Simulating the combustion of gaseous fuels

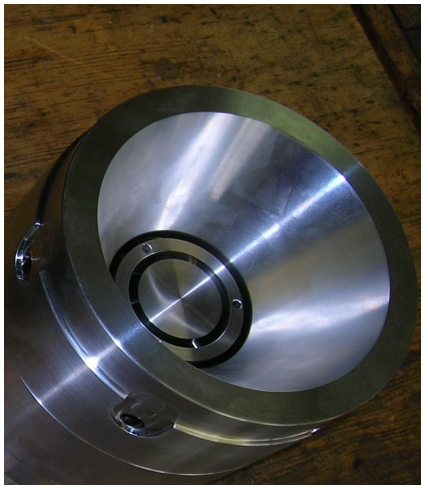
6th OpenFoam Workshop Training Session

Dominik Christ

Institute of Heat
and Mass Transfer
RWTH Aachen University
Univ.-Prof. Dr.-Ing. R.Kneer

RWTH AACHEN

This presentation shows how to use OpenFoam to simulate gas phase combustion



Overview

Theory

Tutorial case

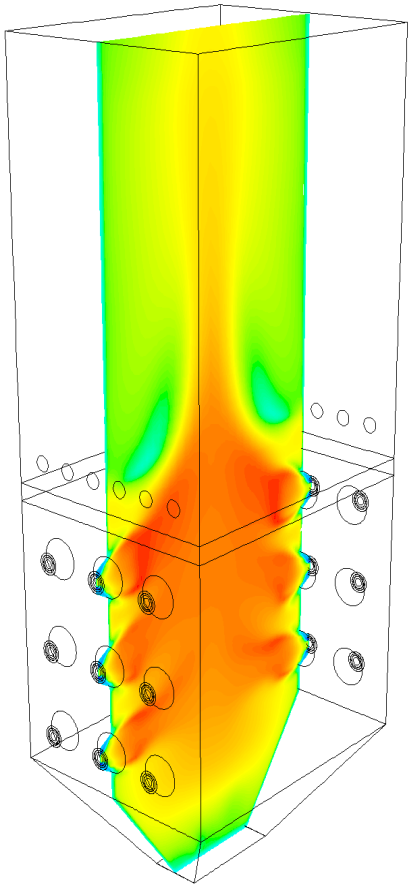
Solution strategies

Validation

The focus of combustion simulation depends on the application

Burner design

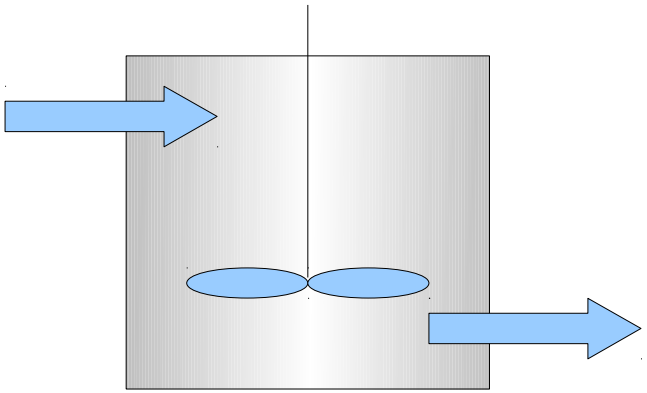
Pollutant formation



Furnace operation/retrofit

The focus of the present tutorial is simulating a model flame

- Model flames are a basis to test and evaluate combustion solvers
- Tutorial case is a turbulent methane/air flame ("Flame D" from Sandia/TNF workshop)
- Solver applications used are
  - `rhoReactingFoam` (PaSR model)
  - `edcSimpleFoam` (EDC model)
- Validation with experimental data to assess the solver/model accuracy



Overview

Theory (combustion; radiation)

Tutorial case

Solution strategies

Validation

Combustion simulation is characterized by chemical reactions

Global reactions summarize the combustion process:

$$CH_4 + 2O_2 \Leftrightarrow CO_2 + 2H_2O$$

Detailed chemical mechanisms describe events on molecular level:

$$CH_4 + O \Leftrightarrow OH + CH_3$$
$$CH_4 \Leftrightarrow CH_3 + H$$
$$CH_4 + H \Leftrightarrow CH_3 + H_2$$
$$CH_4 + OH \Leftrightarrow CH_3 + H_2O$$
$$\vdots$$

from GRI-Mech 3.0 (325 reactions, 53 species)

- *Chemical mechanisms need to be used within their specification limits, eg. GRI-Mech 3.0: methane/natural gas, T in 1000-2500 K, Φ in 0.1-5*

- *Detailed mechanism are more accurate (e.g. NO_x, ignition delay), but computationally much more expensive*
  → level of detail needs to be chosen by the user

Chemical reactions can be described with equilibrium or kinetic rates (incl. “infinite rate”)

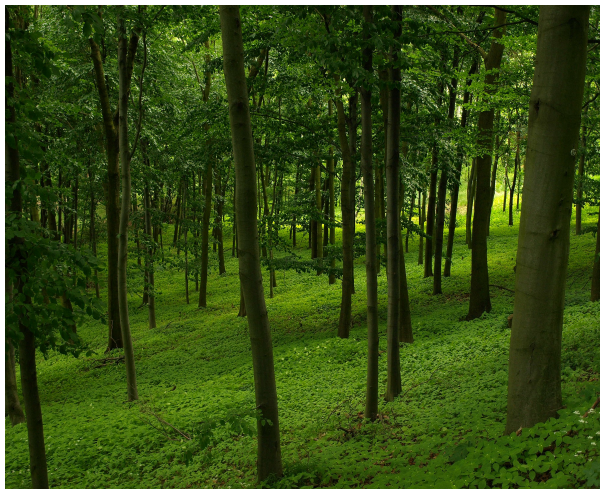
Equilibrium calculation depends only on thermodynamic data: h°, s°, cp°

But concerning combustion, many things are not in equilibrium!

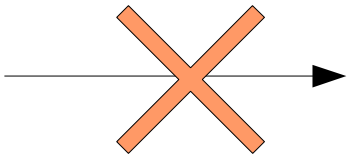
Chemical kinetics determine the reaction rate e.g. with an Arrhenius type formulation:

$$R = A\,T^{b} \exp\left(-\frac{E}{\Re\,T}\right) C_{CH4}\,C_{O2}^{0.5}$$

“Infinite rate” chemistry is a special case, where reaction rates are assumed to be infitely fast



kinetically inhibited



In turbulent flows, turbulence/chemistry interaction defines the reacting flow

Turbulent flow ⟷ **Chemical kinetics**

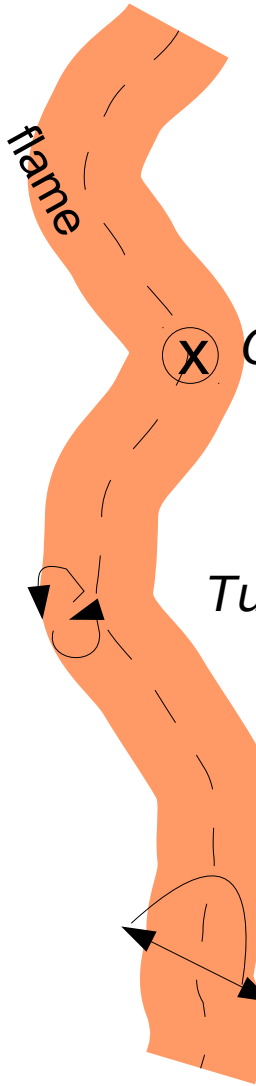
- Turbulence enhances mixing of species such as fuel, oxidizer and products
- Strong turbulence can suppress combustion
  → local extinction

- In a laminar flow, combustion is controlled exclusively by chemical kinetics
- Combustion leads to flow acceleration
  → modification of flow field

Different approaches exist to model the turbulence/chemistry interaction

FUEL
or
FRESH MIXTURE

OXIDIZER
or
BURNT MIXTURE



One-point statistics (PDF)

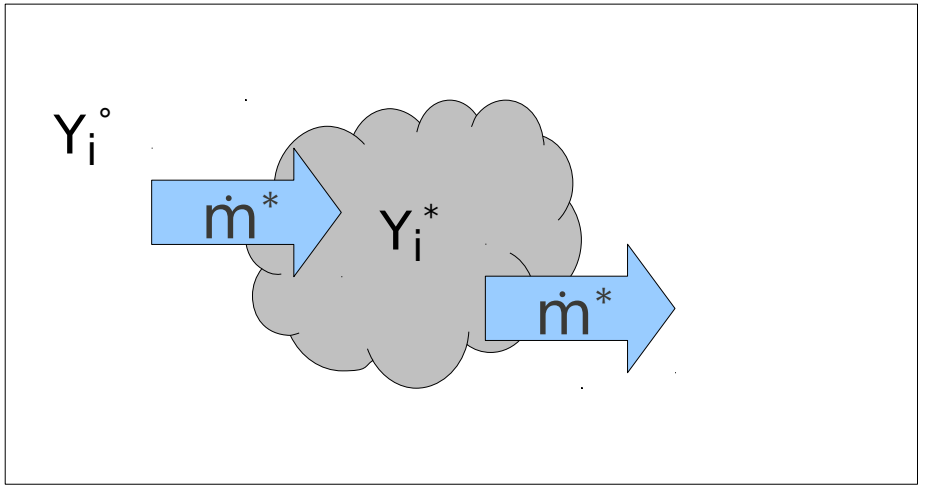
Turbulent mixing (e.g. EDC, PaSR)

Geometrical analysis (flamelet)

cf. Poinsot, Veynante “Theoretical and Numerical Combustion”

The Eddy-Dissipation Concept (EDC) assumes reactions in *fine structures*

$$\overline{R_i} = \overline{\rho}\,\frac{\gamma^{*}\,\dot{m}^{*}}{(1-\gamma^{*})}\,(\overline{Y_i} - Y_i^{*})$$



Fraction of the flow occupied by *fine structures:*

$$\gamma^{*}$$

Relation of mean, *fine structure* and *surrounding* state:

$$\overline{Y_i} = \gamma^{*}\,Y^{*} + (1-\gamma^{*})\,Y^{o}$$

EDC reaction rate depends on turbulent flow properties and chemical kinetics approach

