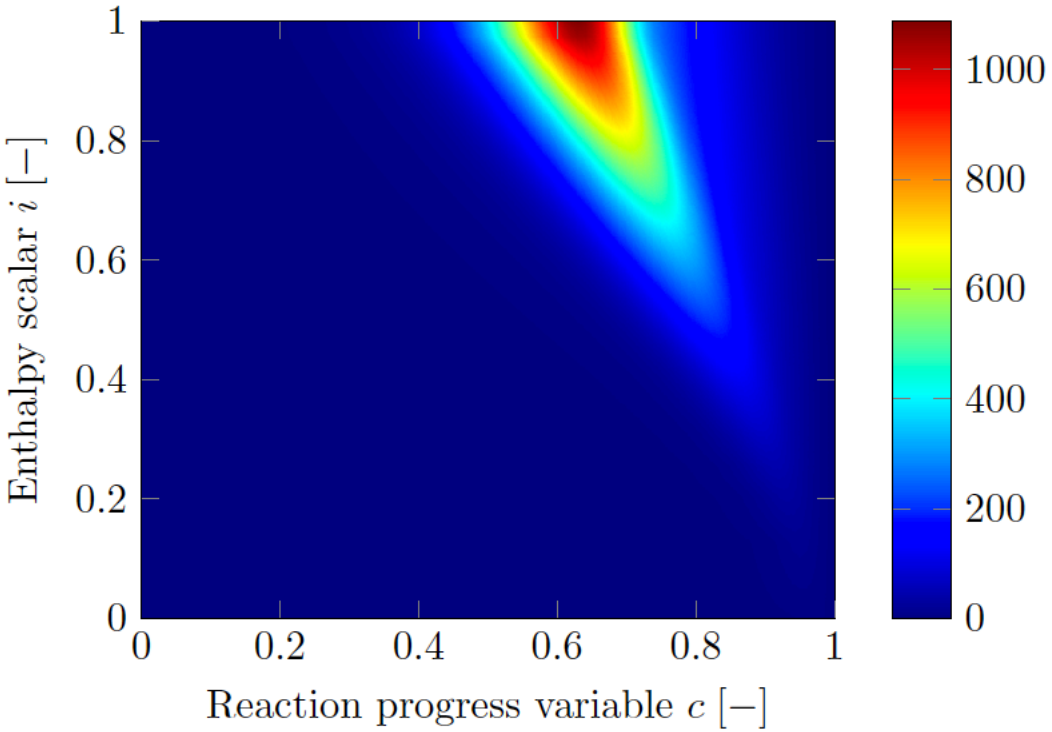
- Enthalpy and mixture fraction (Z) are constant along the flame
- Solution are calculated at Z values within the flammability limits
- Space variable changed to reaction progress variable:

$$c = \frac{\sum a_k\left(Y_k - Y_{k,in}\right)}{\sum a_k\left(Y_{k,out} - Y_{k,in}\right)}$$

- Presumed Beta-PDF for the calculation of the mean Favre-averaged quantities
- RPV source term, transport properties and NASA polynomial coefficients are tabulated

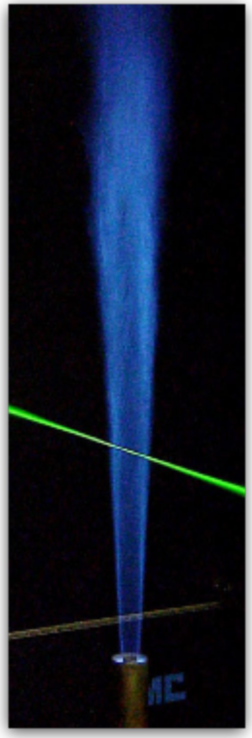
Source term and properties are computed tabulated for several non-dimensional enthalpy values

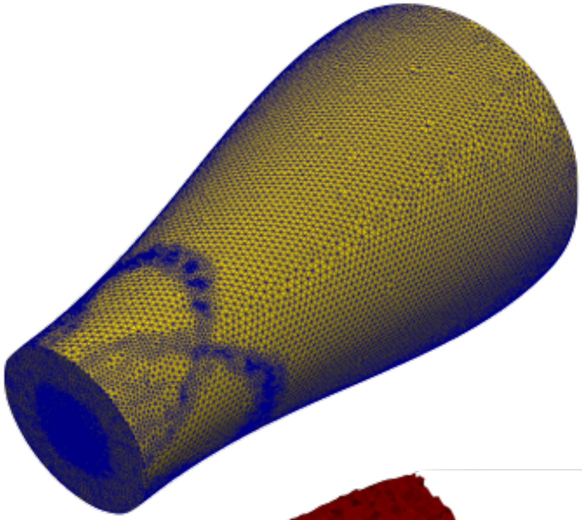
$$i = \frac{h - h_{min}}{h_{max} - h_{min}}$$

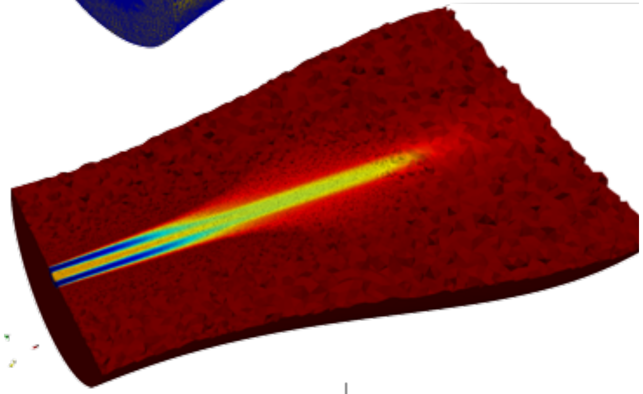


- h_{max} is defined from adiabatic conditions
- h_{min} is determined from the value at which the flame speed is almost negligible
- Source term is zero if $h < h_{min}$
- Effect of enthalpy variance is neglected

BIOMASS FOR ENERGY – Sandia D flame





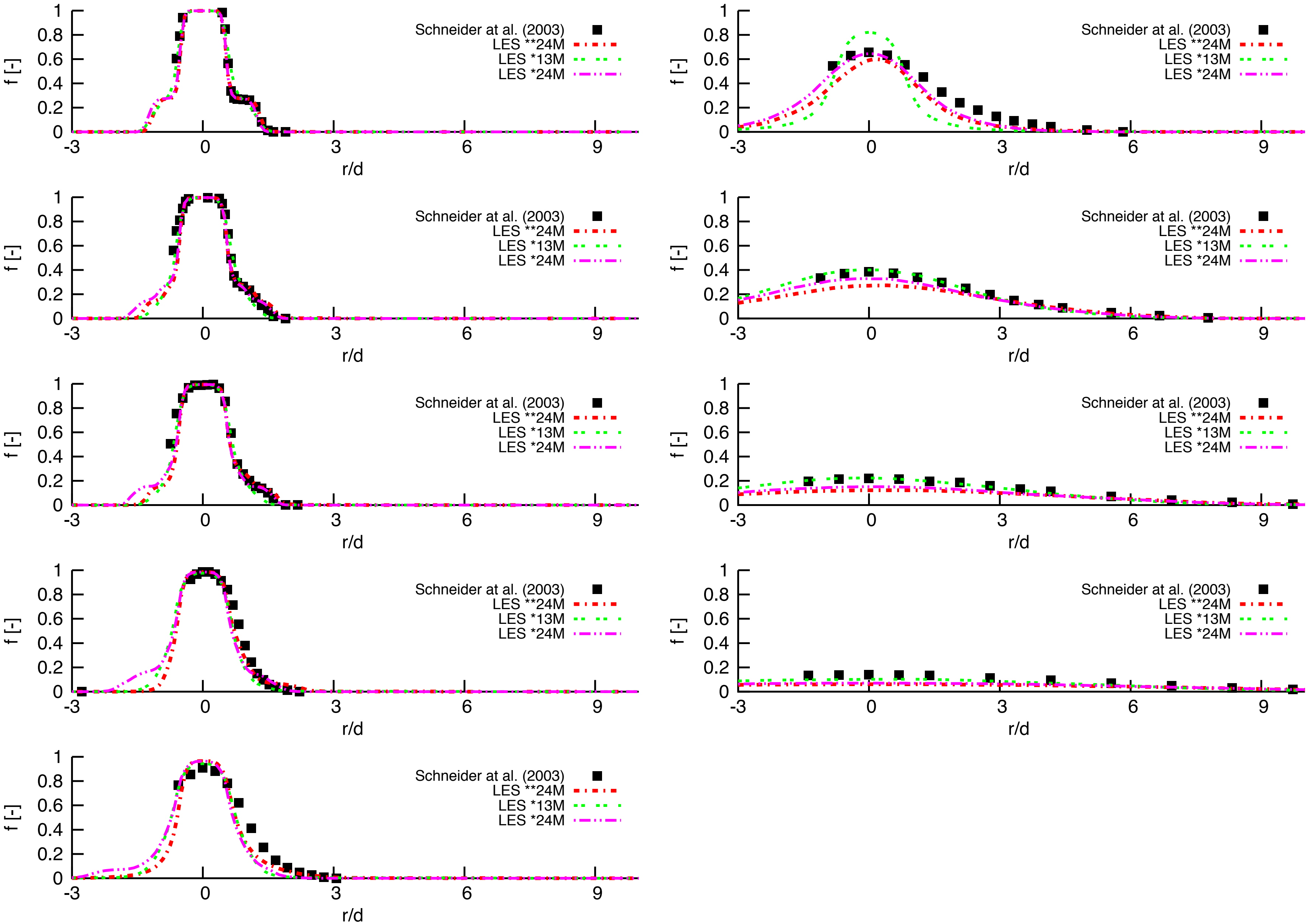


U_{jet}=49.6 m/s; Re=22400

25% CH_4, 75% Dry Air

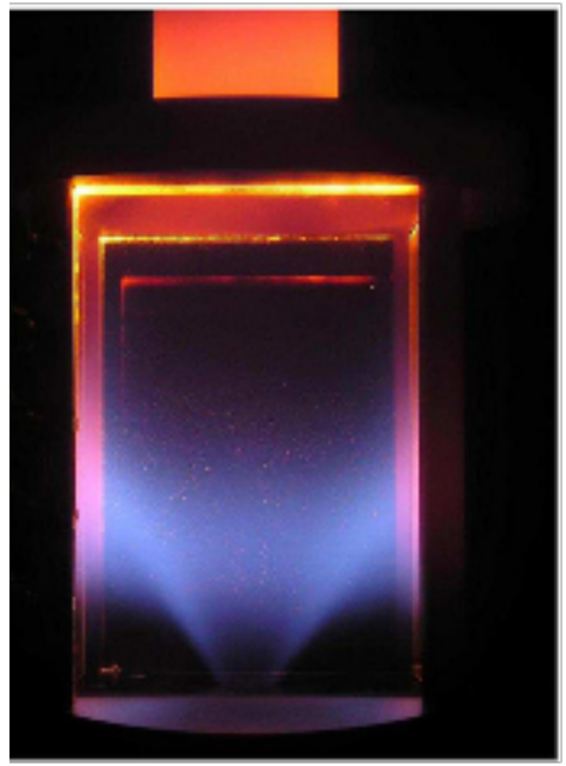
	# Cells
Mesh 1	13M
Mesh 2	24M
Mesh 3	50M

