Towards optimization of reactive flows in SU2

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Bosch – Overview
Corporate Research – RTC-NA

America
Research and Technology Center North America

130 associates

Europe
- Corporate Research Germany
- Research and Technology Office Russia
- Research and Technology Office Tel Aviv

1,400 associates

Asia-Pacific
- Research and Technology Center India
- Research and Technology Center Asia-Pacific

110 associates

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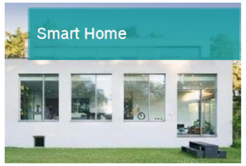
Bosch – Overview
Thermotechnology – Residential Heating

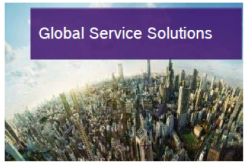
402,166
Bosch associates make these solutions possible

60 countries
–
440 regional subsidiaries

Four business sectors

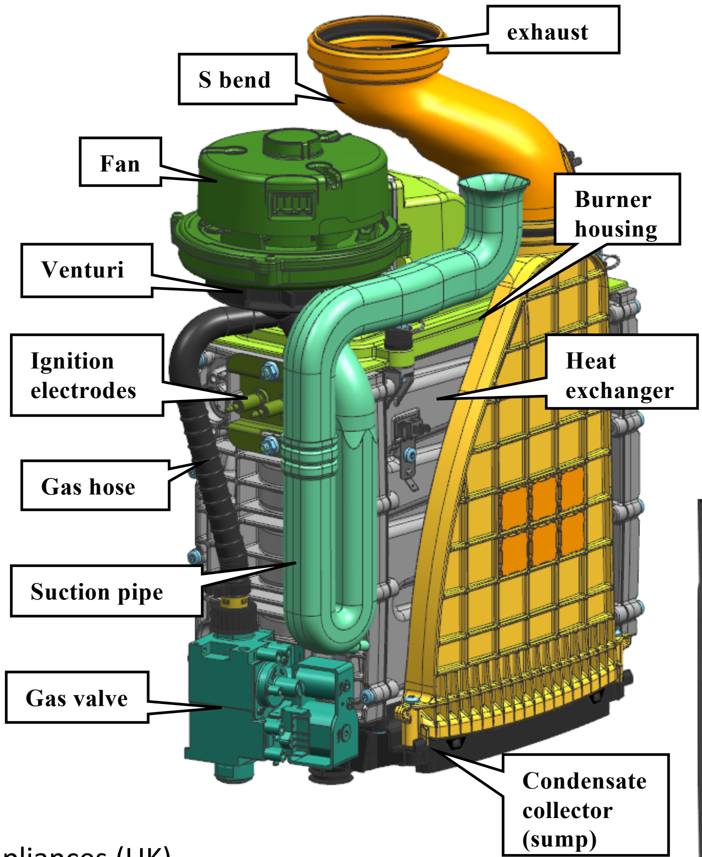
- Mobility Solutions
- Industrial Technology
- Energy & Building Technology
- Consumer Goods

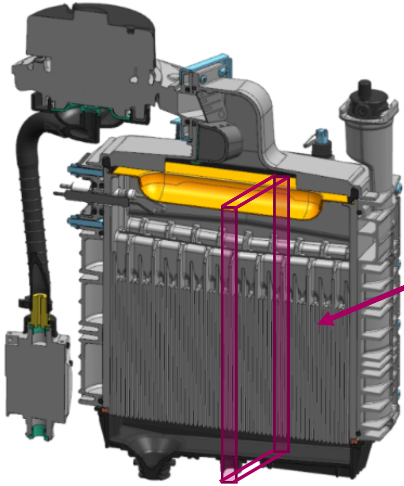




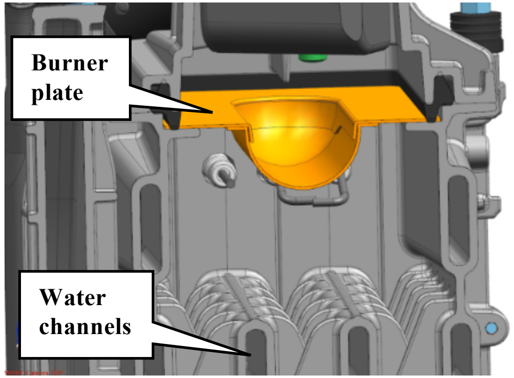
Bosch Thermotechnology – Residential Heating

Domestic wall mounted boiler with WB7 heat exchanger





A slice of the heat exchanger is simulated to assess performance and improve design