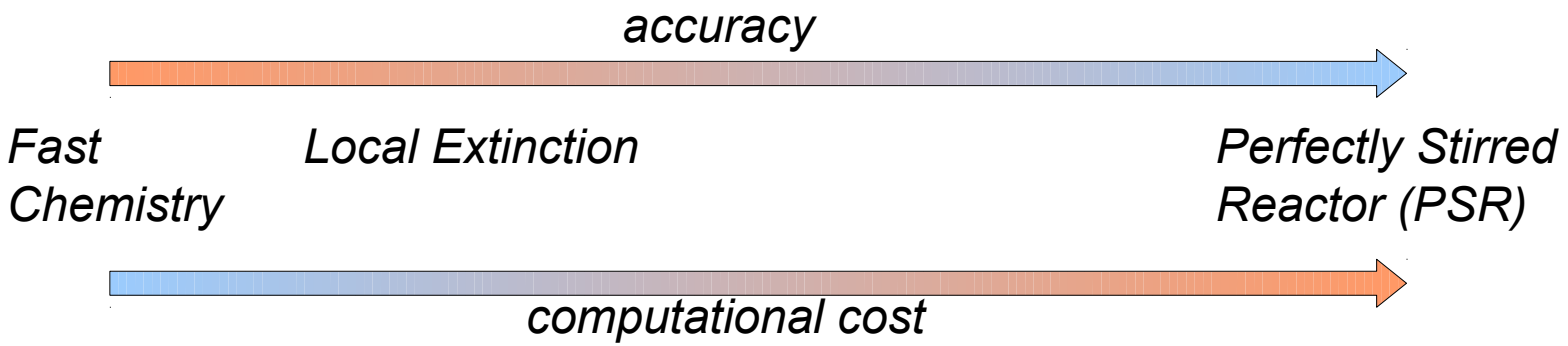
The fraction of the flow occupied by *fine structures:*

$$\gamma^* = 9.7 \left(\frac{\nu \cdot \epsilon}{k^2} \right)^{\frac{3}{4}}$$

Mass transfer rate between the *fine structures* and the *surroundings:*

$$\dot{m}^* = 2.45 \left(\frac{\epsilon}{\nu} \right)^{\frac{1}{2}}$$

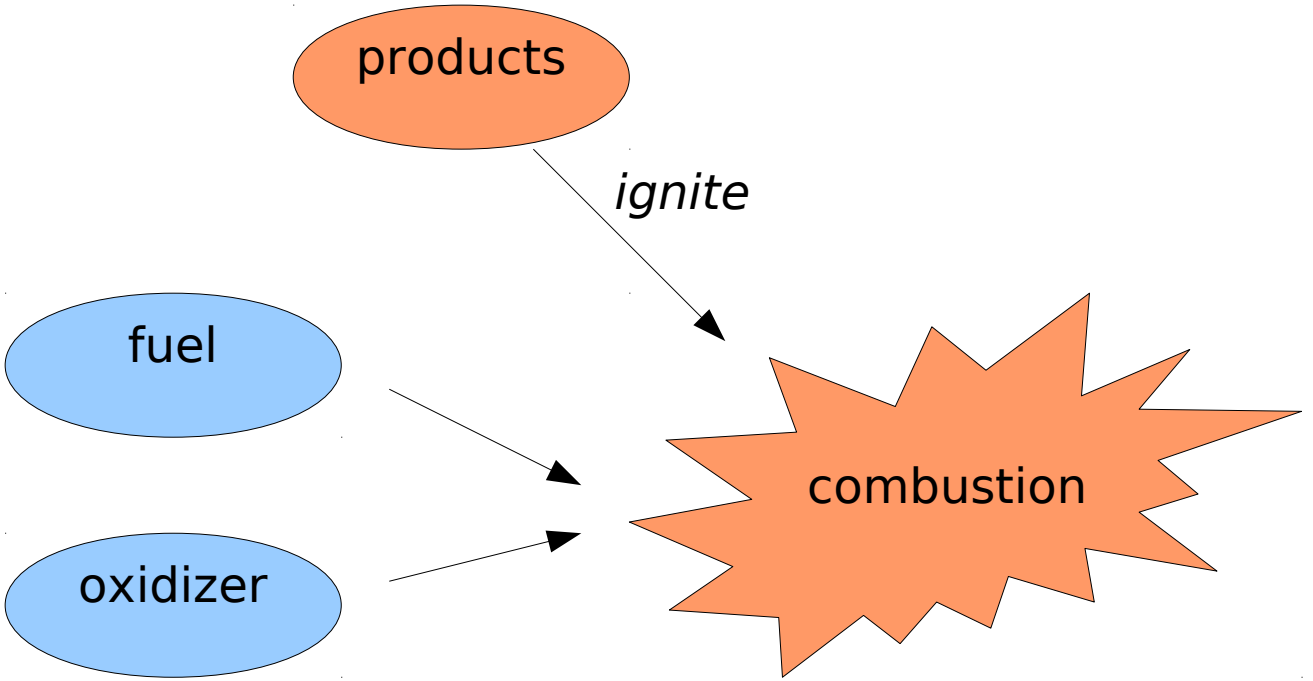
Chemical kinetics approaches for fine structure composition Y_i^*:



The Fast Chemistry approach assumes infinitely fast reactions

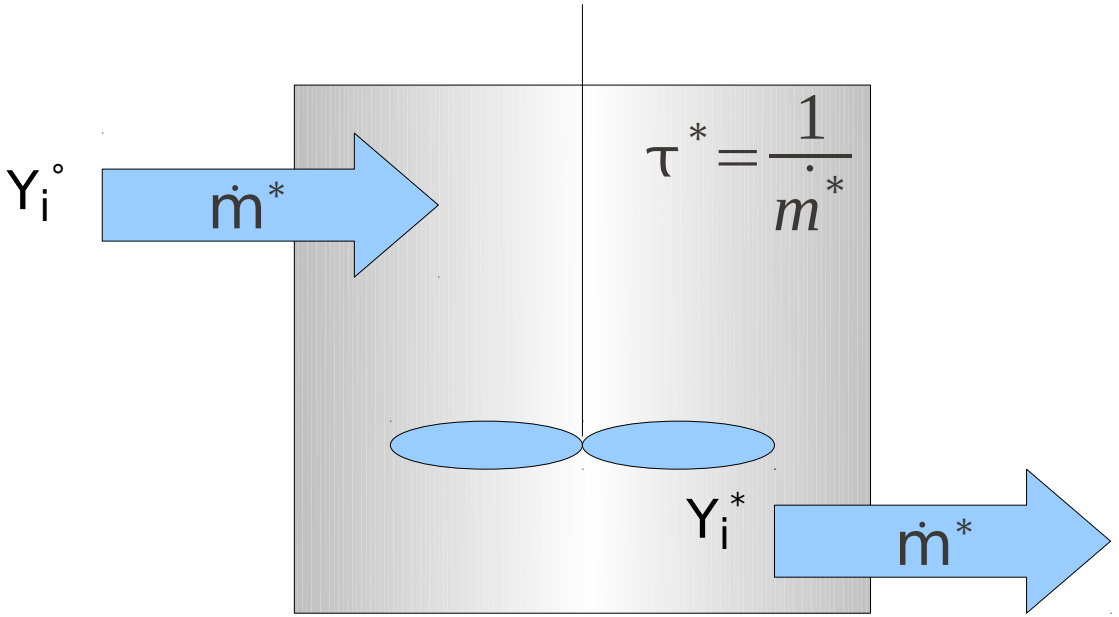
- Assumes sufficient time to achieve equilibrium inside fine structures
- Works only with irreversible global reactions

Combustion occurs if fuel, oxidizer and products meet simultaneously



→ *Product mass fractions must be initialized accordingly*

The PSR approach determines the steady-state of a perfectly stirred reactor



$$\frac{dp^*}{dt} = 0$$

$$\frac{dh^*}{dt} = 0$$

$$\frac{dY_i^*}{dt} = \omega_i + \dot{m}^*\left(Y^o - Y^*\right)$$

Chemical kinetics, $\omega_i = \omega_i\left(p, T, Y_i^*\right)$

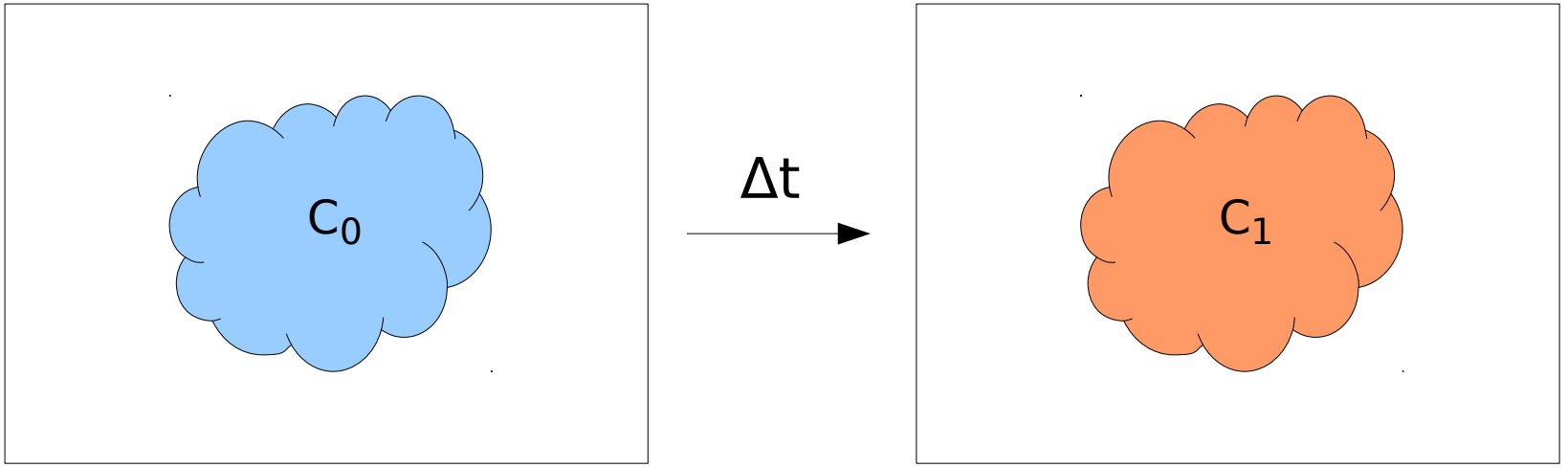
Local Extinction approach employs data from a priori PSR calculations

$$\tau^* < \tau_{ch} \Rightarrow R = 0$$

τ_{ch} is the minimum residence time which sustains combustion in PSR.