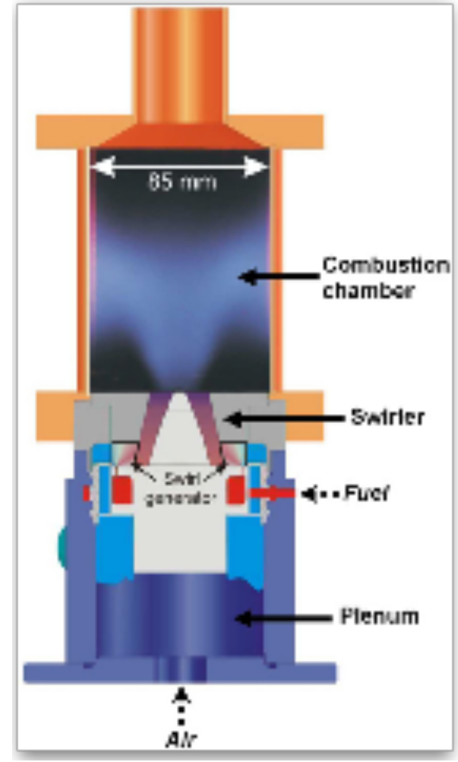
BIOMASS FOR ENERGY – Sandia D flame

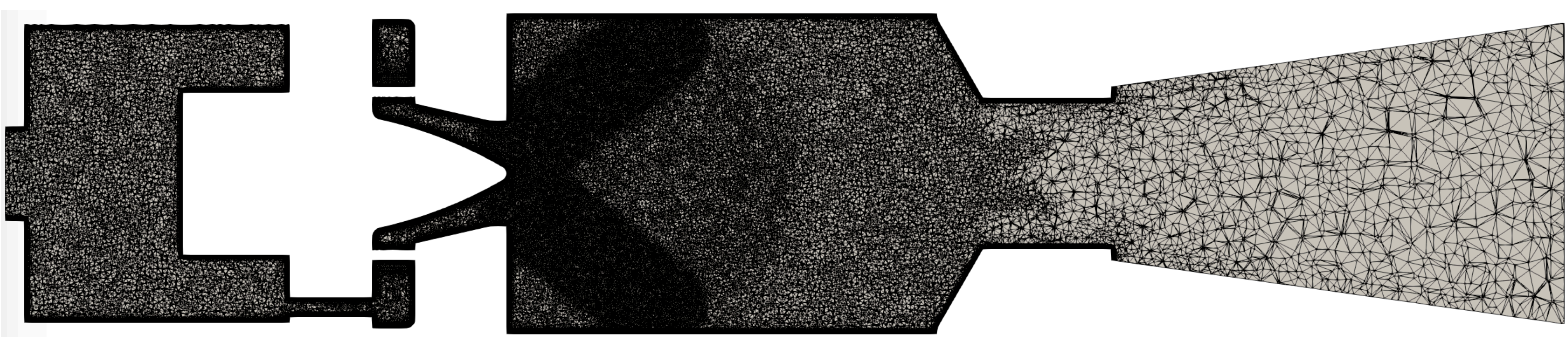


BIOMASS FOR ENERGY – PRECCINSTA setup

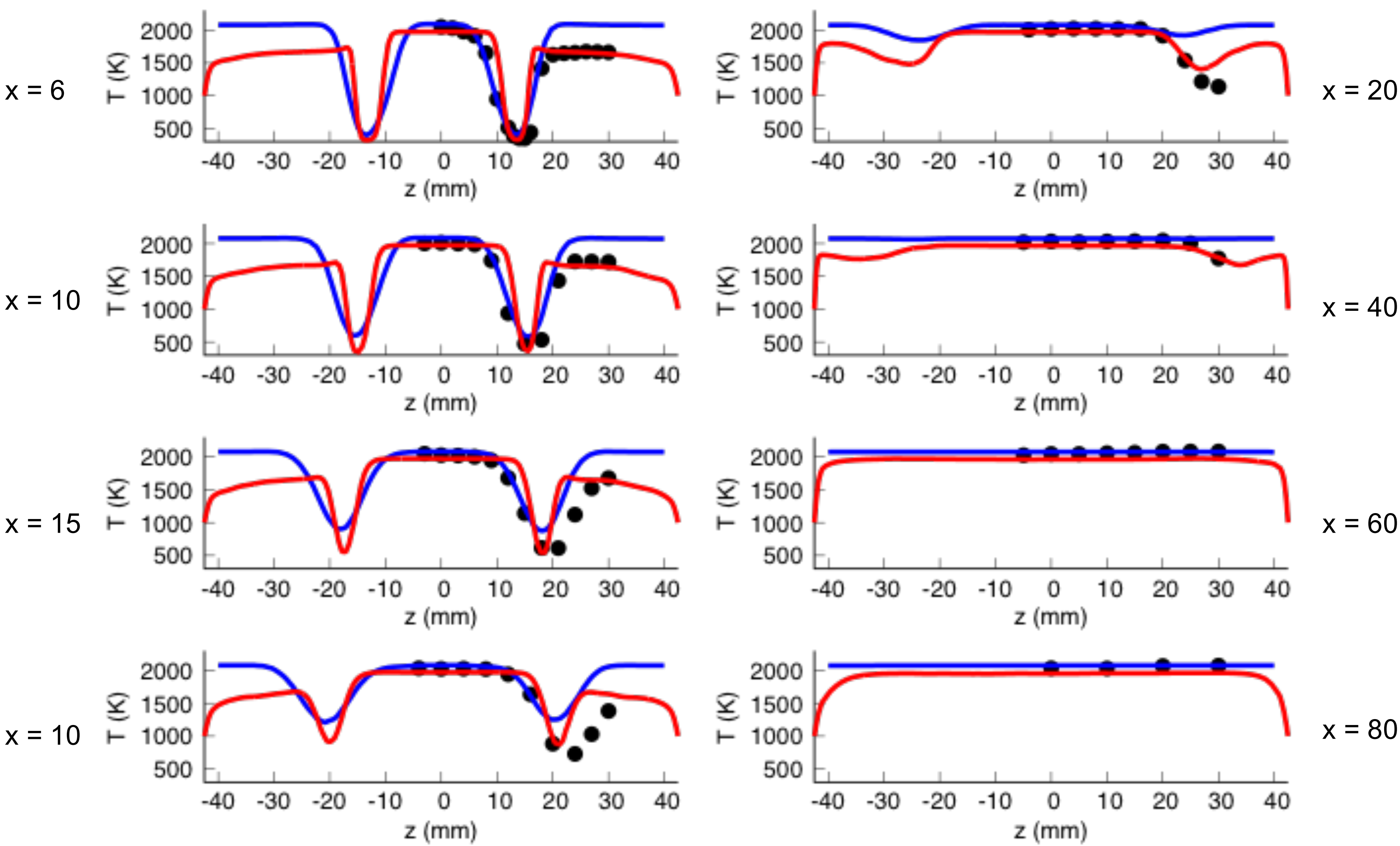
Fuel	$\dot{m}_{air}$ (g/s)	$\dot{m}_f$ (g/s)
CH_4	12.2366	0.5983
75% CH_4 25% CO_2	12.2366	1.1468
50% CH_4 50% CO_2	12.2366	2.2437
50% CH_4 40% CO_2 10% N_2	12.2366	2.1241