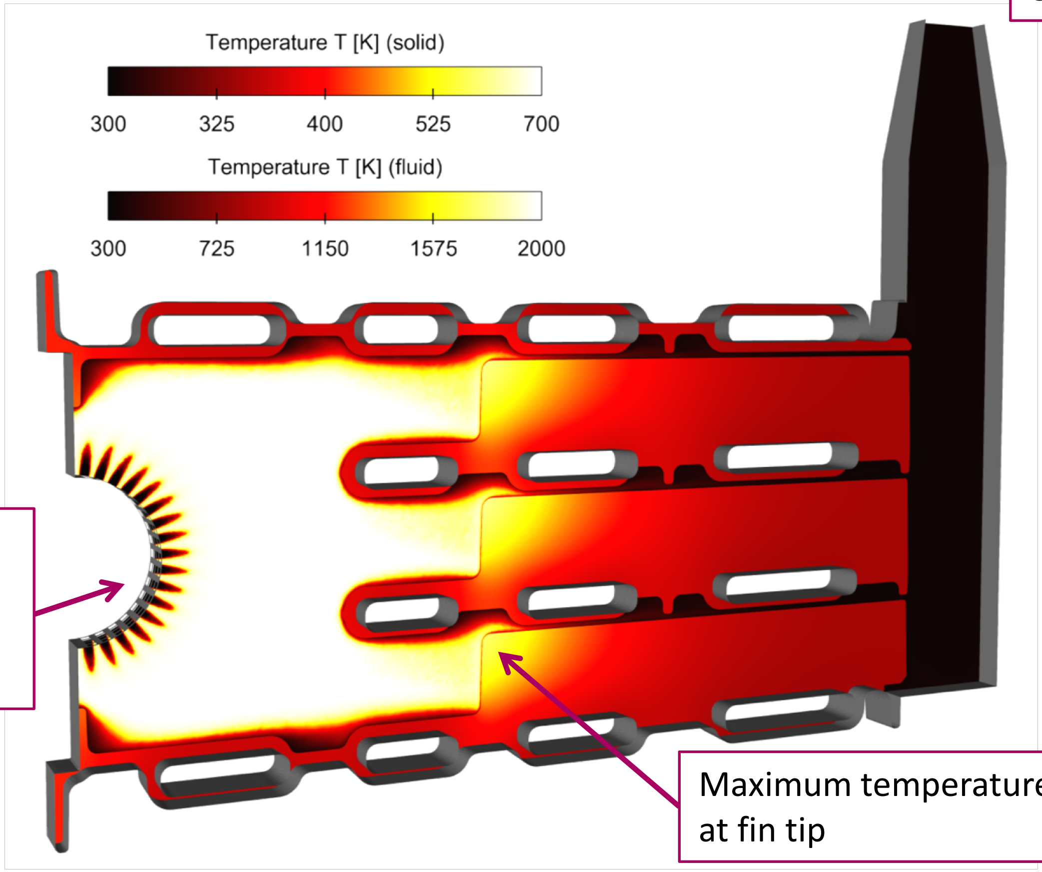
- WB7 Heat exchanger (7-37 kW)
- Used in Trendline (NL) and Greenstar appliances (UK)

We want a good estimate of emissions (CO,NO_x) in early stages of development

Prediction and reduction of emissions in domestic boilers

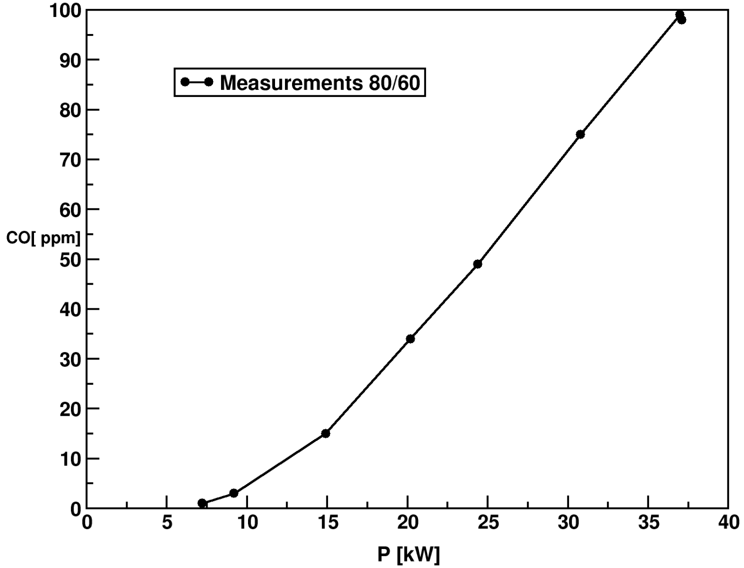
How much CO,NO_x is produced?

How much CO at the exit?



Adiabatic burner wall: attached flames

Maximum temperature at fin tip



We want a good estimate of emissions (CO,NO_x) in early stages of development

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Prediction and reduction of emissions in domestic boilers

For combustion simulations we need the chemical reactions

Detailed description of methane-air combustion consists of many reactions involving many species being produced during the reaction, e.g. The GRI-3.0 mechanism from Berkeley:

53 SPECIES: H2 H O O2 OH H2O HO2 H2O2 C CH CH2 CH2(S) CH3 CH4 CO CO2 HCO CH2O CH2OH CH3O CH3OH C2H C2H2 C2H3 C2H4 C2H5 C2H6 HCCO CH2CO HCCOH N NH NH2 NH3 NNH NO NO2 N2O HNO CN HCN H2CN HCNN HCNO HOCN HNCO NCO N2 AR C3H7 C3H8 CH2CHO CH3CHO

- **325 reactions**:
- (1) O+H2<=>H+OH
- (2) O+HO2<=>OH+O2
- (3) O+H2O2<=>OH+HO2
- ...
- (325) CH3+C3H7<=>2C2H5

Solving 53 transport equations for the species is too expensive for industrial 3D CFD simulations

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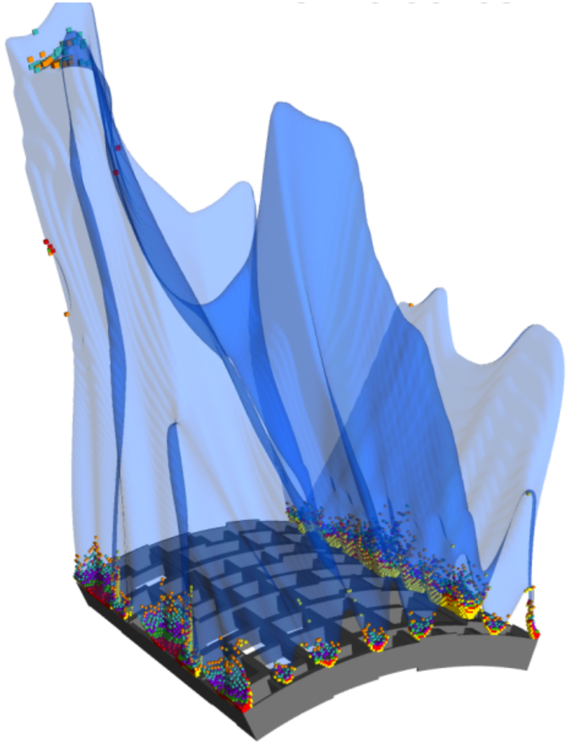
Prediction and reduction of emissions in domestic boilers