Example 1: Close to burner	high turbulence (τ^*=2.e-6)	<	T = 300 K (τ_{ch}= 1.e-4)
Example 2: Free stream reaction zone	medium turbulence (τ^*=2.e-4)	>	T = 900 K (τ_{ch}= 2.e-5)

The PaSR combustion model derives the reation rate in a transient manner



$$\bar{R}_i = \kappa \frac{C_{i,1} - C_{i,0}}{\Delta t}$$

Mixed fraction of cell that can react: κ

The parameter κ is based on two time scales

Turbulent mixing time scale:

$$\tau_m = \sqrt{\frac{k}{\epsilon}\left(\frac{\nu}{\epsilon}\right)^{\frac{1}{2}}}$$

Chemical time scale (infinite or finite rate):

$$\frac{1}{\tau_{ch}} = max\left(-\frac{R_{fuel}}{\rho Y_{fuel}}, -\frac{R_{O_2}}{\rho Y_{O_2}}\right)$$

$$\frac{1}{\tau_{ch}} = -\frac{\partial R}{\rho \partial Y}$$

Mixed fraction that reacts:

$$\kappa = \frac{\tau_{ch}}{\tau_m + \tau_{ch}}$$

In OpenFOAM, mixing time scale is implemented slightly different

In rhoReactingFoam:

$$\tau_m = C_{mix}\sqrt{\frac{\mu_{eff}}{\rho\,\epsilon}}$$

In Chomiak (1996):

$$\tau_m = \sqrt{\frac{k}{\epsilon}\left(\frac{\nu}{\epsilon}\right)^{\frac{1}{2}}}$$

Both can be transformed into each other, using:

$$\frac{\mu_t}{\rho} = C_\mu \frac{k}{\epsilon}, \quad Sc_t = 1, \quad Re_t = \frac{k^2}{\epsilon\,\nu}$$

As result, we obtain:

$$C_{mix} = \sqrt{\frac{1}{1 + C_\mu Re_t}}$$

Chomiak (1996): *Flame Liftoff in Diesel Sprays* 25th Symp. Int. on Comb. pp. 2557-2564

The value for C_{mix} needs to be estimated a priori

$$C_{mix} = \sqrt{\frac{1}{1 + C_{\mu} Re_t}}$$

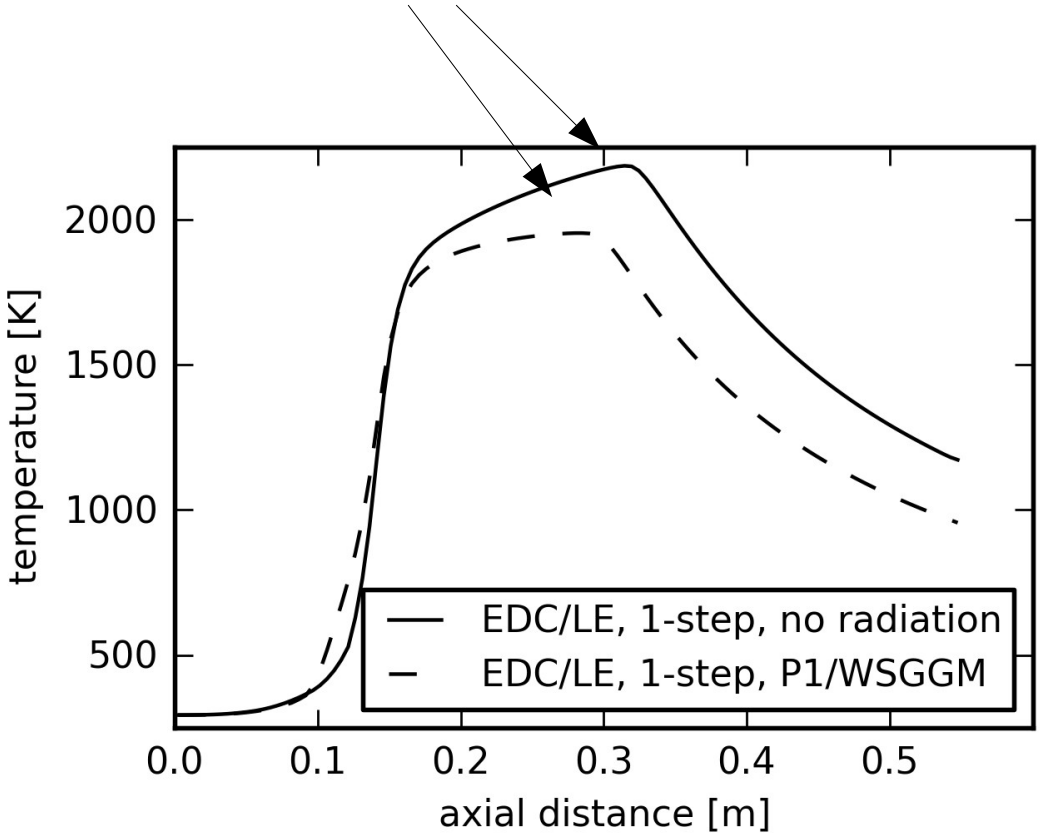
Laminar flow	Typical turbulent flow	Extremely turbulent flow
$Re_t = 0$	$Re_t \approx 1000$	$Re_t \rightarrow \infty$
$C_{mix} = 1.0$	$C_{mix} \approx 0.1$	$C_{mix} \rightarrow 0.0$

Typical values for C_{mix}: 0.001 – 0.3; cf. Nordin (2001)

Nordin (2001): *Complex Chemistry Modelling of Diesel Spray Combustion,* PhD-Thesis

Radation heat transfer needs to be considered in combustion simulation

Peak temperature ≈250 K higher without radiation modelling

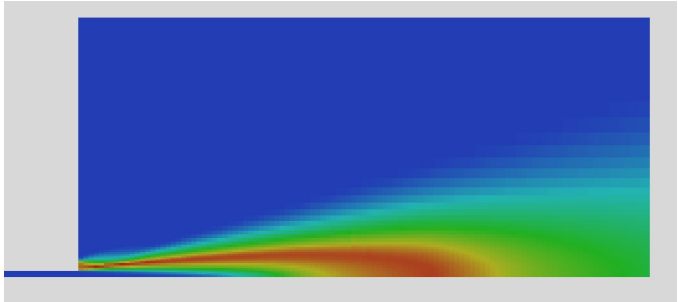


Radiation Transport Equation:

- P1 - Transport
- Discrete Ordinates (DOM)

Gas-Absorption Modelling:

- constant
- RADCAL-Polynomials
- WSGGM (custom)



Overview

Theory

Tutorial case

Solution strategies

Validation

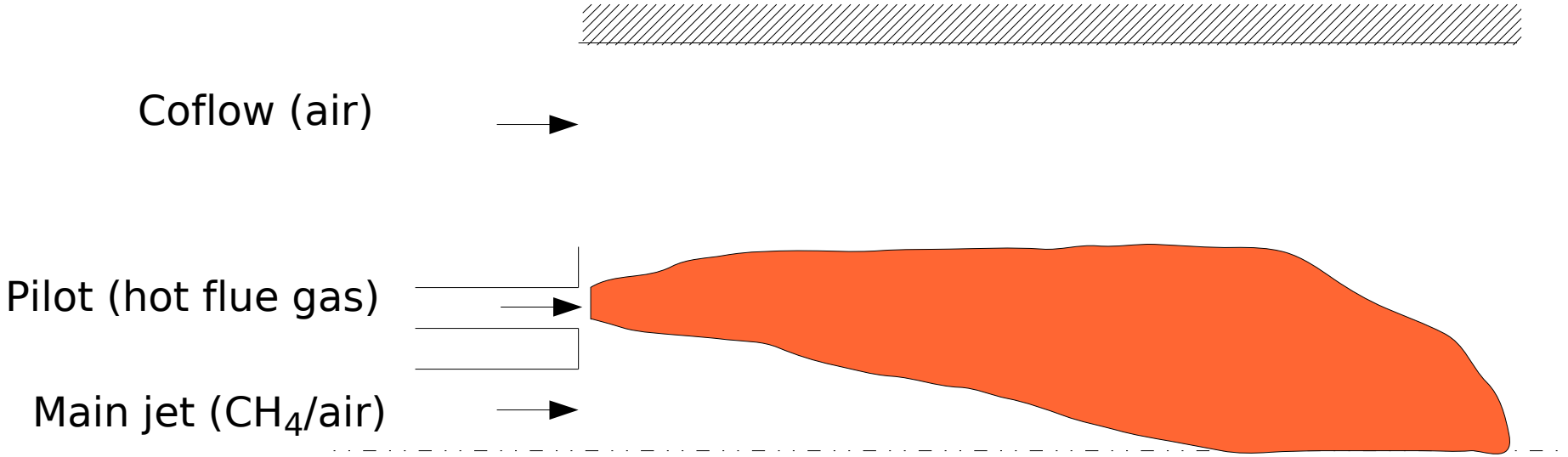
The tutorial case is a non-premixed piloted flame (“Flame D”)

Characteristics:

Steady-state, piloted, methane/air, diffusion flame, some local extinction

Geometry:

Axi-symmetric, 2D



The boundary conditions are identical for `rhoReactingFoam` and `rhoSimpleFoam`

	Ux [m/s]	p [Pa]	T [K]	Yi [-]	k [m²/s²]	epsilon [m²/s³]
Main jet	49.6	zeroGradient	294	fixedValue	I_{turb}=0.0458	L_{turb}=5.04e-4
Pilot	11.4	zeroGradient	1880	fixedValue	I_{turb}=0.0628	L_{turb}=7.35e-4
Coflow	0.9	zeroGradient	291	fixedValue	I_{turb}=0.0471	L_{turb}=0.0197
Outlet	zeroGradient	100000	zeroGradient	zeroGradient	zeroGradient	zeroGradient
Walls	0.0	zeroGradient	zeroGradient	zeroGradient	wall function	wall function

Front and backside of axi-symmetric domain are specified as 'wedge'.

edcSimpleFoam: Flow field initialized as required by chemical kinetics approach

- Fast Chemistry and Local Extinction: Set CO_2 and H_2O mass fraction to 0.01 everywhere.
- Perfectly Stirred Reactor: Initialize with Fast Chemistry or Local Extinction solution.
- Setup chemistryProperties:

```
edcFastChemCoeffs
{
    oxidiserName O2;
    mainFuelName CH4;
}
```

```
edcLECoeffs
{

    oxidiserName O2;
    mainFuelName CH4;
    autoIgnitionTemperature
        868;


    curve1
    {
        temperature 300;
        tauChMin  7.00E-005;
    }
…
}
```

```
edcPSRCoeffs
{
    relativeTolerance 1.e-6;
    absoluteTolerance 1.e-14;
    maxIterations 1.e8;

    useBinaryTree off;
    binaryTreeTolerance 1e-4;
    binaryTreeSize 1.e7;
}
```

no local extinction above this temperature

rhoReactingFoam: Choosing C_{mix} and ODE intergrator

- Estimate turbulent Reynolds number:

$$Re_t = 500 \rightarrow C_{mix} = 0.15$$

SIBS is stable enough for solving detailed chemistry

- Setup `chemistryProperties`:

```
odeCoeffs
{
    ODESolver       SIBS;
    eps             5.0e-4;
    scale           1.0;
}
```

Setting-up discretization schemes

- *Convective term*: Linear upwind discretization (2nd order accurate)

```
default    Gauss linearUpwind cellLimited Gauss linear 1;
```

For species Y_i (for rhoReactionFoam: Y_i and hs)

```
div(phi,Yi) Gauss  multivariateSelection
{
    //hs     linearUpwind cellLimited Gauss linear 1;
    CH4      linearUpwind cellLimited Gauss linear 1;
    O2       linearUpwind cellLimited Gauss linear 1;
    …
}
```

- *Time discretization:* (Pseudo) steady-state

edcSimpleFoam (steady-state solver)

```
    default         steadyState;
```

rhoReactingFoam (transient solver)

```
    default         SLTS phi rho 0.7;
    default         CoEuler phi rho 0.4;
```

global under-relaxation factor

max. CFL number

Setting-up fvSolution

Numerical solver precision depends on solver type:

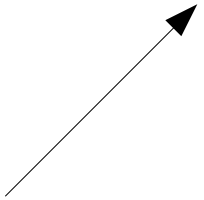
Transient solver requires each time-step to be accurate

all variables: relTol = 0. ;

Steady state solver can reach solution through intermediate results

pressure: relTol 0.001;

other variables: relTol 0.1;



intermediate results will not be accurate

Chemical mechanisms can be defined in Chemkin or OpenFOAM native format

Example: Arrhenius type kinetics

$$R = A\, T^{b} \exp\left(-\frac{E}{\Re\, T}\right) C_{CH4}^{0.7}\, C_{O2}^{0.8}$$

Chemkin format uses units: mol, cm³, s, K; cal

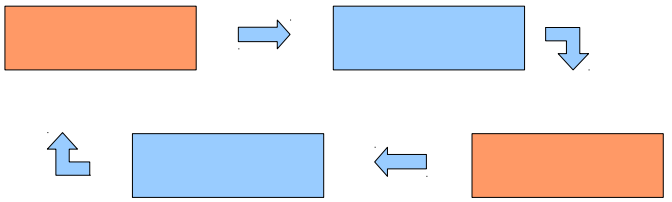
```
CH4 + 2O2 => CO2 + 2H2O     3e13  0.0   47e3
        FORD    / CH4   0.7 /
        FORD    / O2    0.8 /
```

OpenFoam native format uses units: kmol, m³, s, K; K

```
irreversibleArrheniusReaction

    CH4^0.7 + 2O2^0.8 = CO2 + 2H2O (9.48683e+11 0 23650)
```

Use `chemkinToFoam` *to convert chemkin files (or to check their consistency)*



Overview

Theory

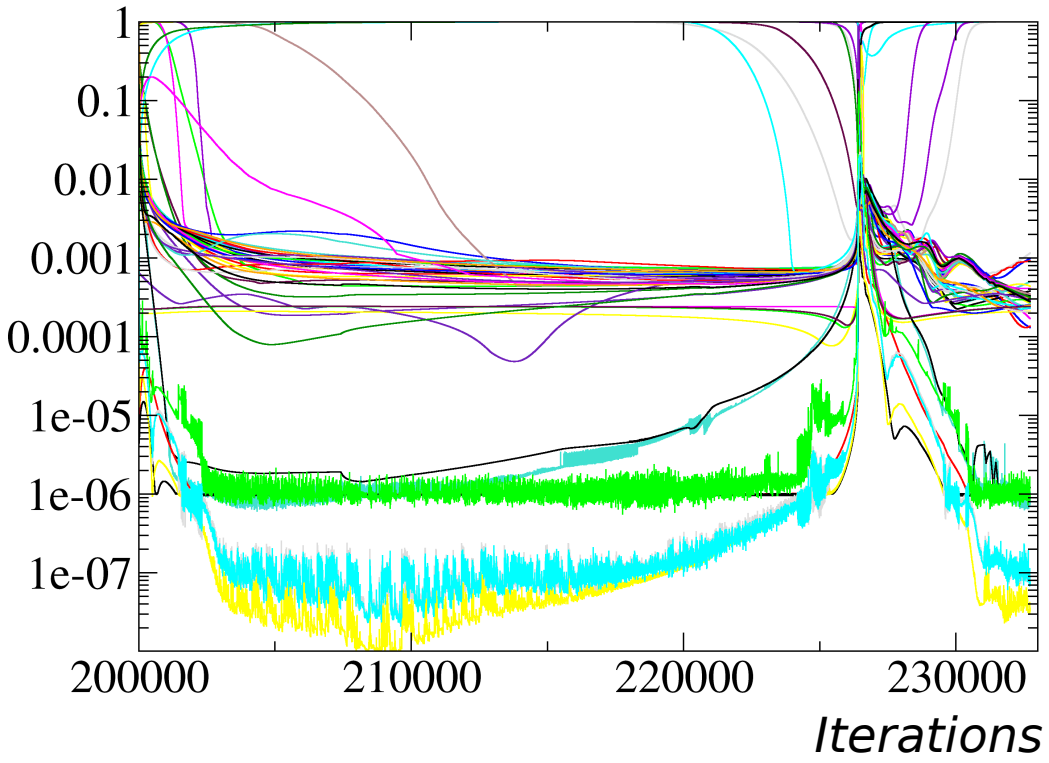
Tutorial case

Solution strategies

Validation

Combustion simulation often faces stability issues

Residuals



Many error sources are possible because numerous models are applied simultaneously, for example:

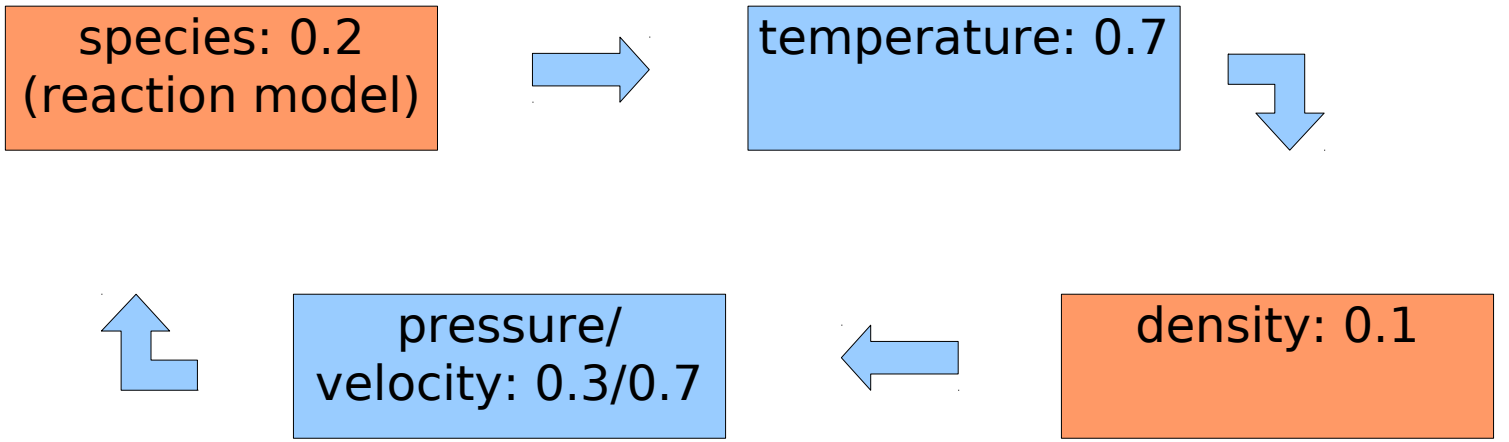
- Compressible flow
- Coupling of transport equations
- Numerically stiff reaction mechanisms

Solution strategies include good initialization and under-relaxation

Possible “well initialized” flow fields are:

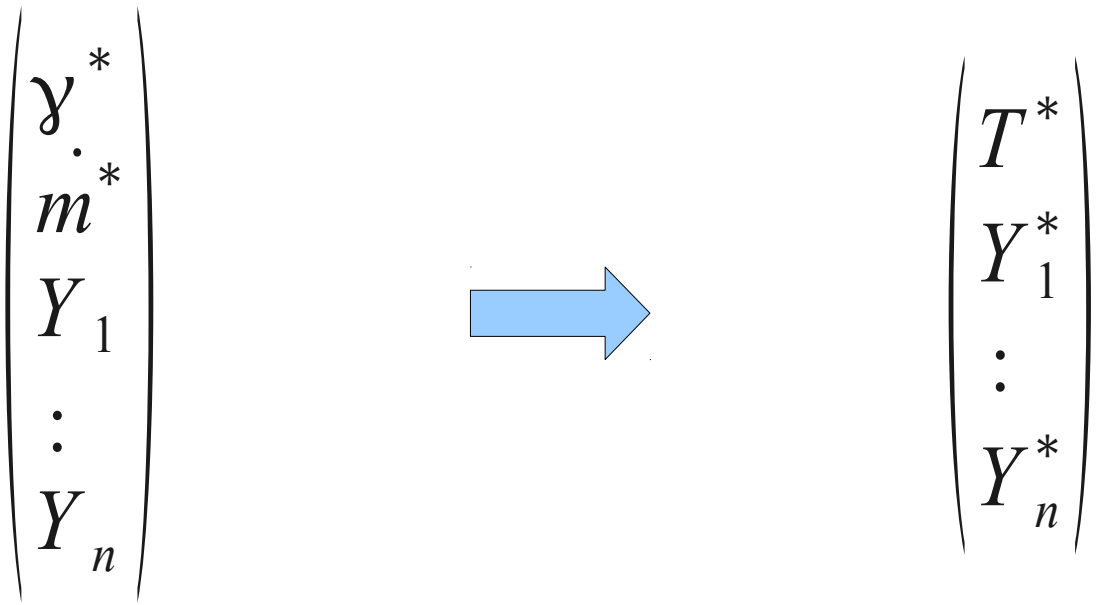
- Cold flow
- Starting solution (steady-state; 1- or 2-Step)
- Products

Strong coupling between transport equations may be broken with different under-relaxation factors.



Under-relaxation only applicable to steady-state cases.
Unsteady solver based on Transient-SIMPLER needed?

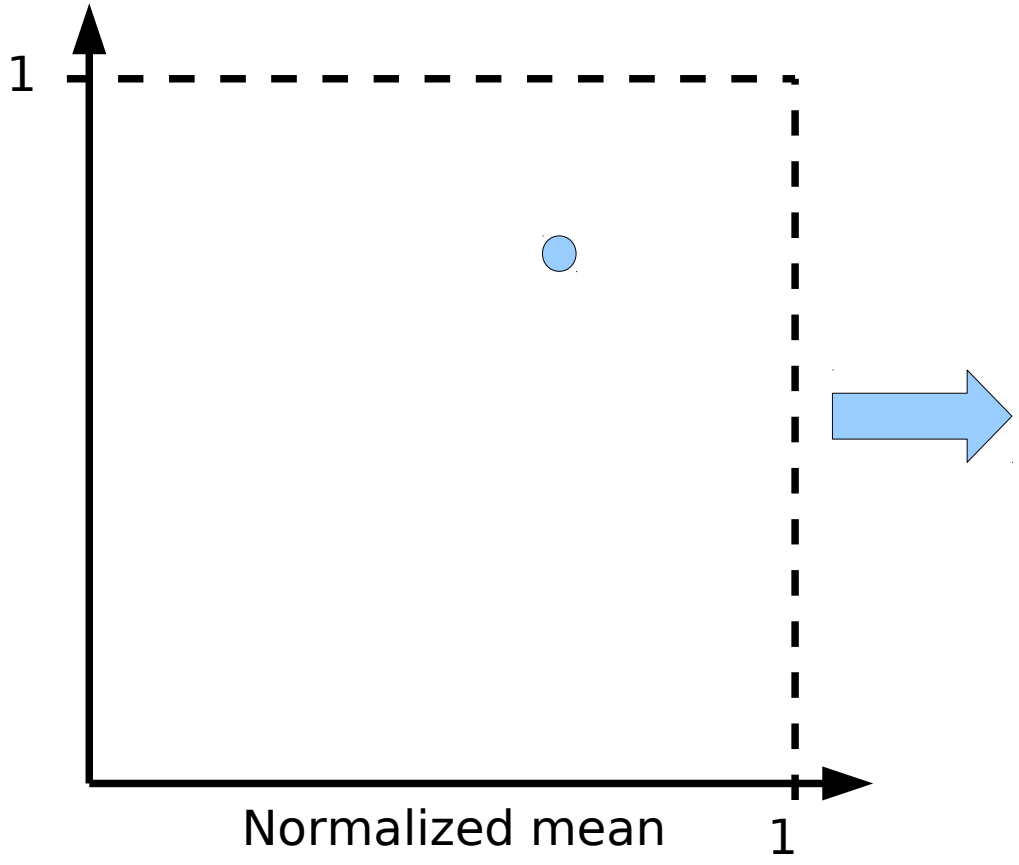
Tabulation of PSR reactor results can provide speed-up and additional stability



Mean flow data

PSR integration results

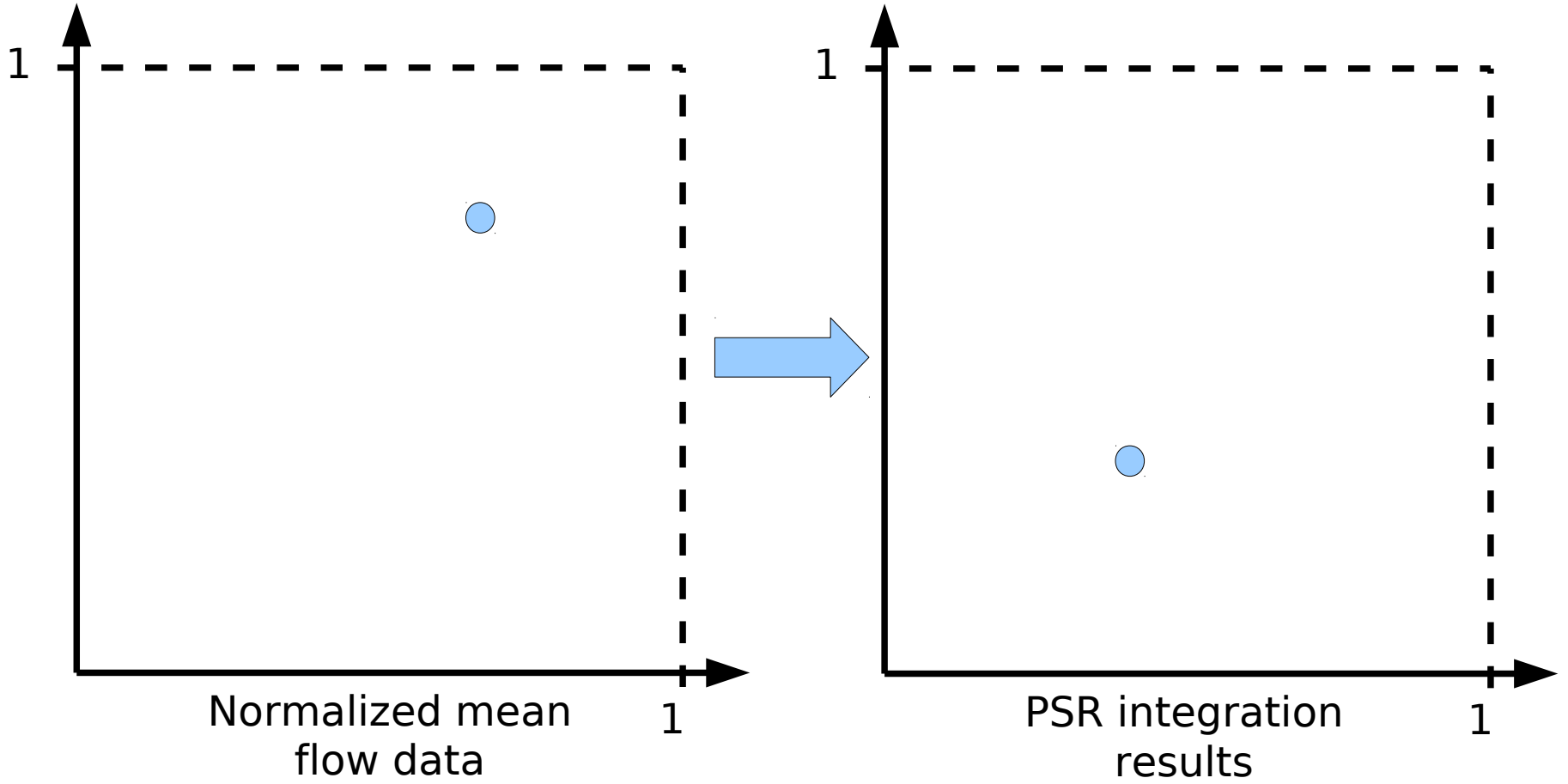
Tabulation of PSR reactor results can provide speed-up and additional stability