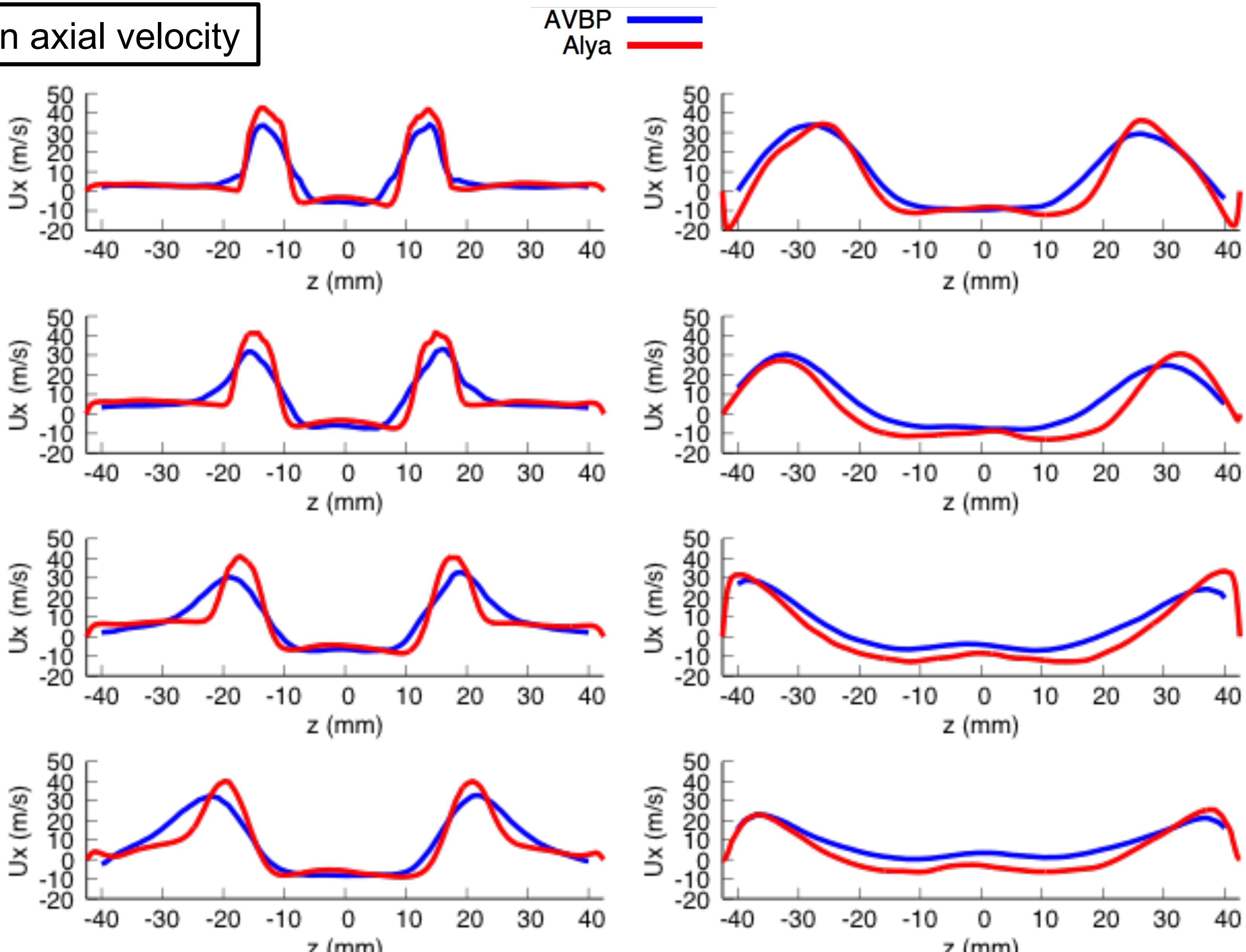


Mean Temperature



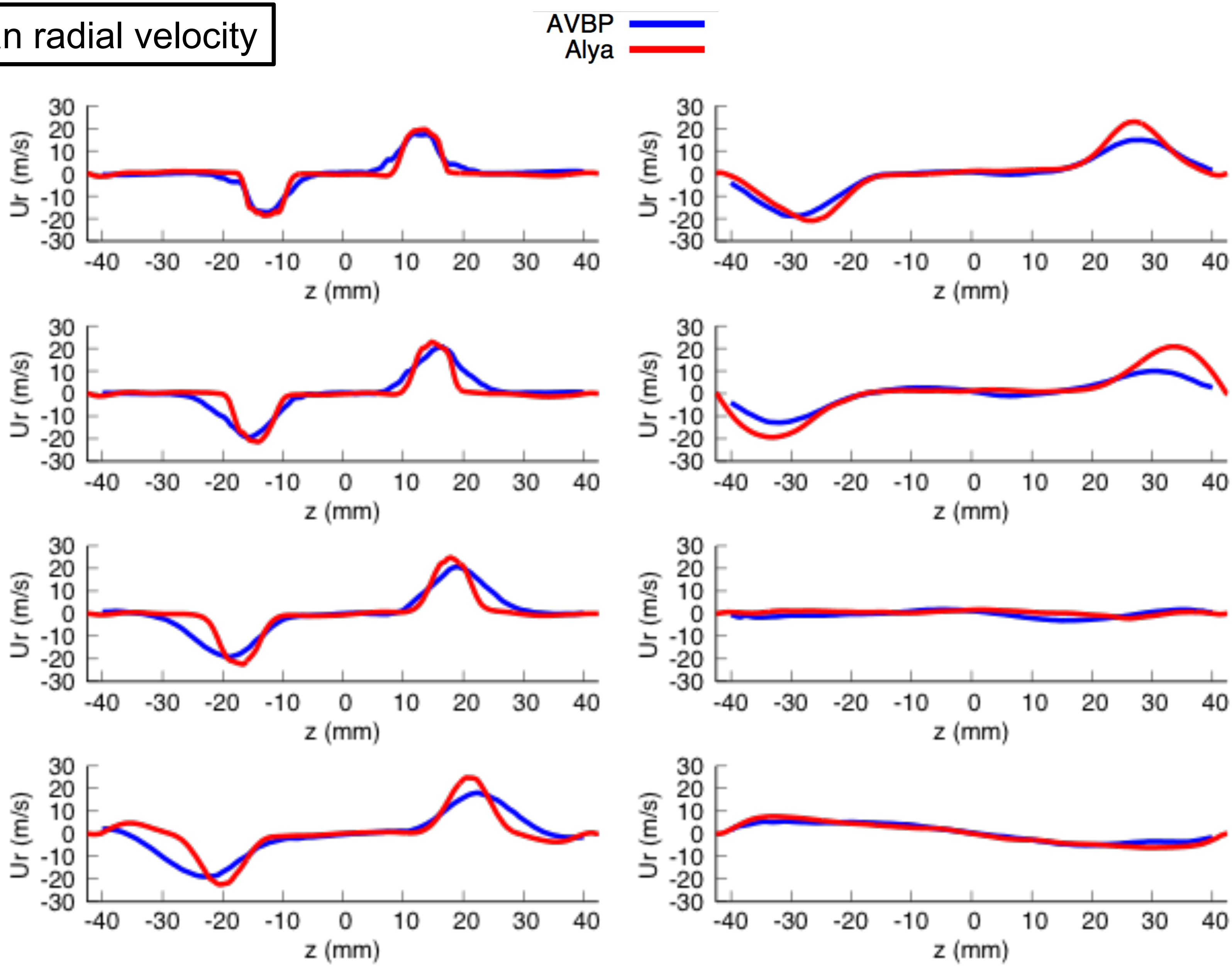
BIOMASS FOR ENERGY – PRECCINSTA CH4

Mean axial velocity



BIOMASS FOR ENERGY – PRECCINSTA CH4

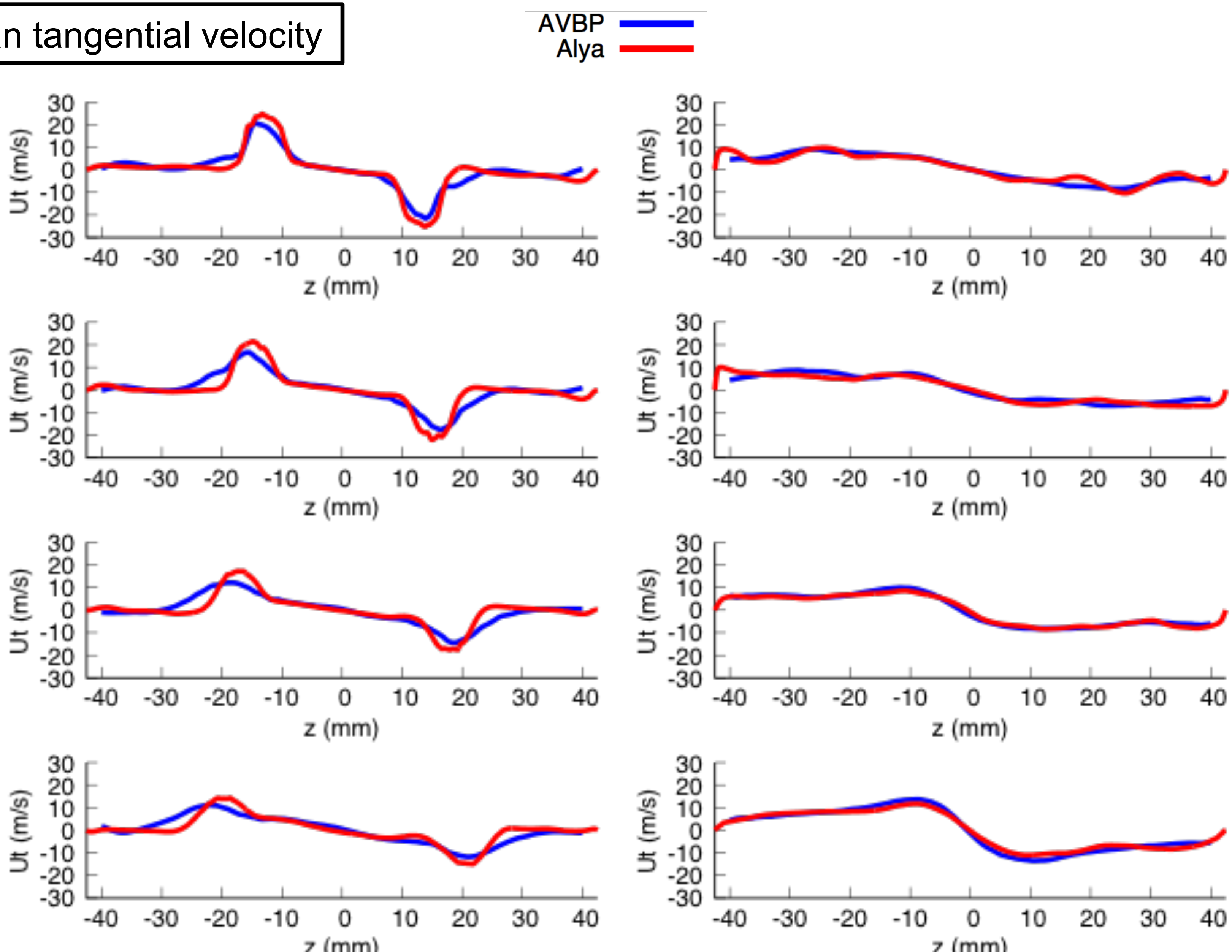
Mean radial velocity



BIOMASS FOR ENERGY – PRECCINSTA CH4

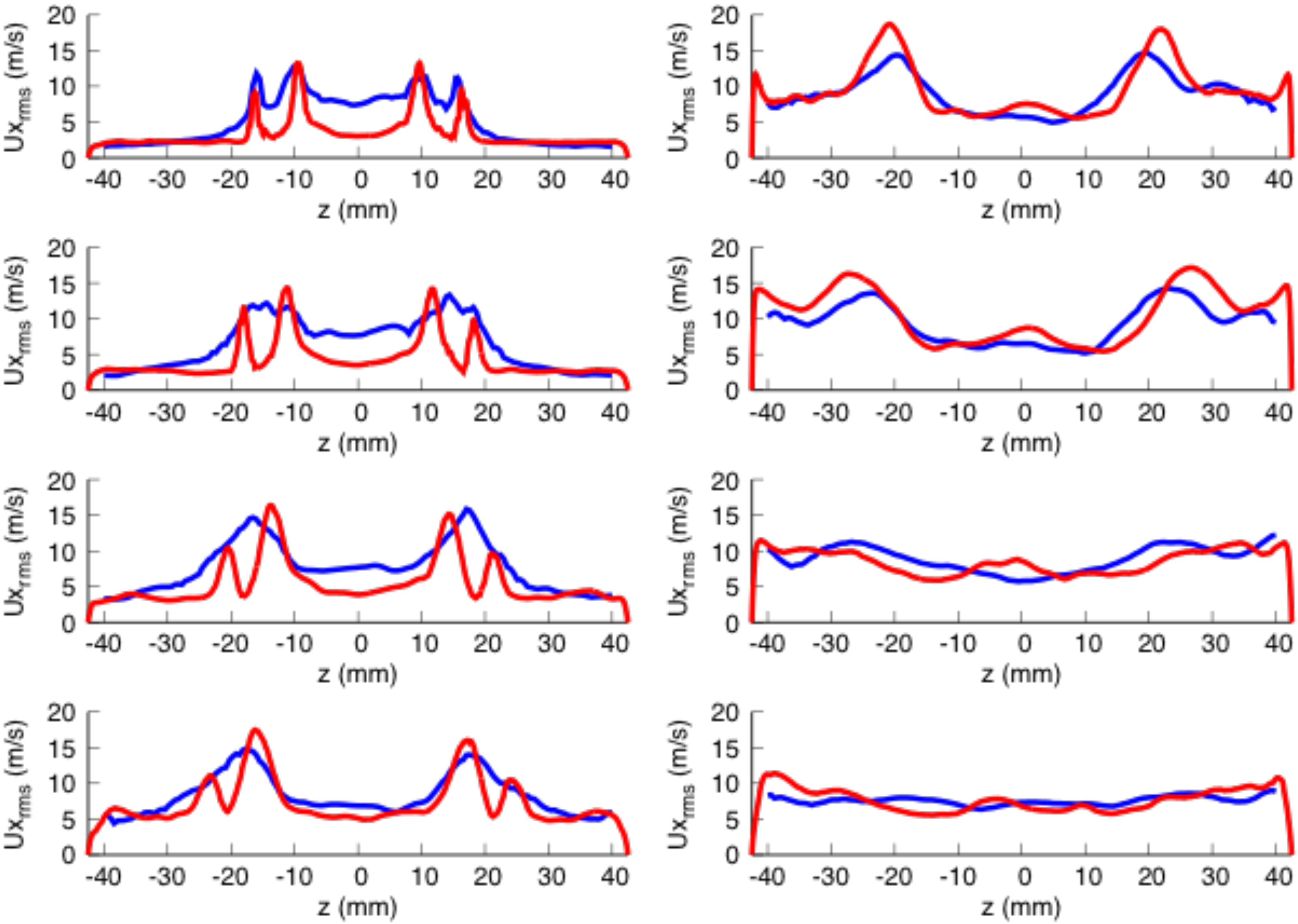