General idea of flamelets: observation

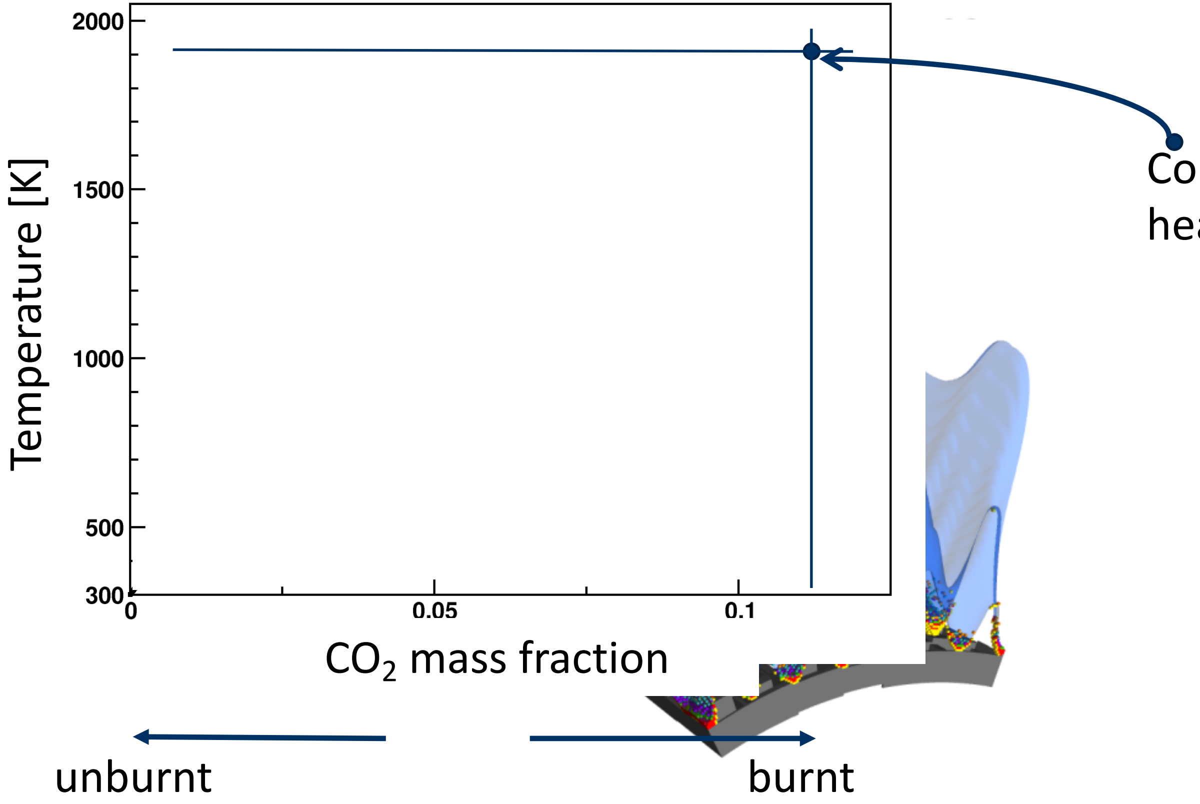


Consider an adiabatic flame, where no heat losses occur

Flame properties (temperature, concentrations) are complex structures in 3D

Prediction and reduction of emissions in domestic boilers

General idea of flamelets: observation



Consider an adiabatic flame, where no heat losses occur

Plot temperature etc. as function of a combustion progress variable, e.g. CO_2

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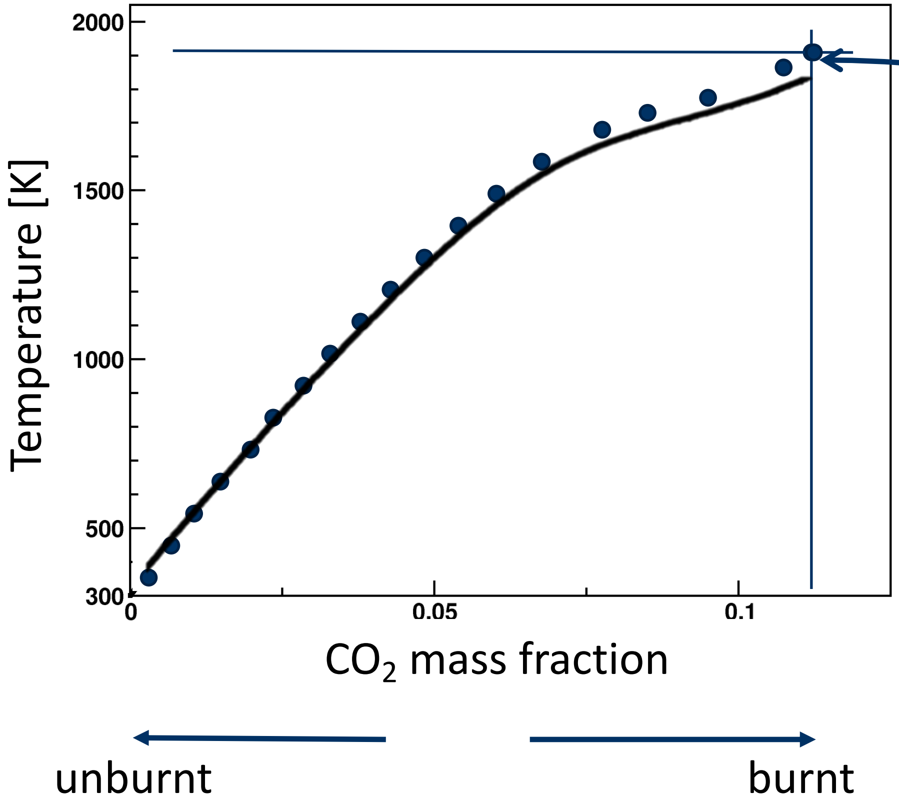
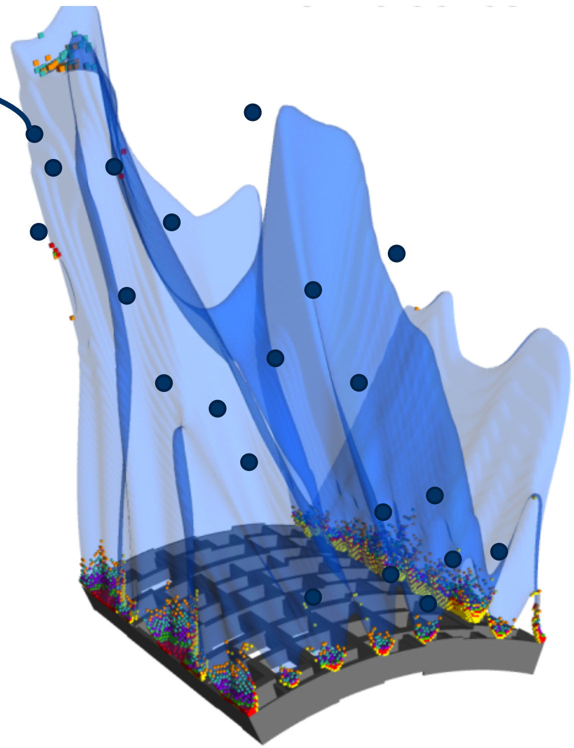
Prediction and reduction of emissions in domestic boilers