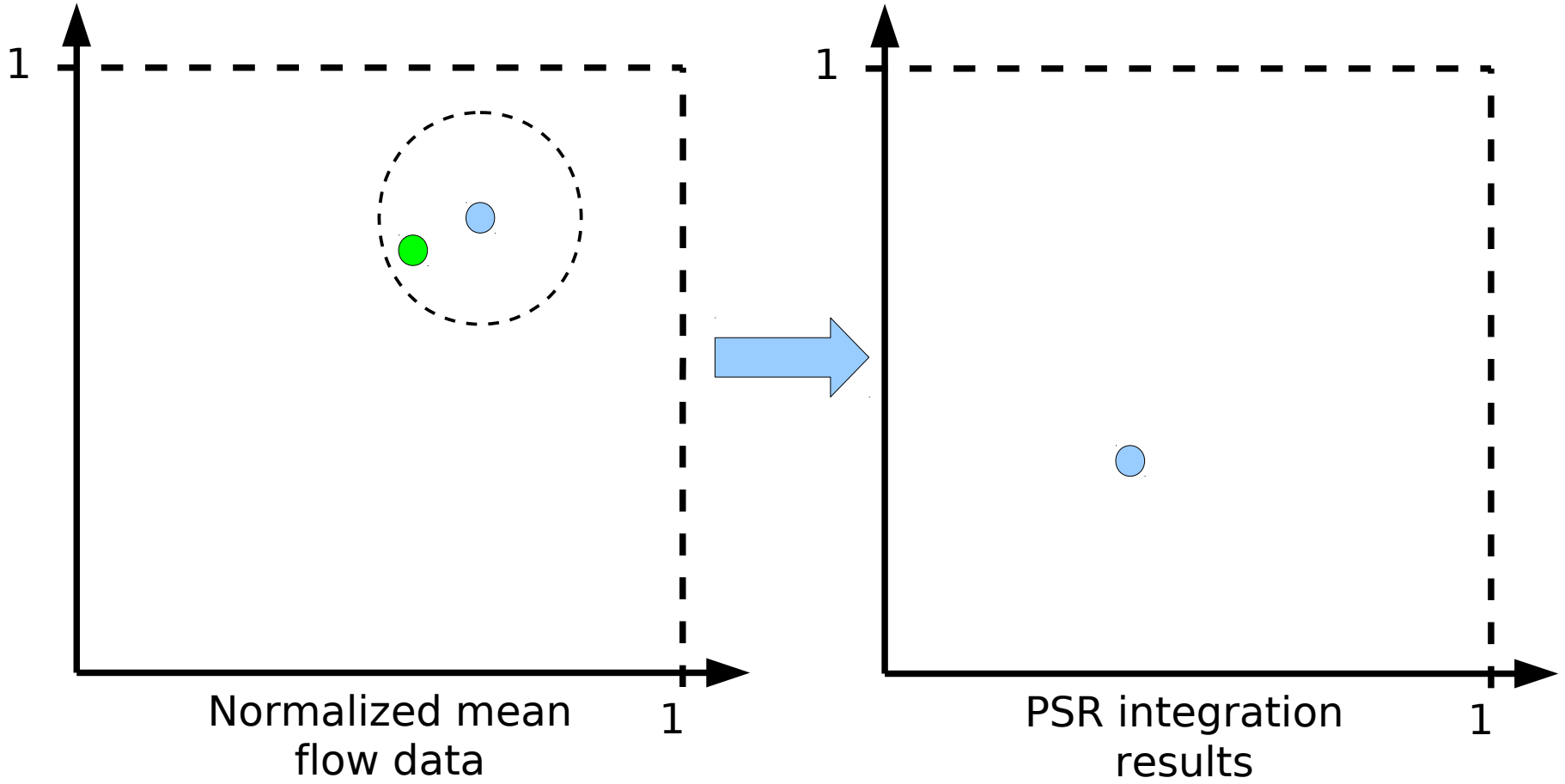
$$\begin{pmatrix} T^* \\ Y_1^* \\ \vdots \\ Y_n^* \end{pmatrix}$$

PSR integration
results

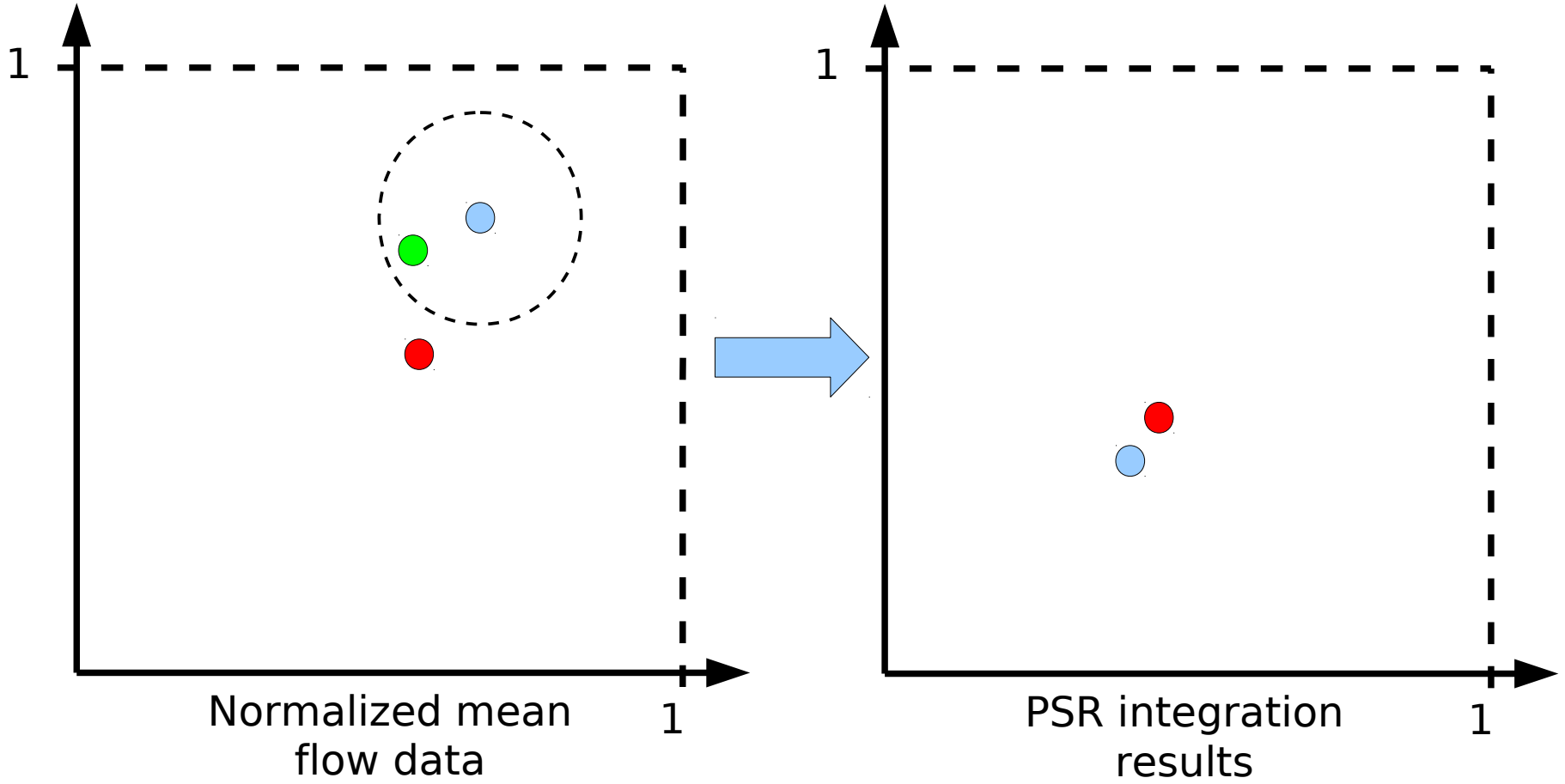
Tabulation of PSR reactor results can provide speed-up and additional stability



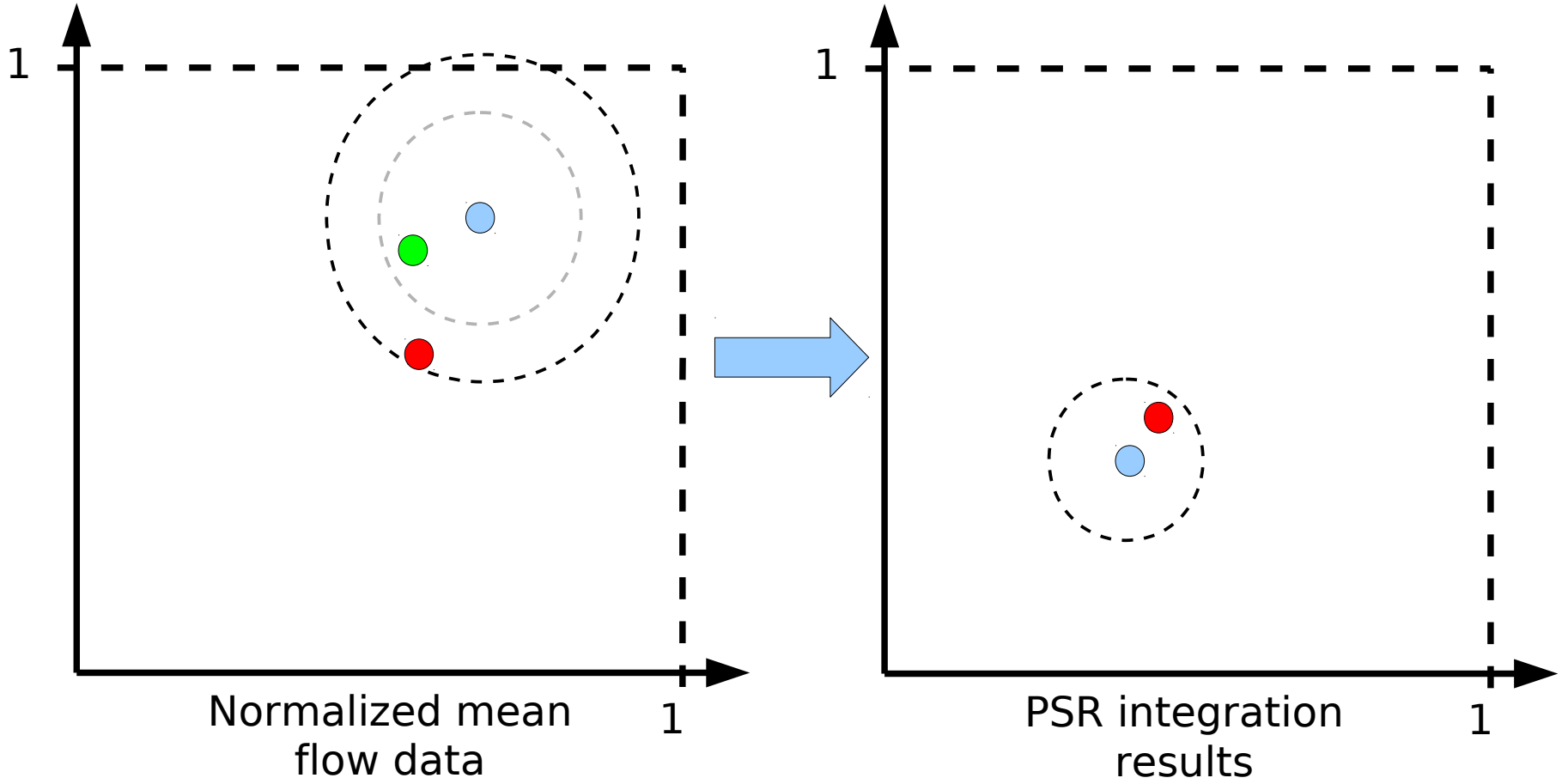
Tabulation of PSR reactor results can provide speed-up and additional stability