HPC

Mean tangential velocity



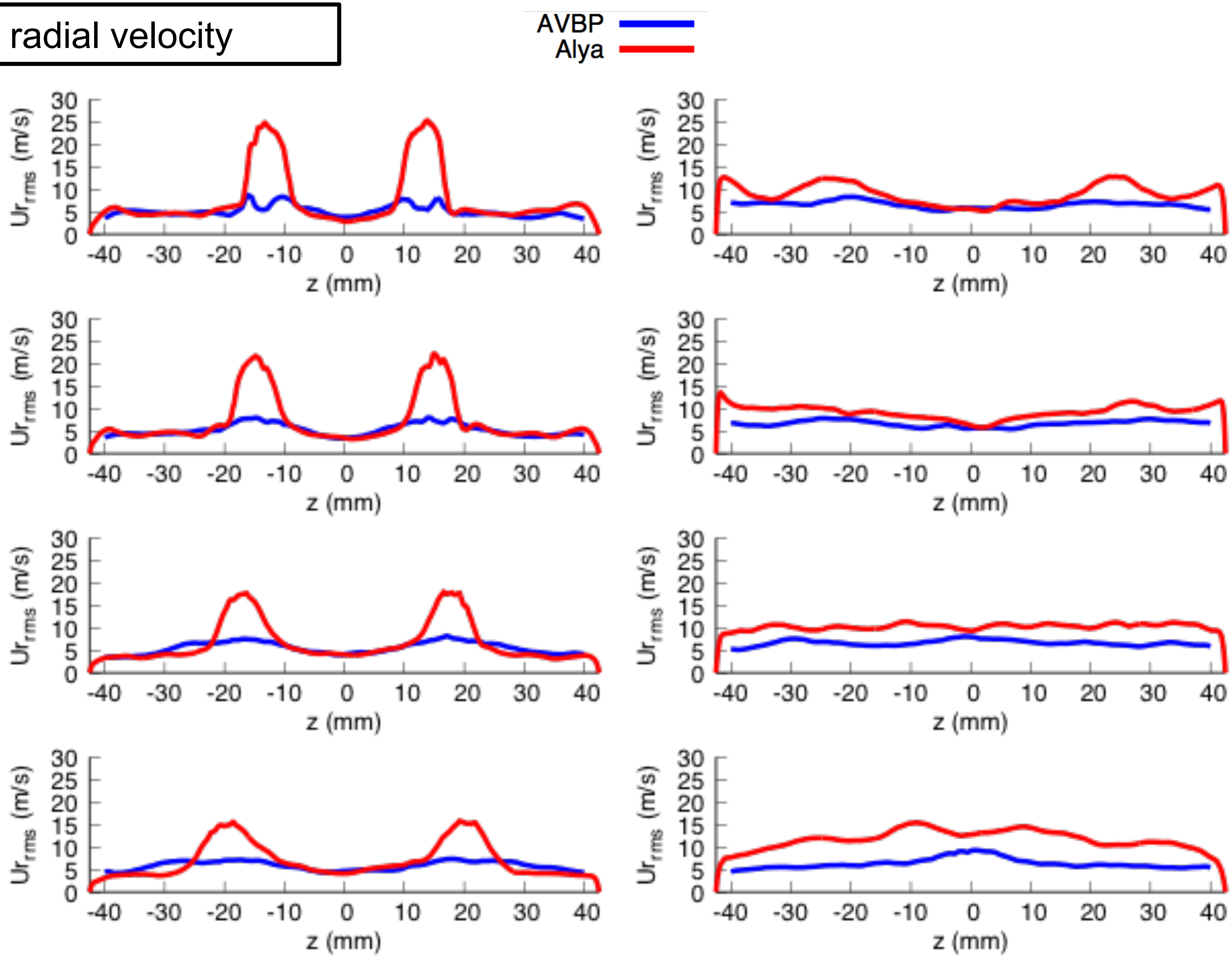
BIOMASS FOR ENERGY – PRECCINSTA CH4

Rms axial velocity

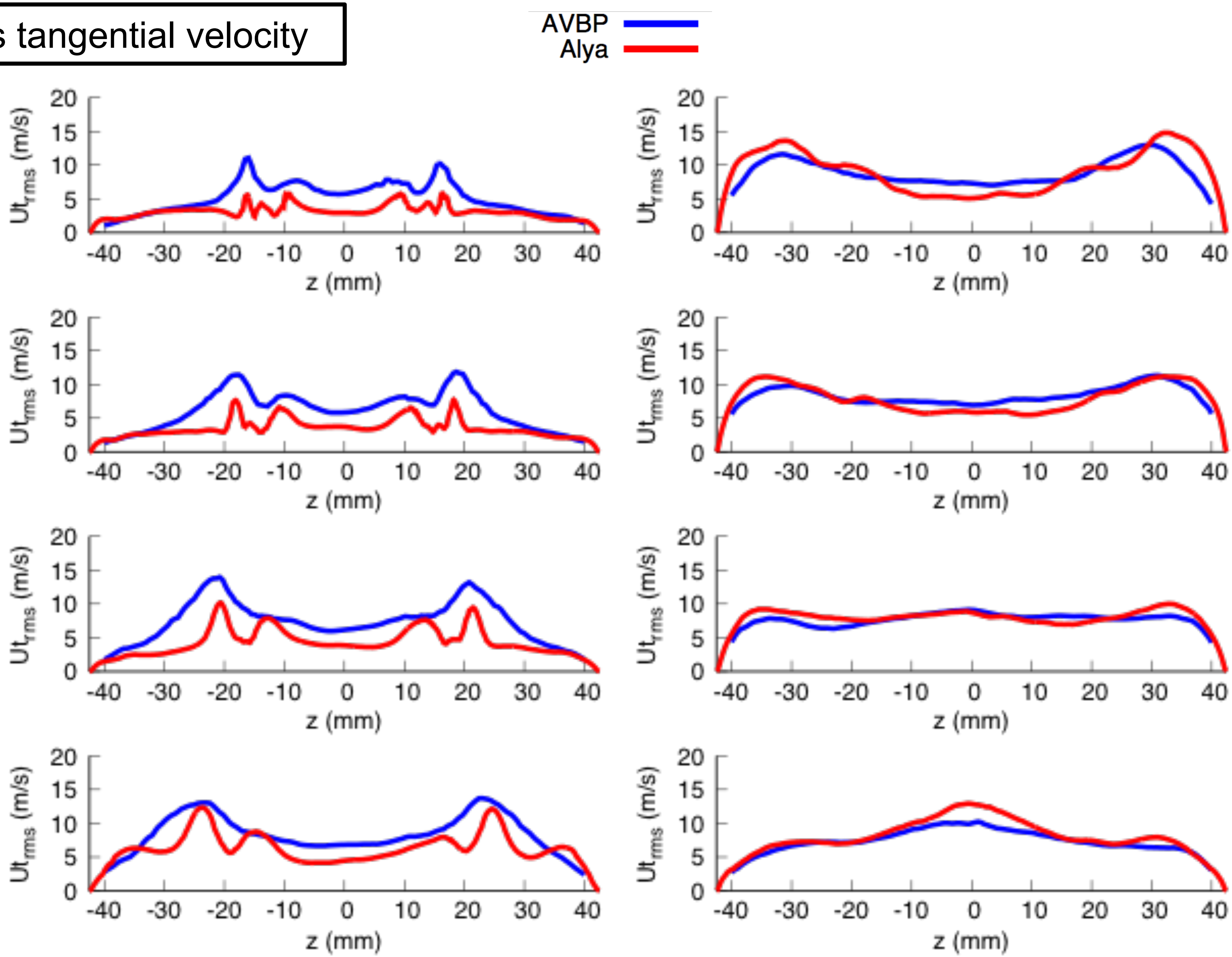


BIOMASS FOR ENERGY – PRECCINSTA CH4

Rms radial velocity

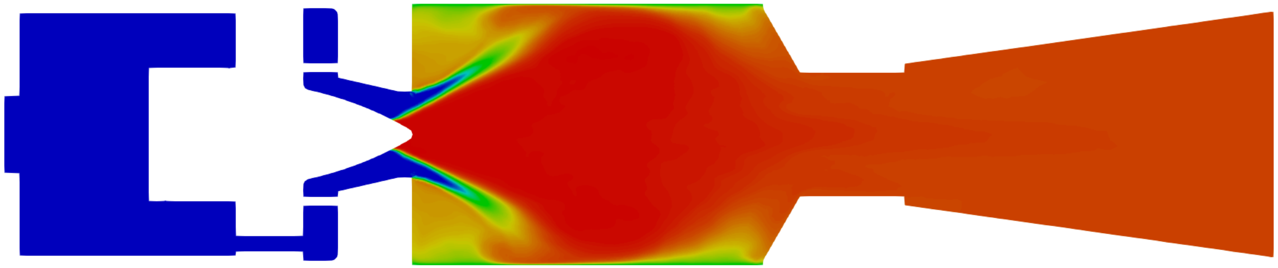


Rms tangential velocity