General idea of flamelets: observation

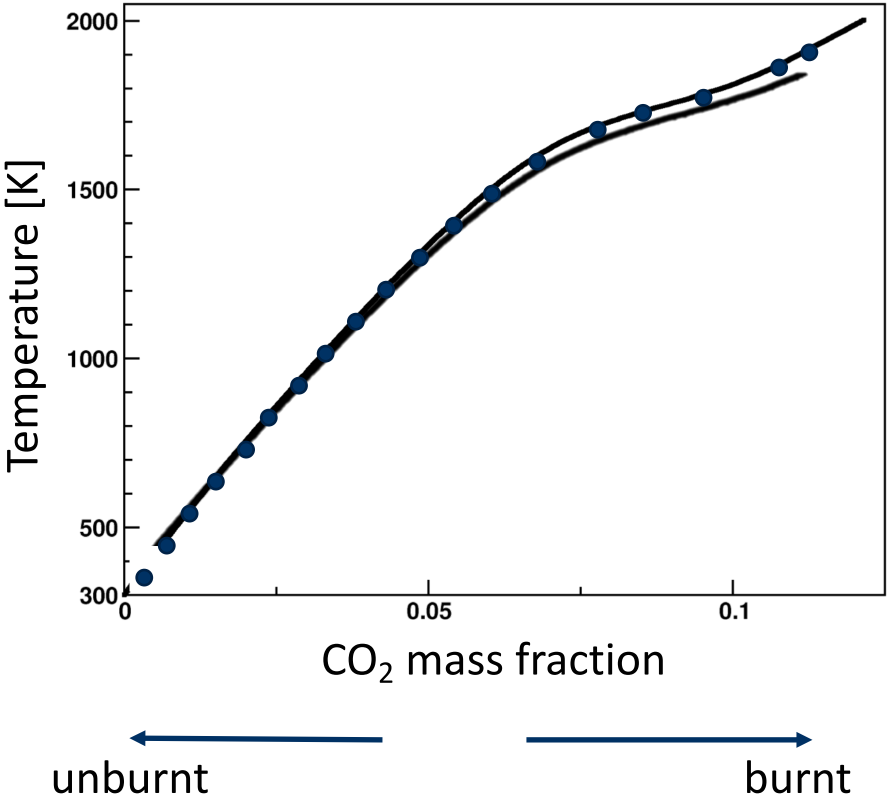




All points fall on a single line: flames are one-dimensional in progress variable space

Prediction and reduction of emissions in domestic boilers

General idea of flamelets: observation



Enthalpy is constant in adiabatic flame

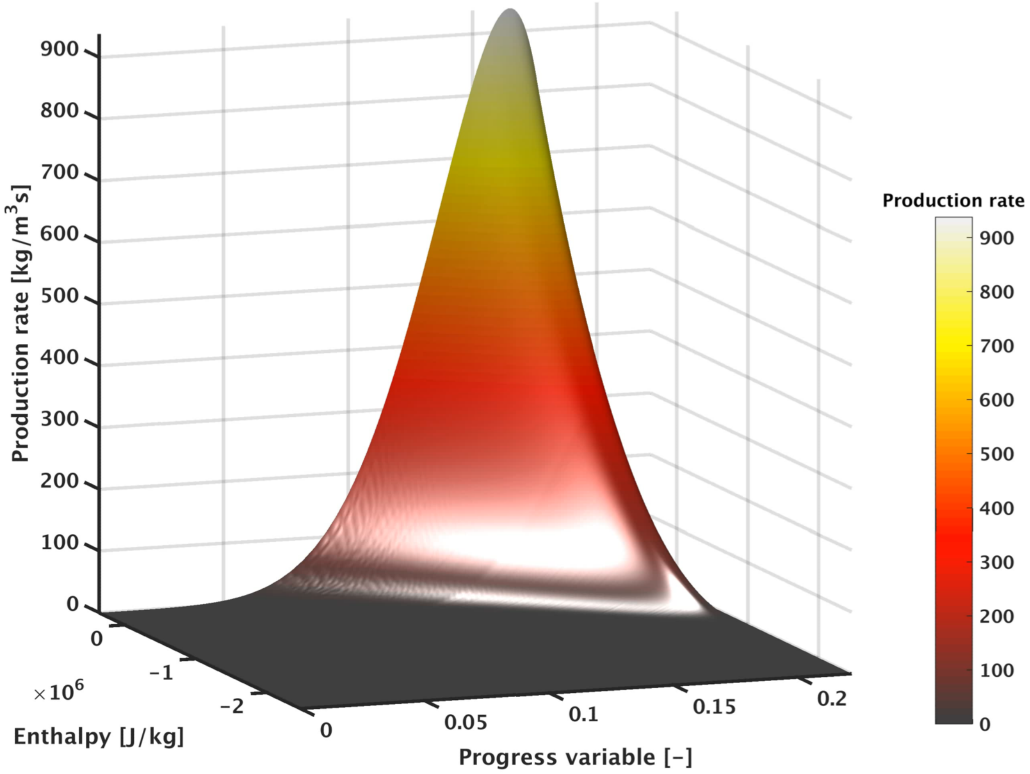
Enthalpy decreases if e.g. the inlet temperature is decreased