Tabulation of PSR reactor results can provide speed-up and additional stability



Tabulation of PSR reactor results can provide speed-up and additional stability



Limiting temperature is possible in steady-state cases

In a steady state case, intermediate “time steps” are not accurate.
→ Temperature may temporarily increase and needs to be limited

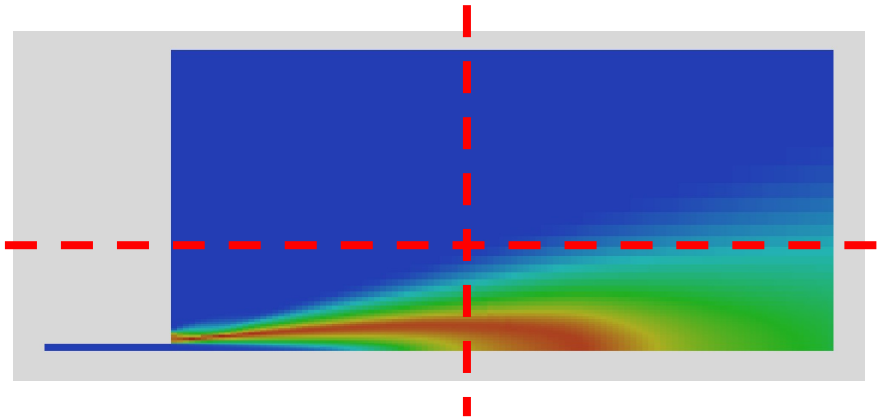
Solver level implementation in edcSimpleFoam:

- New enthalpy field calculated from species mass fractions and T_{min}
- Another enthalpy field calculated for T_{max}
- Both fields are used to limit enthalpy field
- T_{max} and T_{min} are specified in `thermophysicalProperties`

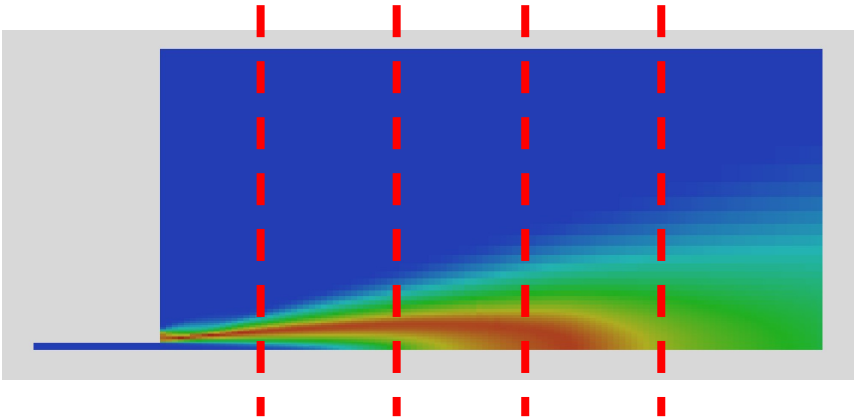
Request for integrated limitation filed in OpenCFD's bugtracker (Issue #57).

Optimal parallelization depends on the complexity of the chemical model

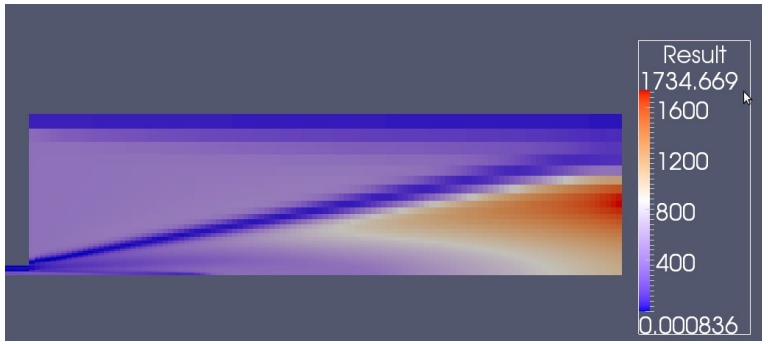
Integrating complex chemical mechanisms is computationally much more expensive than solving transport equations (even if there are many)!