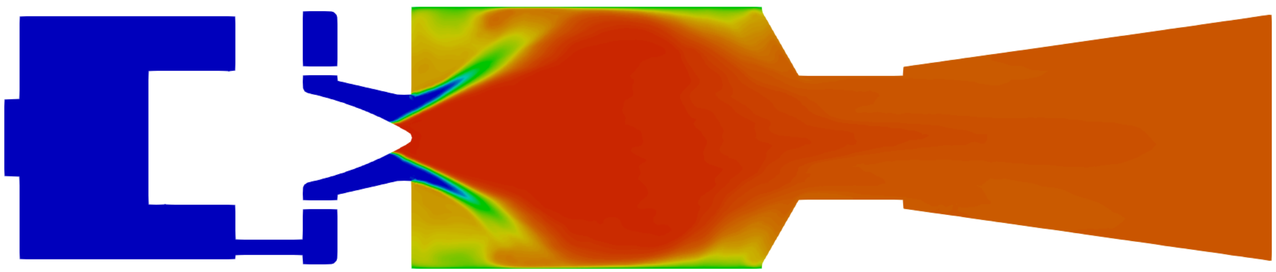


BIOMASS FOR ENERGY – Averaged temperature fields

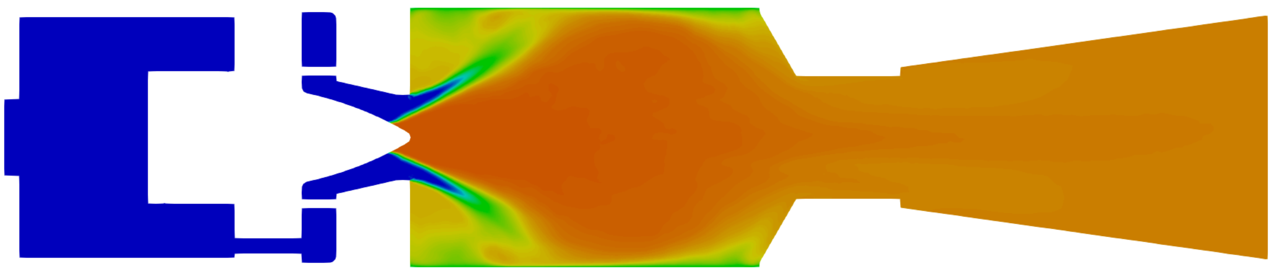
CH4:



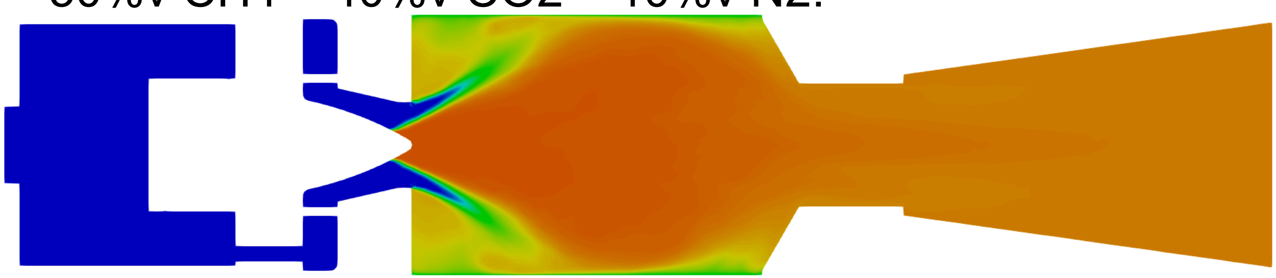
75%v CH4 – 25%v CO2:

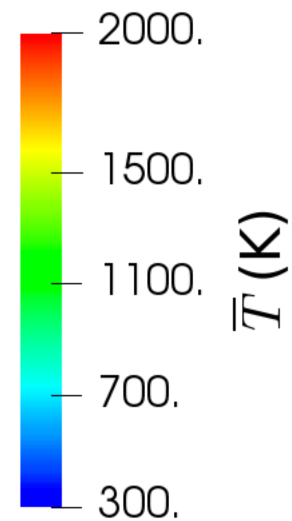


50%v CH4 – 50%v CO2:



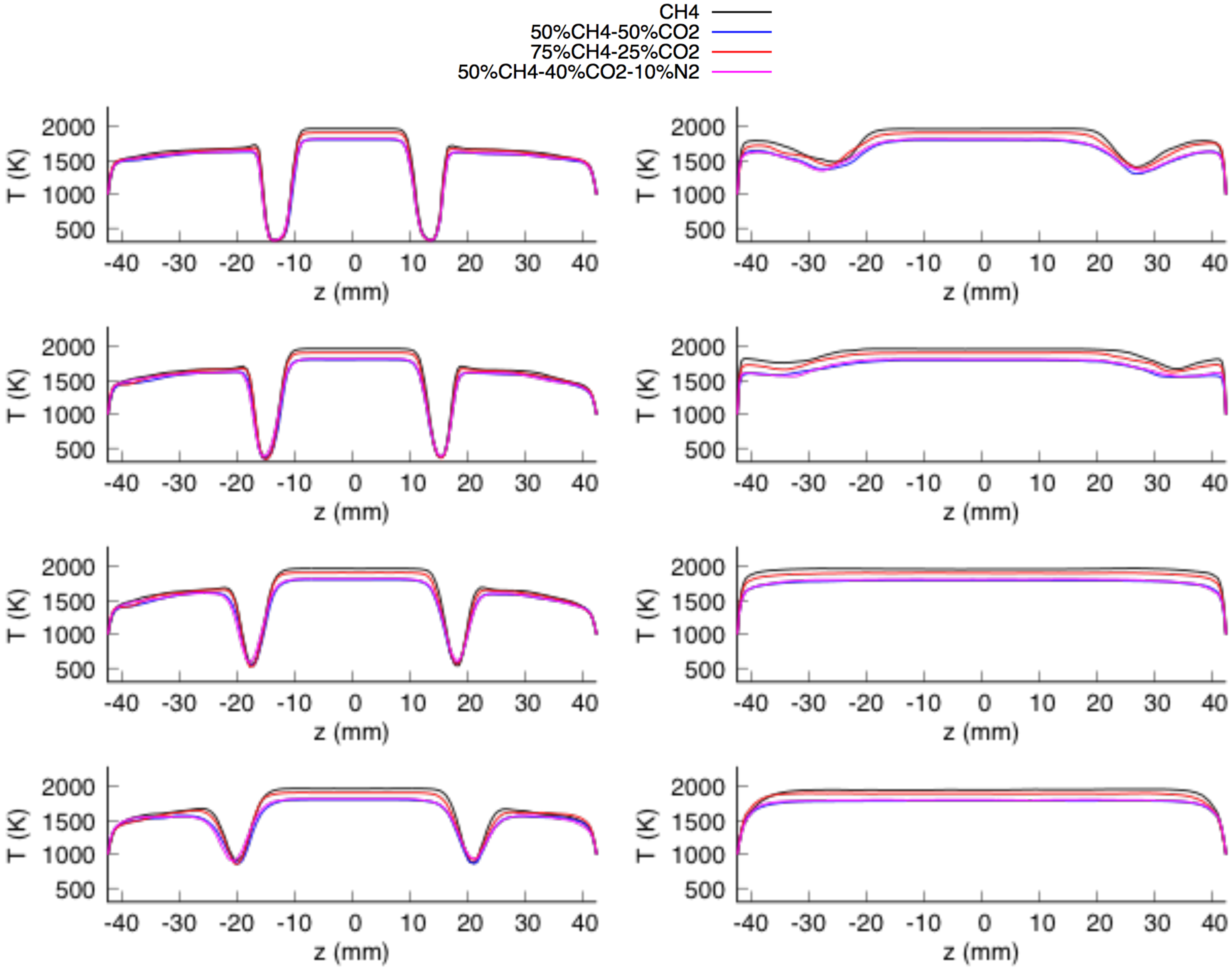
50%v CH4 – 40%v CO2 – 10%v N2:



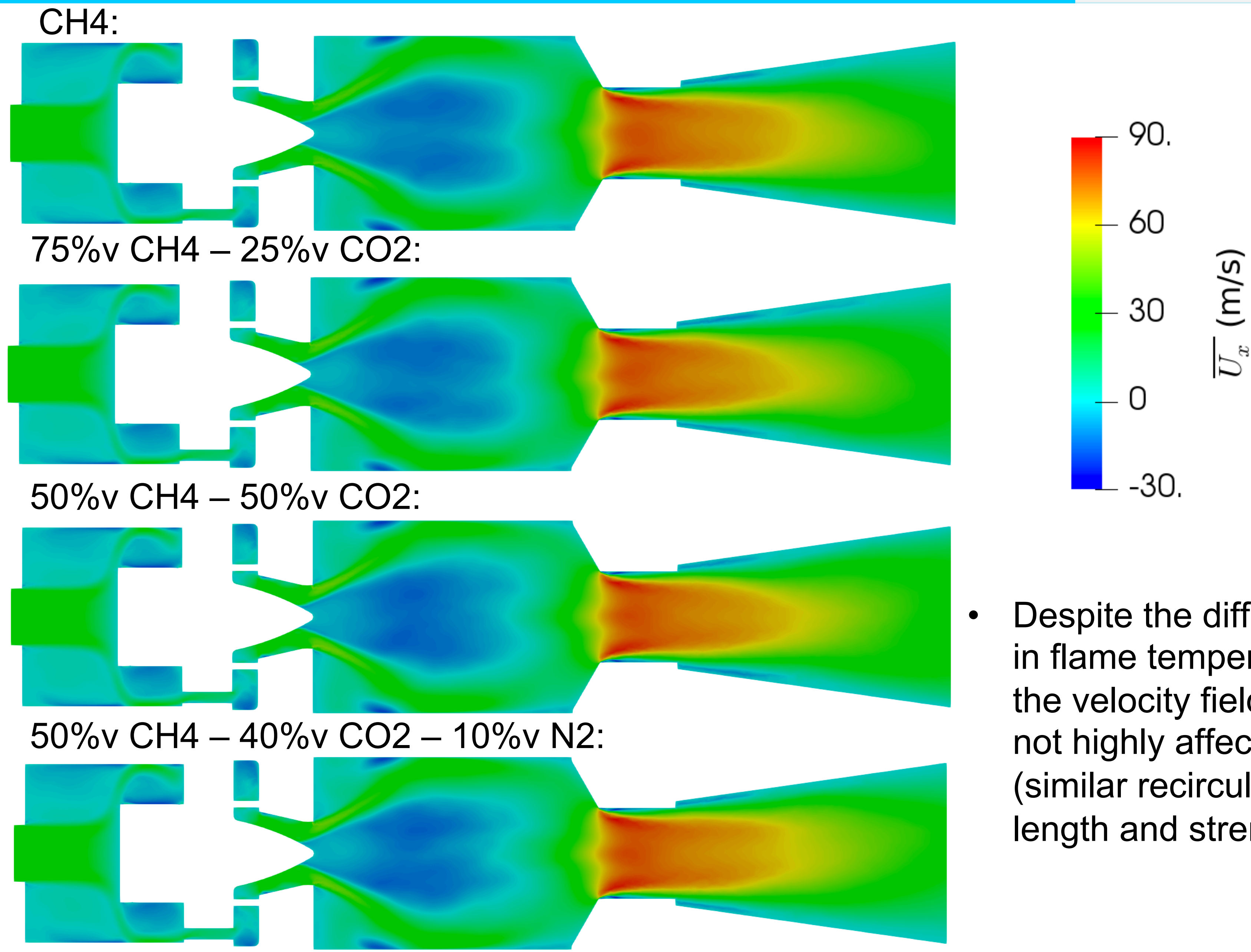


- Flame temperature decreases because of the dilution effect (lower NOx emissions)
- Reaction zone is more compact with higher CH_4 content