This can be used in simulations with heat losses

The lines compose a unique 2D flamelet generated manifold in progress variable-enthalpy space

Prediction and reduction of emissions in domestic boilers

Flamelet modelling of combustion



- Solve transport equation for progress variable and enthalpy:

$$\frac{\partial(\rho C)}{\partial t} + \vec{\nabla}\cdot(\rho\vec{v}C) - \vec{\nabla}\cdot\left(\rho\mathcal{D}_C\vec{\nabla}C\right) = \rho\dot{\omega}_C$$

$$\frac{\partial(\rho h)}{\partial t} + \vec{\nabla}\cdot(\rho\vec{v}h) - \vec{\nabla}\cdot\left(\rho\mathcal{D}_h\vec{\nabla}h\right) = 0$$

- Retrieve production rate (source term) from FGM lookup table
- Retrieve temperature, density, viscosity etc. from FGM lookup table

Implementation models in SU2
General idea of implementation (in progress)

- General framework for solving system of transport equations of species:

$$\frac{\partial \rho y_i}{\partial t} + \nabla \cdot (\rho u y_i) = \nabla \cdot (\rho D_i \nabla y_i) + S$$

- Specific implementations for species transport, non-premixed and premixed combustion, as well as finite rate chemistry:

e.g. $S_{prem} = \rho_u S_L \nabla |c|$

- Fluid properties from
  - Built-in functions (for simple problems, e.g. constant properties per species, implementation of mixing rules)
  - Lookup tables (for combustion)
  - External library (e.g. mutation++ or fluidprop)

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SU2 - scalar transport

Transport equation for a scalar has been added

Example 1: transported scalar

```
%scalar transport. Options: PASSIVE_SCALAR, PROGRESS_VARIABLE
KIND_SCALAR_MODEL= PASSIVE_SCALAR
% mass diffusivity. Options: CONSTANT_DIFFUSIVITY, CONSTANT_SCHMIDT
DIFFUSIVITY_MODEL=CONSTANT_DIFFUSIVITY
DIFFUSIVITY_CONSTANT= 0.002
% write diffusivity to file
WRT_DIFFUSIVITY=yes
% initialization of the domain
SCALAR_INIT=0.0
% in case of turbulence  we need the turbulent Schmidt number
%SCHMIDT_TURB=0.7
% scalar clipping
SCALAR_CLIPPING= YES
SCALAR_CLIPPING_MIN= 0.0
SCALAR_CLIPPING_MAX= 1.0
```

Example 2: premixed combustion

```
% scalar transport. Options: PASSIVE_SCALAR, PROGRESS_VARIABLE
KIND_SCALAR_MODEL= PROGRESS_VARIABLE
% laminar flamespeed for premixed combustion [m/s]
PREMIXED_LAMINAR_FLAMESPEED= 0.5
% adiabatic flame temperature for premixed combustion
% note that unburnt temperature comes from reference values
PREMIXED_FLAME_TEMPERATURE= 1800
```


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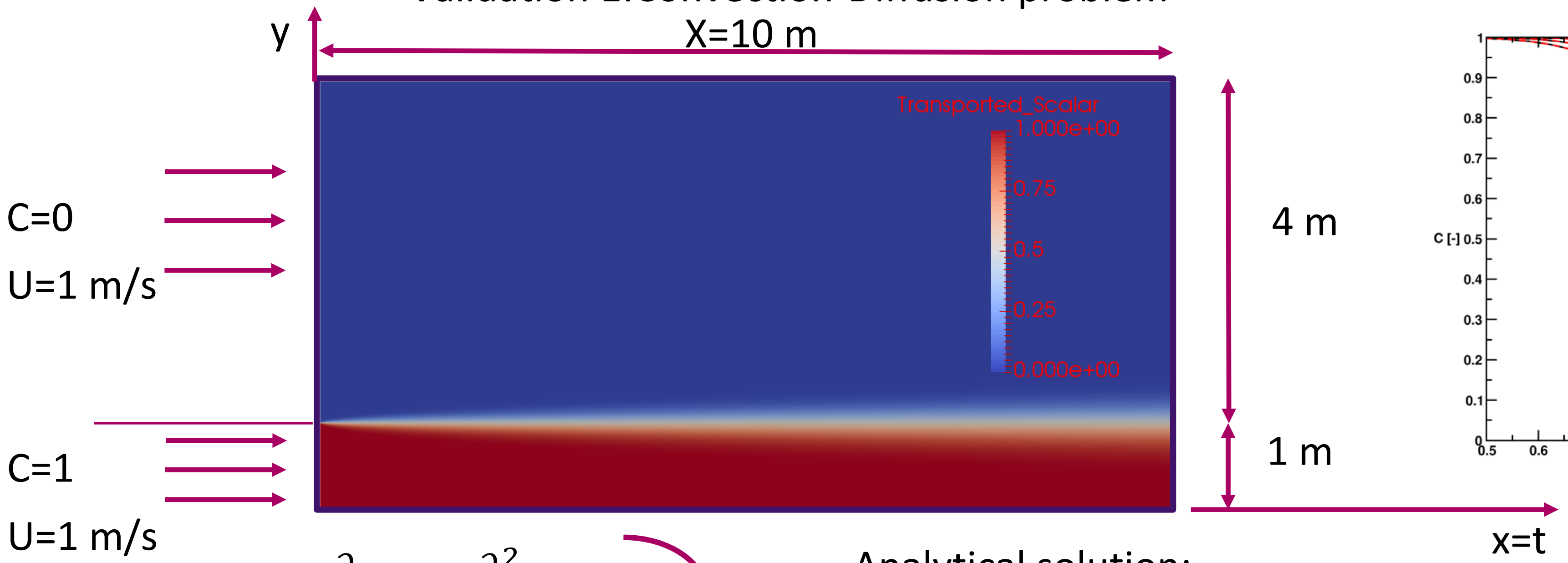
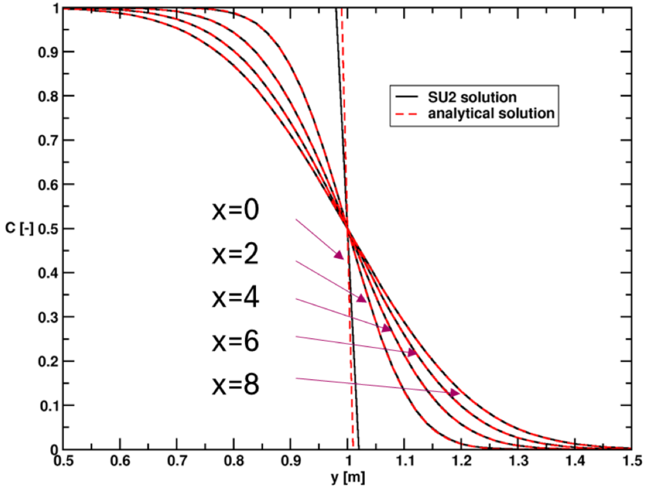
VALIDATION