optimized for network bandwidth



optimized for PSR-integration



Overview

Theory

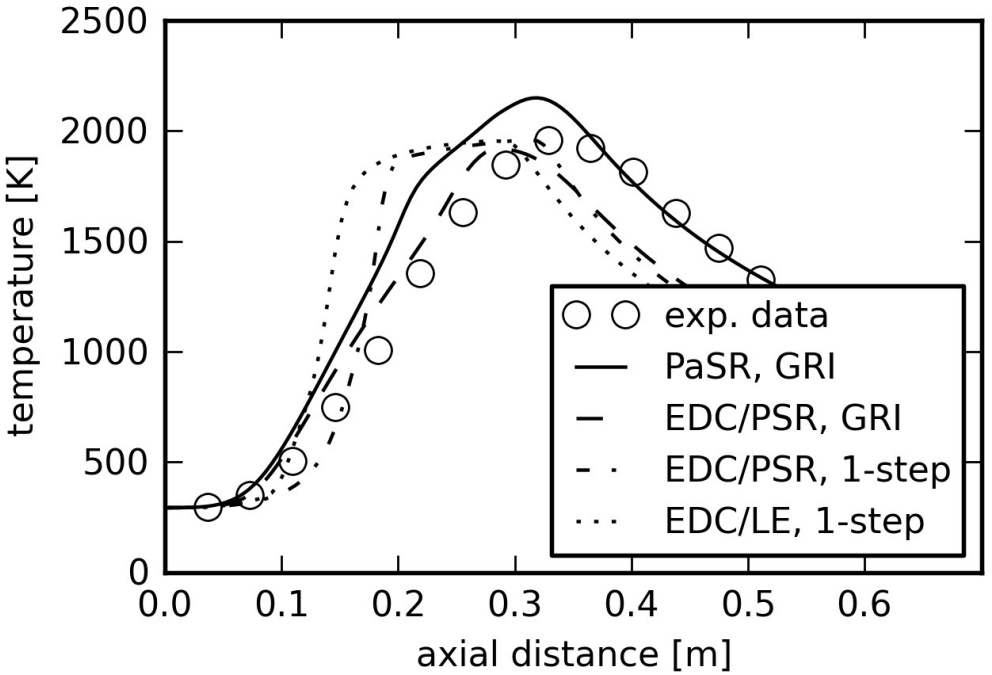
Tutorial case

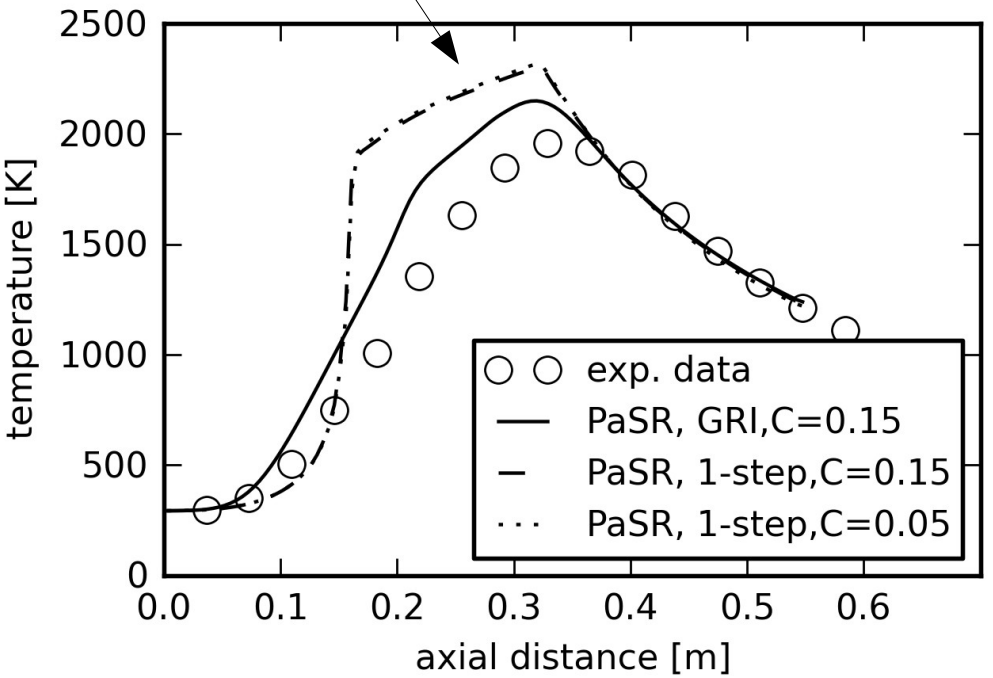
Solution strategies

Validation

Detailed reaction mechnism predicts temperature profile accurately

Influence of C_{mix} is minimal

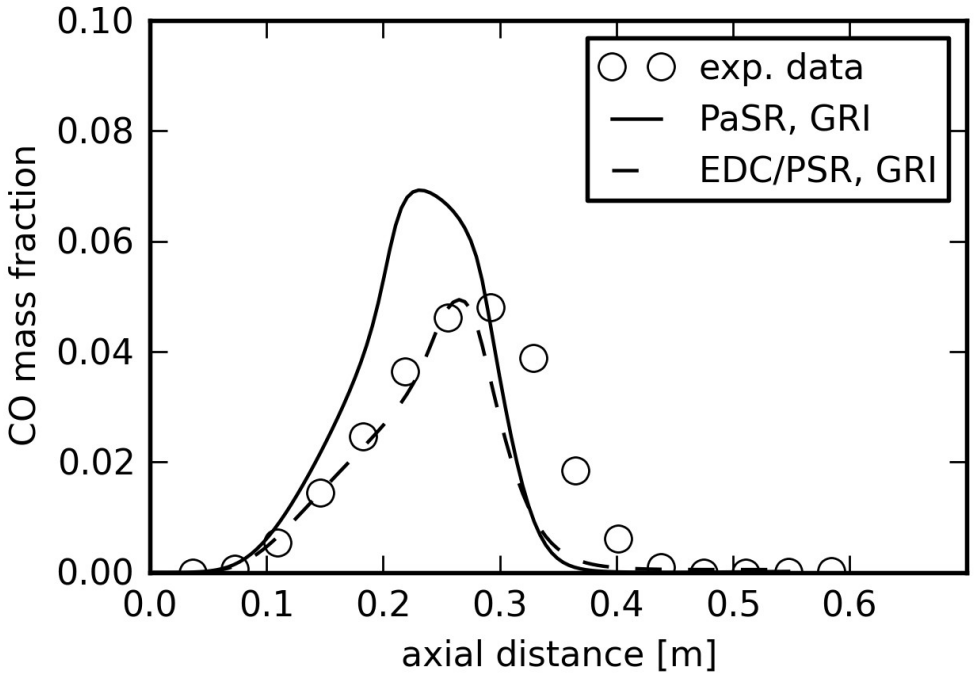


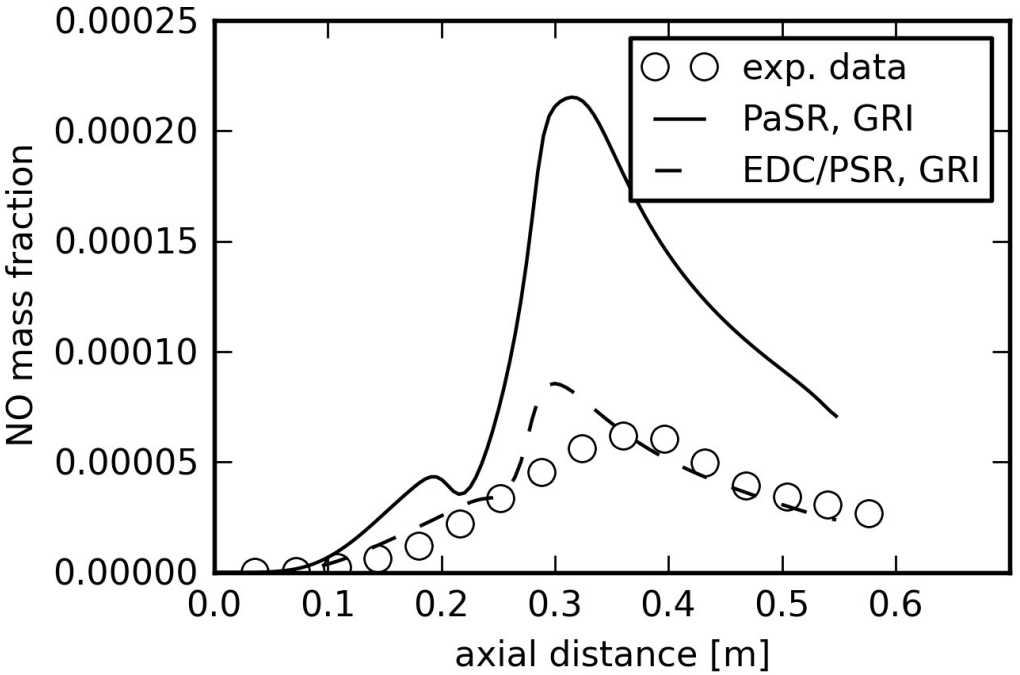


Radiation modeling used with EDC, not used with PaSR.

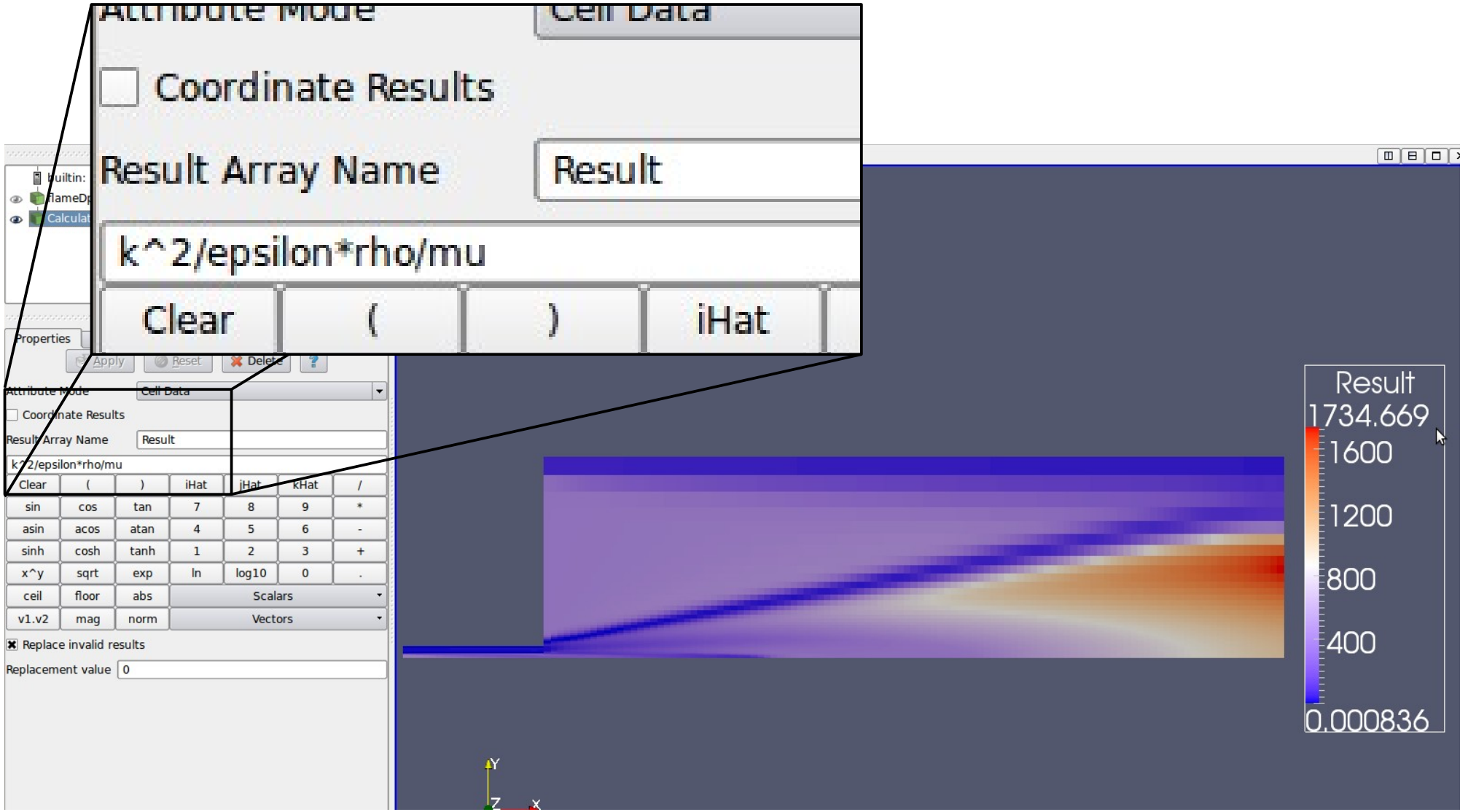
exp. data: Barlow, R. S. and Frank, J. H., Proc. Combust. Inst. 27:1087-1095 (1998)

Intermediate species and pollutants are more difficult to predict





ParaFoam's “calculator” can be used to check Re_t assumption



Comparison with measurements may require special post-processing

Common difficulties when comparing simulated mass fractions with measurements:

- Measured data are often mole fractions or concentrations

  If not all (major) species are measured, correct conversion to mass fractions impossible

- Flue gas or emission monitoring can be measured in “dry gas”, i.e. after water vapor has been condensed out

  Simulated data comprise a complete set, therefore they can be accurately converted

New utility massToMoleFraction *handles conversion together with* “-dryGas” *option*

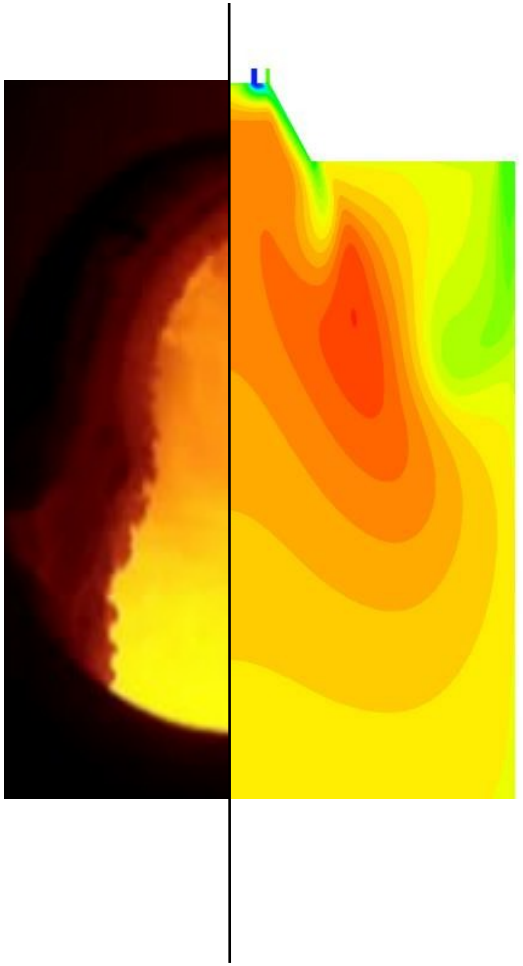
Final note: When using edcSimpleFoam or edcPisoFoam, please cite

for the EDC model:

B. Magnussen: *The Eddy Dissipation Concept: A Bridge between Science and Technology,* ECCOMAS Thematic Conference on Computational Combustion, Lisbon, Portugal, 2005

for the validation of the OpenFoam implementation:

B. Lilleberg, D. Christ, I.S. Ertesvåg, K.E. Rian, R. Kneer, *Numerical simulation with an extinction database for use with the Eddy Dissipation Concept for turbulent combustion* (submitted)



Thank you for your attention!