BIOMASS FOR ENERGY – Averaged temperature lines

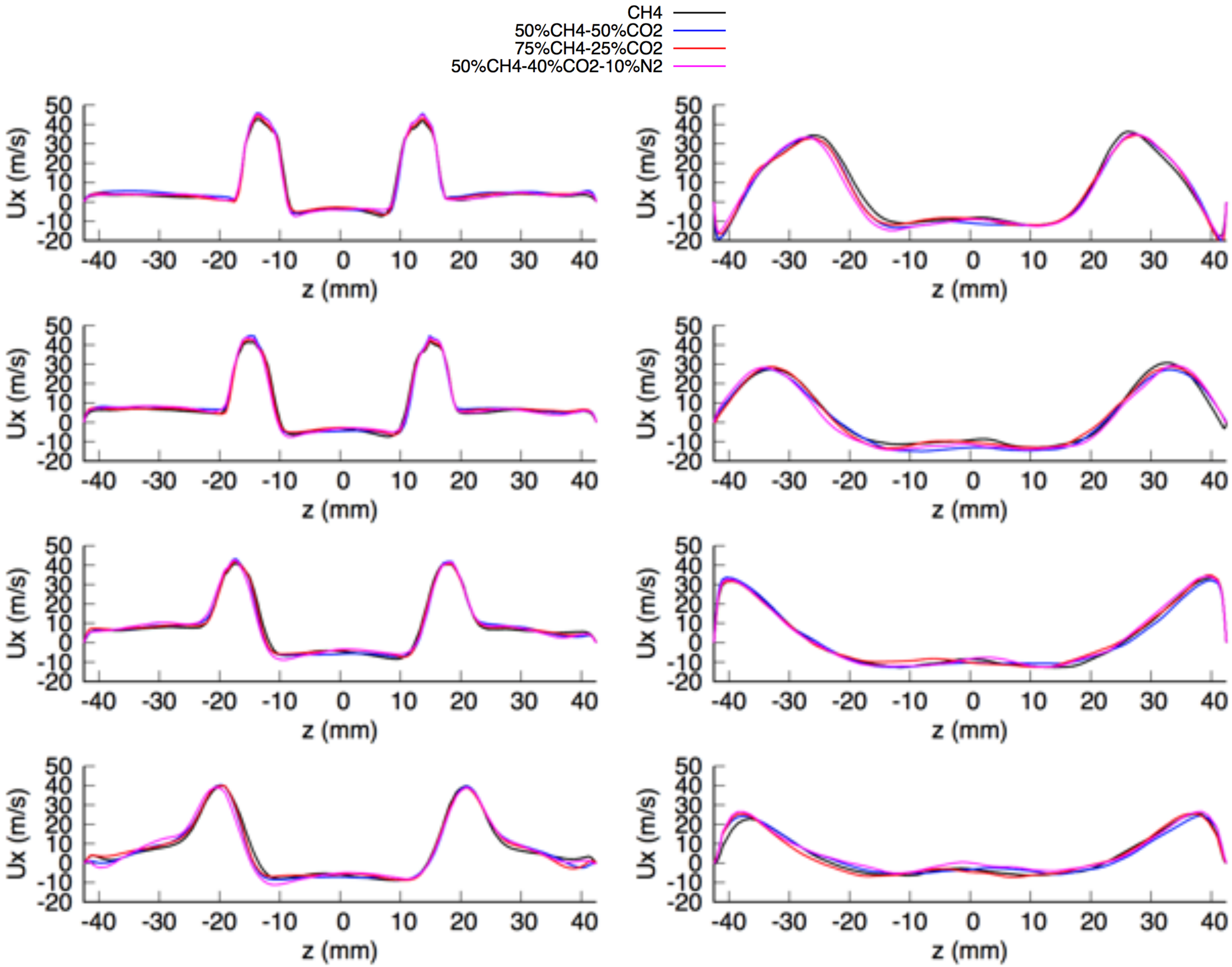


BIOMASS FOR ENERGY – Averaged velocity fields

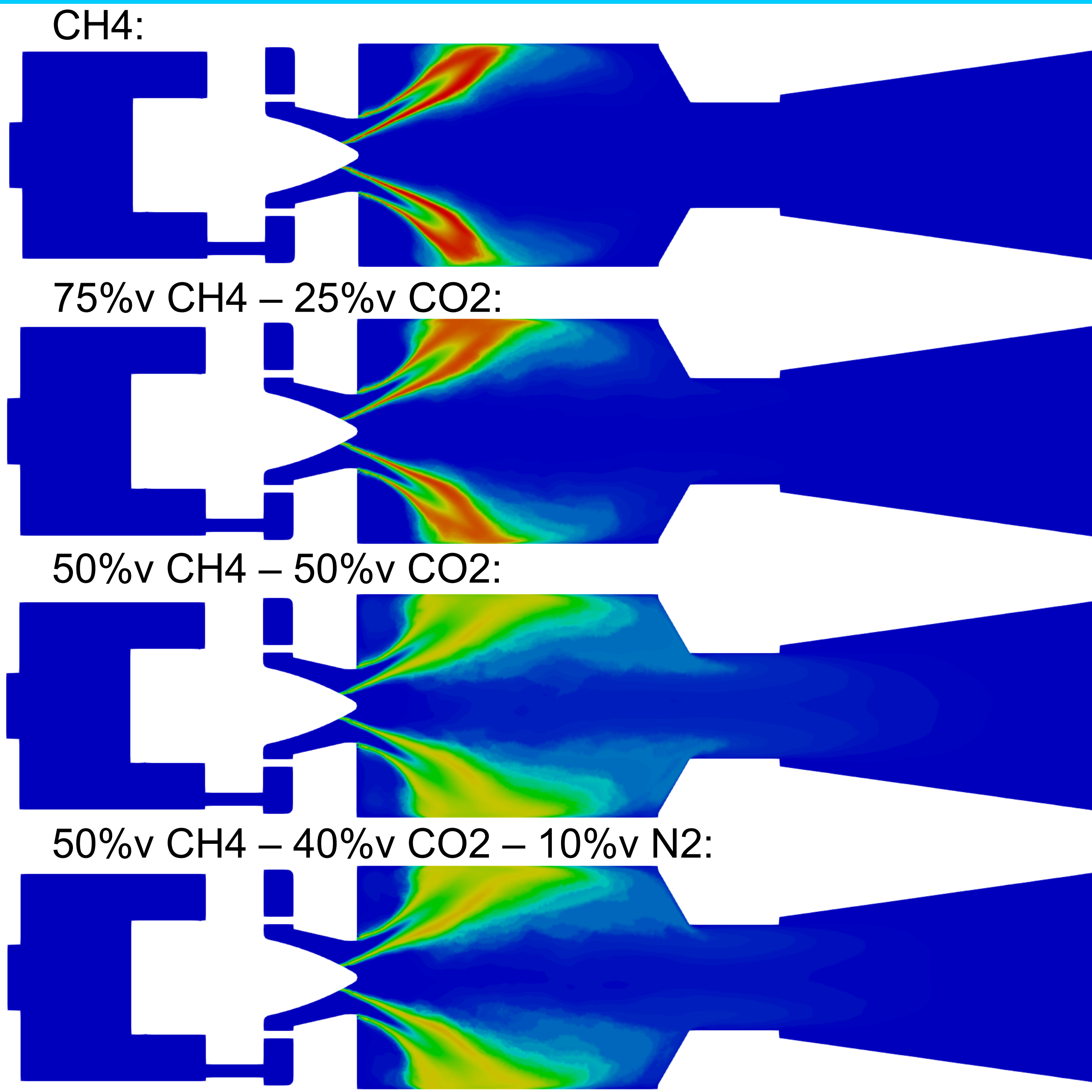


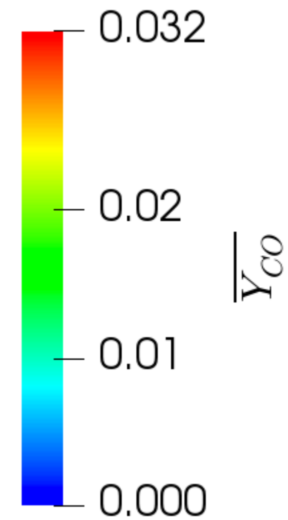
- Despite the difference in flame temperature, the velocity fields are not highly affected (similar recirculation length and strength)

BIOMASS FOR ENERGY – Averaged velocity lines



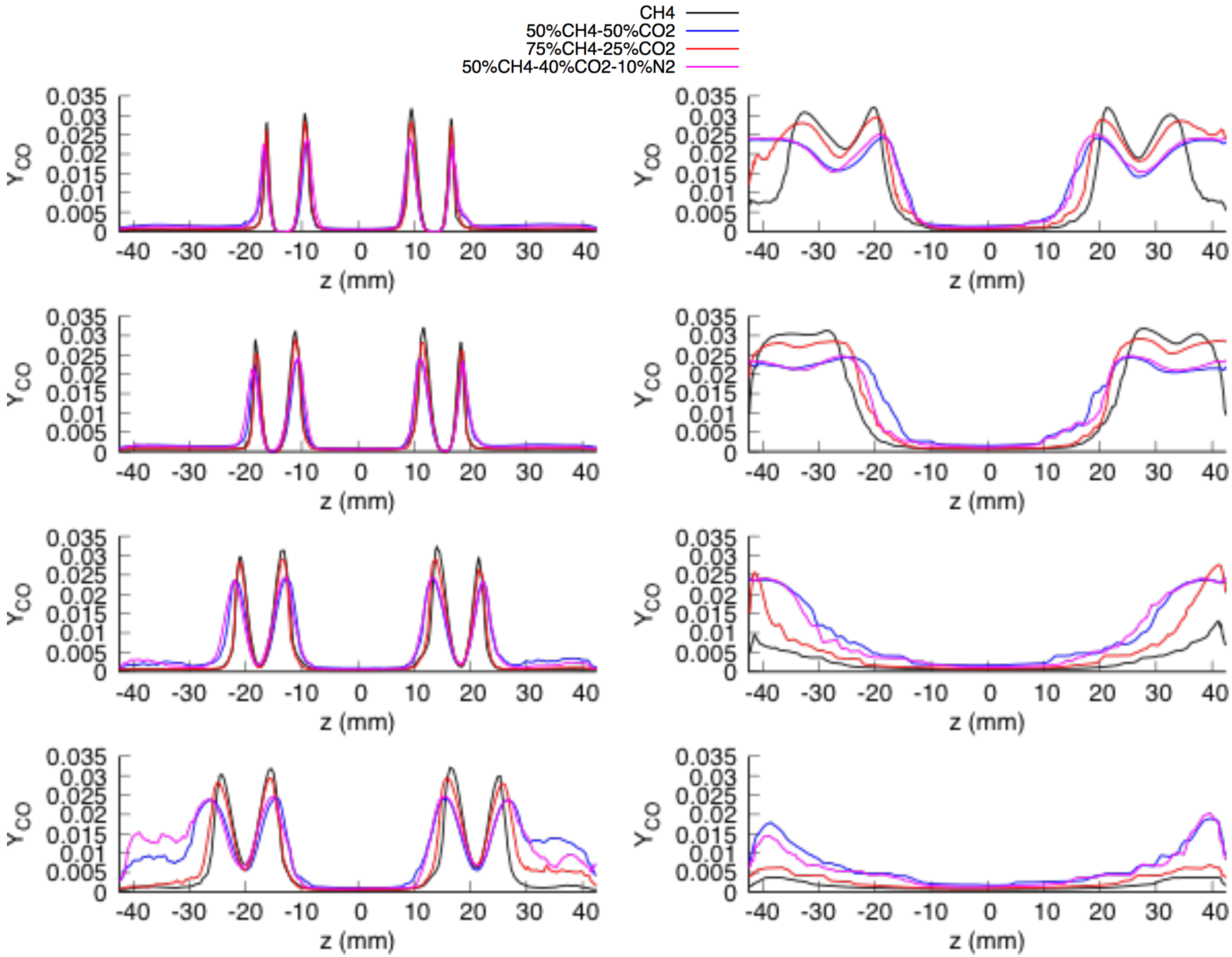
BIOMASS FOR ENERGY – Averaged CO fields



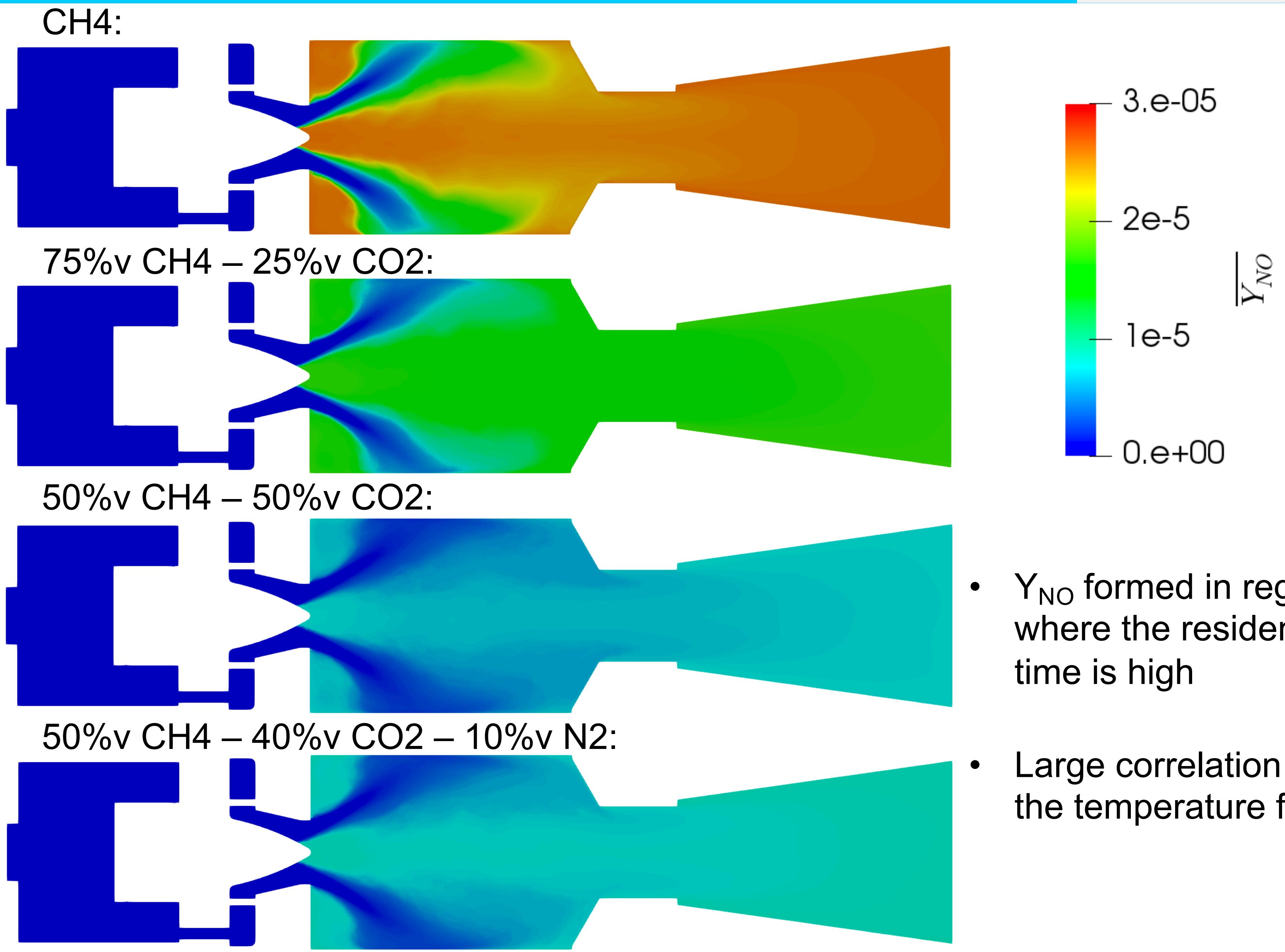


- Higher flame-wall interaction for lower CH_4 content
- Maximum CO reduces with the dilution, but mean value at the exit is higher