SU2 – passive scalar transport

Scalar transport equation has been added to SU2

Validation 1:Convection-Diffusion problem





$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial y^2}$$

Boundary condition:

C(y<1,0)=1

C(y>1,0)=0

Analytical solution:

$$c(y,t) = \frac{1}{2}\left(1 + \mathrm{erf}\left(\frac{y}{\sqrt{4Dt}}\right)\right)$$

D=0.02

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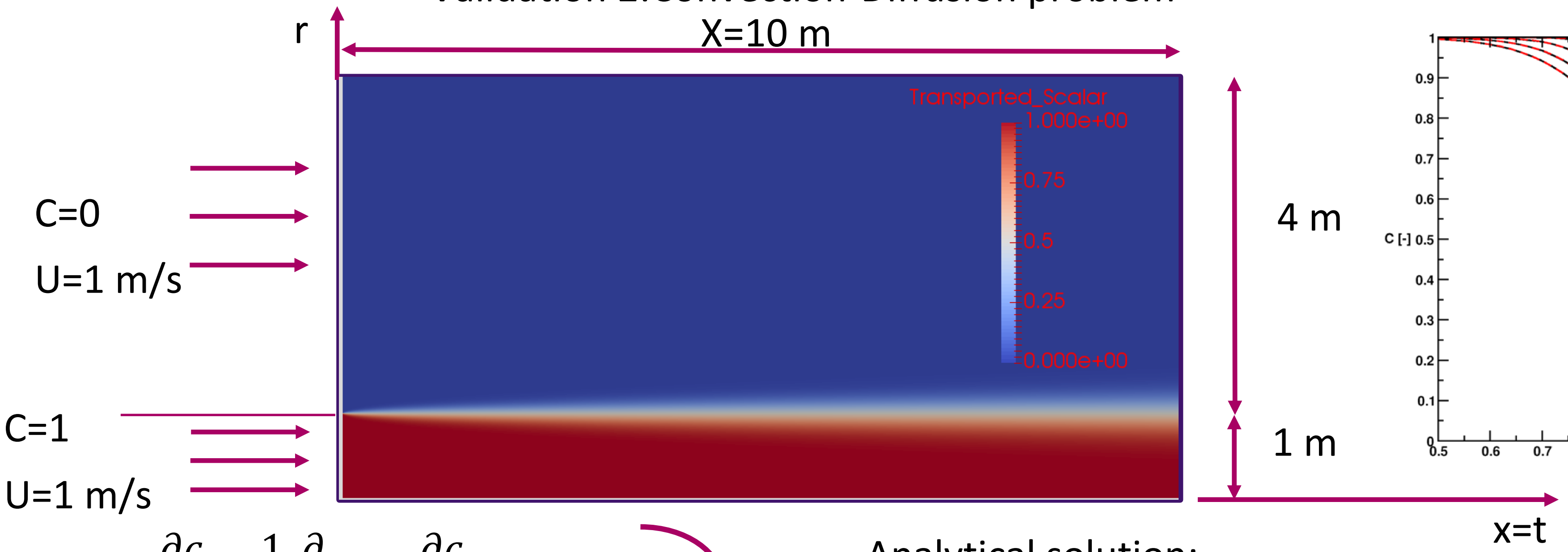
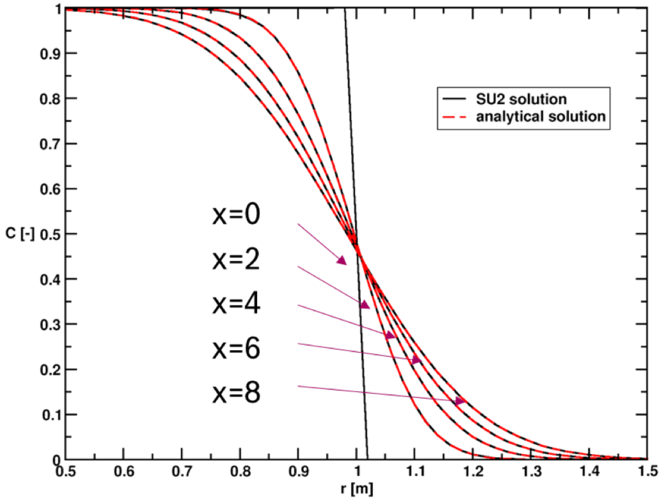
SU2 – passive scalar transport

Axisymmetric case

Validation 2:Convection-Diffusion problem





$$\frac{\partial c}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(Dr\frac{\partial c}{\partial r}\right)$$

Boundary condition: c(r,0)=f(r)

c(r,0)=1, r<1

c(r,0)=0, r>1

Analytical solution:

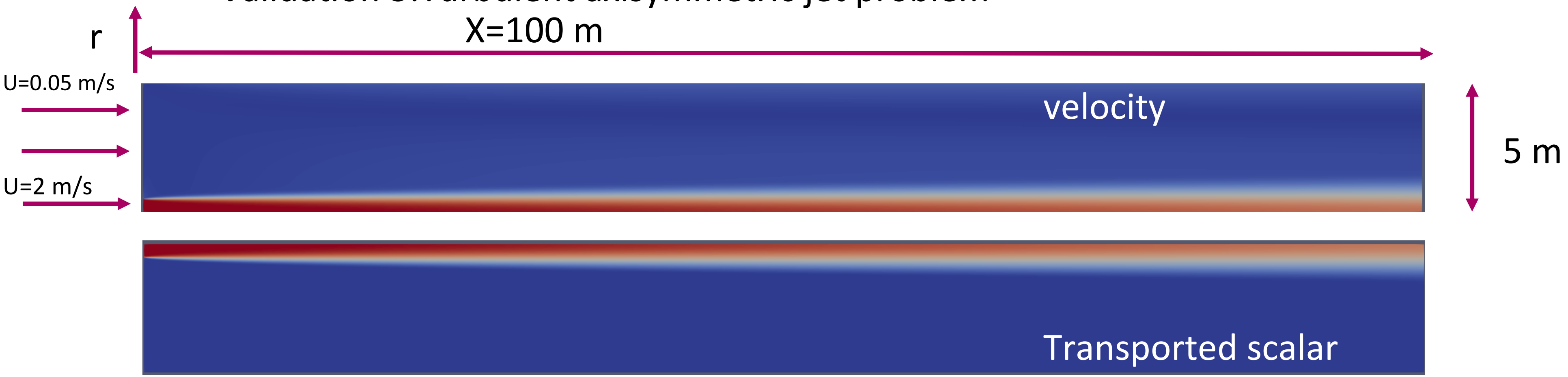
$$c(r,t) = \frac{2}{R^2}\sum_{n=1}^{\infty} e^{-D\alpha_n^2 t}\frac{J_0(r\alpha_n)}{J_1(R\alpha_n)}\int_0^R rf(r)J_0(r\alpha_n)dr$$

D=0.02, R=5,

α_n are roots of $J_0(R\alpha_n)$

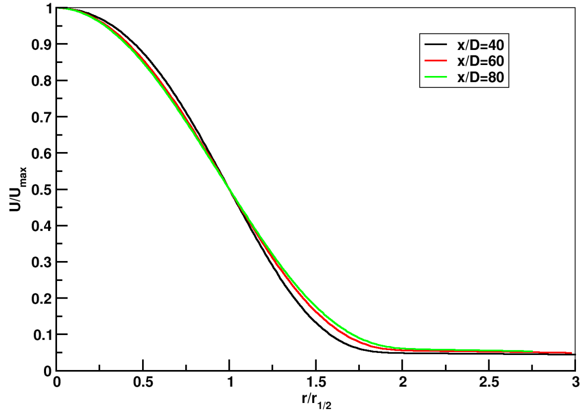
SU2 – passive scalar transport

Turbulent jet with SA turbulence model



Validation:

- Velocity and scalar should be self-similar downstream
- Other validation: spreading rate (~0.11), measurements (e.g. Wygnanski& Fiedler)
- Note that SA is known to perform badly for round jet



SU2 - scalar transport

Laminar premixed flame with laminar flamespeed model

The mean reaction rate of a premixed flame can be modelled as:

$$S = \rho_u S_L \frac{A_T}{A} |\nabla c|$$

In turbulent flames, the flame wrinkling is nonunity:

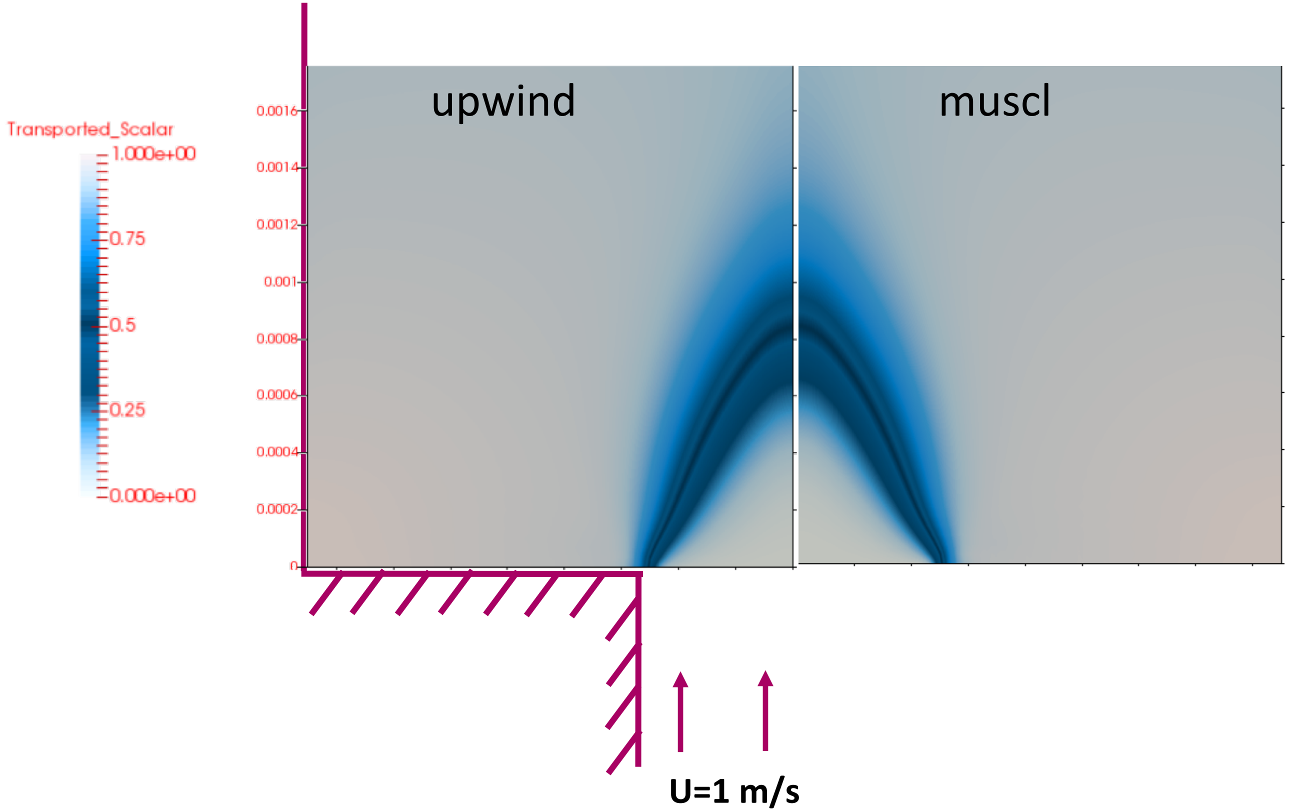
$$\frac{A_T}{A} = 1 + \frac{0.46}{Le} Re_t \frac{u'}{S_L}^{0.3} \frac{p}{p_0}^{0.2}$$

Temperature is linear function of progress variable:

$$T = T_u \cdot (1 - c) + T_f \cdot c$$

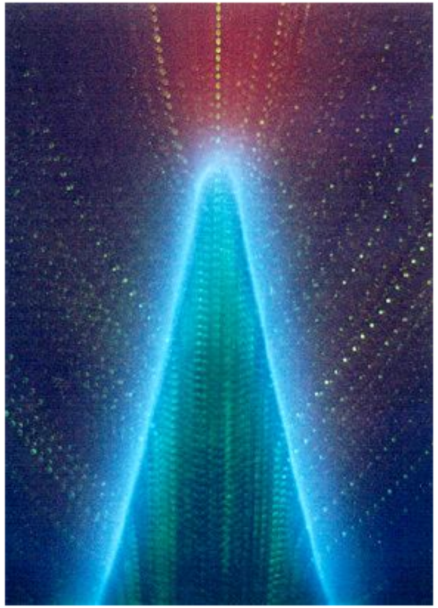
SU2 - scalar transport

Planar laminar premixed flame



- A premixed 'no-chemistry' flame simulation is possible now in SU2
- Temperature is a function of progress variable: T=T(c)
- Density is multicomponent ideal gas law $\rho = \rho(T, c)$
- Currently, other properties like viscosity not coupled directly
- Convergence is not so good yet

Outlook: Adjoint optimization of Bunsen burner
Determine laminar flame speed from flame angle



Bunsen Burner Methane-Air Premixed Flame

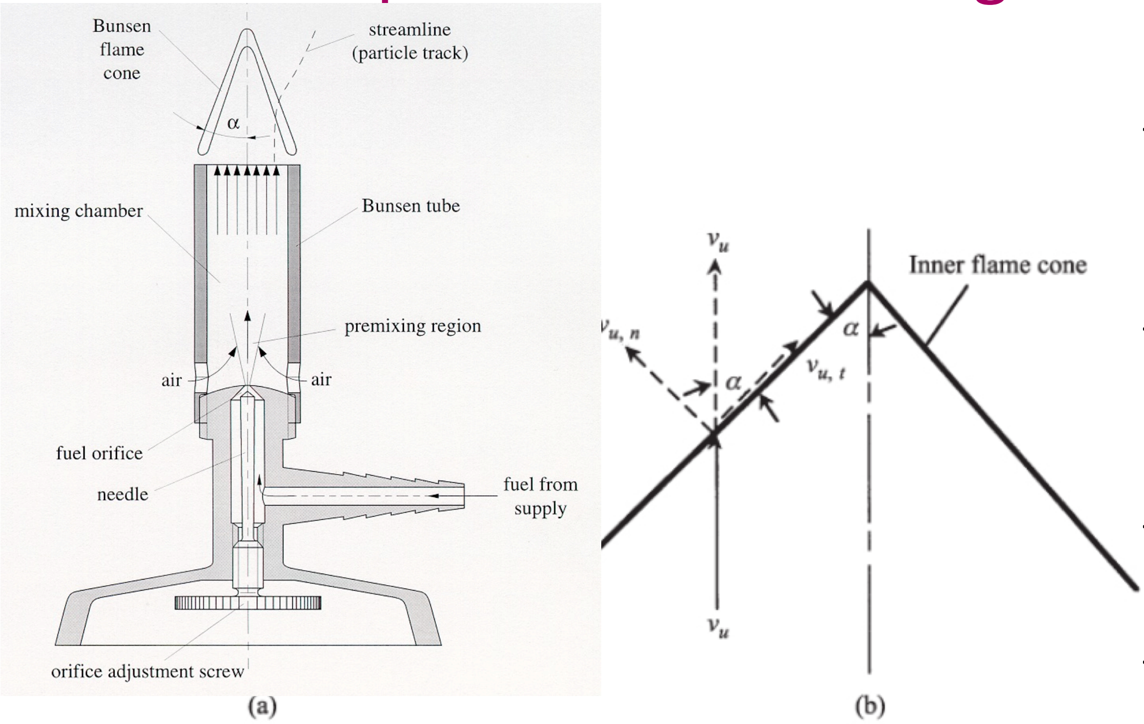


Figure 8.3 (a) Bunsen-burner schematic. (b) Laminar flame speed equals normal component of unburned gas velocity, $v_{u,n}$.

$$S_L = v_{u,n} = v_u \sin\alpha$$

- Laminar flame speed determines flame shape (angle)
- For accurate measurements of flame speed a straight flame profile is necessary
- A uniform velocity profile is crucial
- Objective: optimization of uniformity of velocity profile at Bunsen tube exit

Combustion models in SU2
Final words

- Basic framework for transported scalars was implemented
- Work on lookup table approach will start soon (in collaboration with
- Besides implementing models, convergence needs attention
- Code is available on github in branch feature_scalar
- Looking forward to a good collaboration!