BIOMASS FOR ENERGY – Averaged CO lines

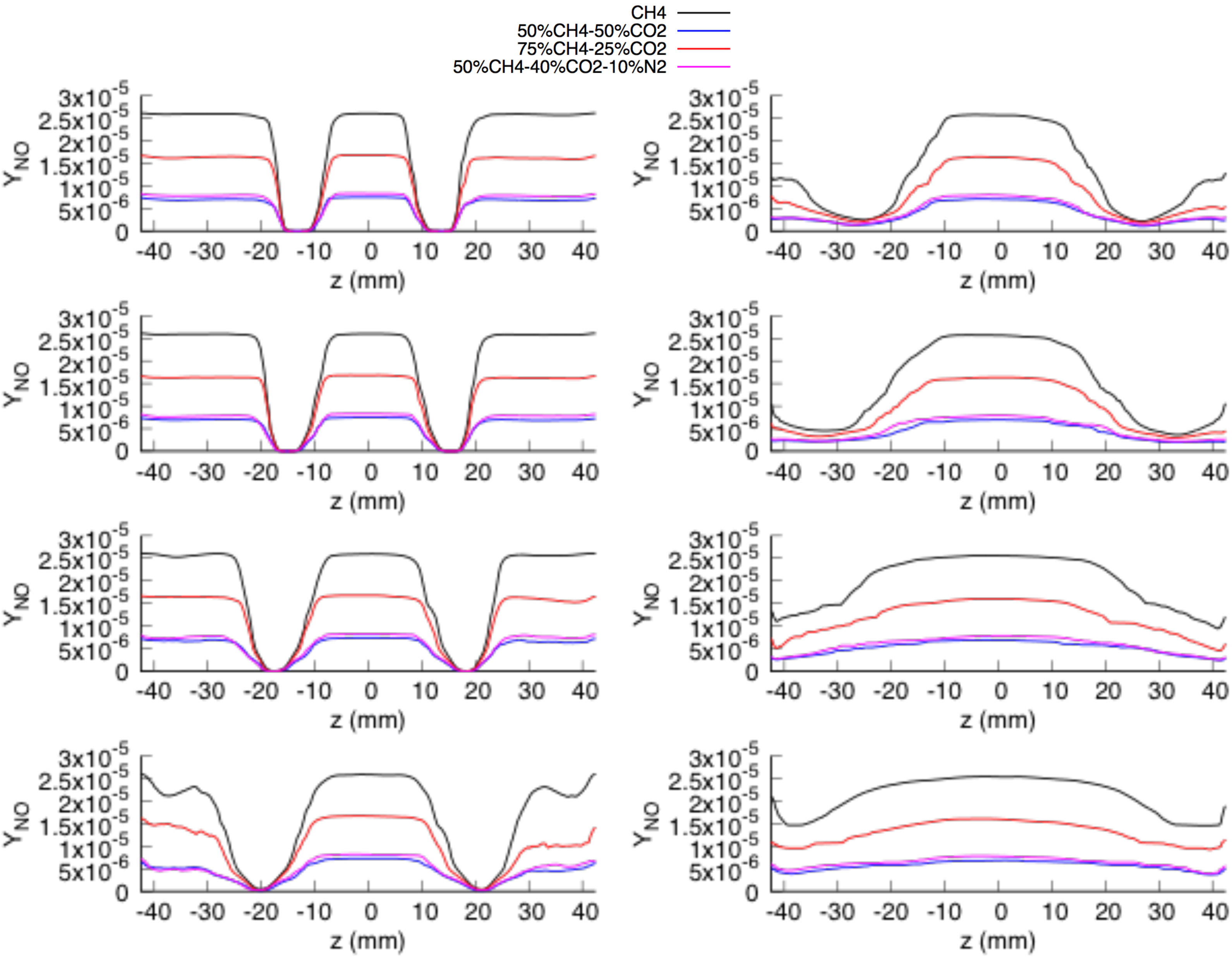


BIOMASS FOR ENERGY – Averaged NO fields

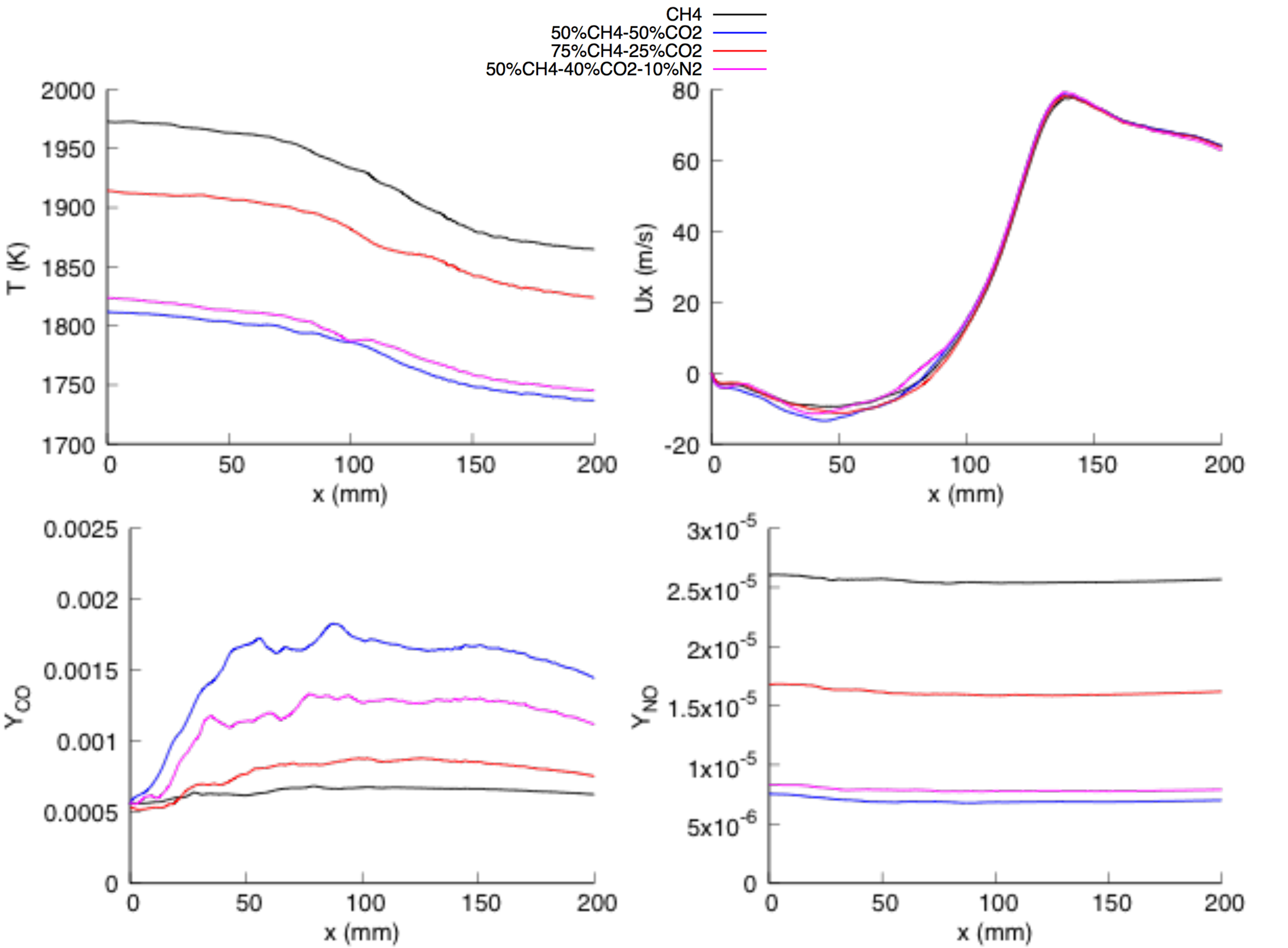


- Y_{NO} formed in regions where the residence time is high
- Large correlation with the temperature fields

BIOMASS FOR ENERGY – Averaged NO lines



BIOMASS FOR ENERGY – Axial line



- Alya has a high potential for performing **large-scale simulations** of practical combustion systems.
- The turbulent combustion model uses **tabulated source terms and properties** that depend on the progress variable, the mixture fraction, their variances and a non-dimensional enthalpy
- Model gives reasonable results when compared to experimental data
- Despite the difference in flame temperature, the velocity fields are not highly affected by the fuel type

- Simulations with a non-premixed setup should introduce further velocity discrepancies between the cases
- Combination of premixed tables with diffusion tables can potentially improve the accuracy of the results

BIOMASS FOR ENERGY – Acknowledgements

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