# Steady-state RANS simulation of a swirling, non-premixed industrial methane-air burner using edcSimpleFoam

Michael Harasek, András Horváth*, Christian Jordan,
Christian Kuttner, Christian Maier, József Nagy, Stefan Pohn

December 2011

Research Divison Thermal Process Engineering &
Computational Fluid Dynamics
Institute of Chemical Engineering, Vienna University of Technology
Getreidemarkt 9/166, 1060 Vienna, Austria

---

## Introduction

At the 6th OpenFOAM workshop in June 2011 new solvers for turbulent non-premixed combustion, edc{Simple,Piso}Foam, including radiation modeling based on the open source CFD-library OpenFOAM were released to the public. This report gives a short evaluation of the steady-state solver edcSimpleFoam. edcPisoFoam is the unsteady counterpart. edcSimpleFoam implements two selectable versions of Magnussen's Eddy Dissipation Concept (see [5], [12] and [13]): EDC/LE and EDC/PSR (Local Extinction and Partially Stirred Reactor respectively).

OpenFOAM is not famous for combustion modeling. Compared to commercial products the selection of solvers and models for reactive flows and combustion is very limited. It was found earlier by the authors that the Chalmers PaSR (Partially Stirred Reactor) model which is the basis of the standard solver reactingFoam can not produce grid-independent results even for simple 2D diffusion flames (this can be tested easily in the included tutorial case in OpenFOAM-1.7.1). Also the solver is unsteady which is a major drawback for industrial applications due to the small time step sizes and the resulting huge CPU-times involved to reach sufficient simulation time for variable averaging (e.g. temperature, species concentration, velocity). Both shortcomings are unacceptable for physically correct and efficient simulations of typical highly turbulent non-premixed burners in the authors' point of view.

## Simulation-setup

The geometry, operating conditions and simulation results of the burner using Fluent 6.3.26 were published in [8]. The same mesh that was used for Fluent was imported into OpenFOAM and the boundary conditions were adapted accordingly.

*Corresponding author: ahorvath@thvt.at

## Boundary conditions

The boundary conditions for temperature (T) and velocity (U) on the outlet patches for an operating temperature of the attached high-temperature oven of 1700 K were set as follows:

```
0/T:
    ".*outlet.*"
    {
        type            inletOutlet;
        inletValue      uniform 1700;
        value           uniform 1700;
    }
```

```
0/U:
    ".*outlet.*"
    {
        type            inletOutlet;
        inletValue      uniform (0 0 0);
        value           uniform (0 0 0);
    }
```

*inletOutlet* is a conditional boundary condition being of Dirichlet type (fixed value) for inflow and a von Neumann type boundary-condition (zero gradient) for outflow. Problems like unphysically high backflow in the simulation were encountered when applying zero-Gradient for U to the outlet patches. The above settings of inletOutlet on T and U are best compared to Fluent's *pressure outlet* with a defined backflow-temperature of 1700 K.

## Applied models

The presented results were simulated using the EDC/LE-submodel. Standard k-$\epsilon$ was the turbulence model, radiation was simulated using the P1 model with an emissivity of $\epsilon = 1$ on all the solid surfaces. Gas radiation was simulated with constant absorption and emission. All variables except the turbulent dissipation rate $\epsilon$, which was set to "Gauss upwind", were discretised using "Gauss linearUpwind cellLimited Gauss linear 1" where applicable. This scheme has 2$^{\text{nd}}$ order accuracy and limits extreme gradients in the variables for numerical stability. Only one chemical reaction was considered:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \ .$$

$N_2$ was the intert specie in the simulation. The inlet stream of the oxidiser was set to air at T=300 K and 20,9 % v/v $O_2$. The flow rates of air and methane were set to yield a power of P=242 kW at an equivalence ratio of $\lambda = 1.04$ accordingly. Like previously published by Harasek et.al. full burn-out of methane is not achieved in the simulated region.

## Solution

The solution of reacting flows is not straight forward, i.e. the correct solver- and boundary-condition-settings don't lead to the desired results right away. The partial differential equation systems involved in reacting flows, that use many different models (advection, diffusion, turbulence and wall functions, species transport, temperature dependent material properties, heat transfer, radiation, reaction, etc.) tend to be numerically "stiff". The usual solution strategies involve solving the cold flow, activating species, reaction and so on in a special order, to avoid a crash of the matrix-solver.

In this work an iteration-method introduced by [7] was modified and applied to the case. The steps necessary to get to a stable and physically correct solution were as follows:

1. Solve the hot flow (1500 K at fuel- and oxidiser inlet) with species transport
2. Solve the hot flow with reaction and lower underrelaxtion-values for species to keep the solver stable

3. Lower the inlet temperatures to 300 K in small steps

4. Activate radiation

5. Set all discretisations to schemes with 2$^{nd}$ order accuracy

6. Increase underrelaxation values of all variables as far as possible

7. Iterate until most residuals are at least below 1e-5

The computational demands are 7.5 GB peak memory during simulation with active species and reaction and approximately (depending on the convergence history) 7 days real time per case when run 32x parallel on Dual Xeon X5500 CPUs (@phoenix new.q). Mostly the phoenix cluster and also VSC2 were used for the simulations. For steady state simulations the disk demands are quite small. The gzip-compressed field variables are stored in 500 MB. The same amount is needed to store one time step when using unsteady solvers.

To test the speed up and the scalability of edcSimpleFoam a benchmark with the much more demanding EDC/PSR-submodel was run on VSC2. The results are presented in the last section.

## Results

Simulation results using edcSimpleFoam and the EDC/LE-submodel of the burner at full load are shown in Figures 1 – 4. The case was converged after approx. 70000 Iterations.

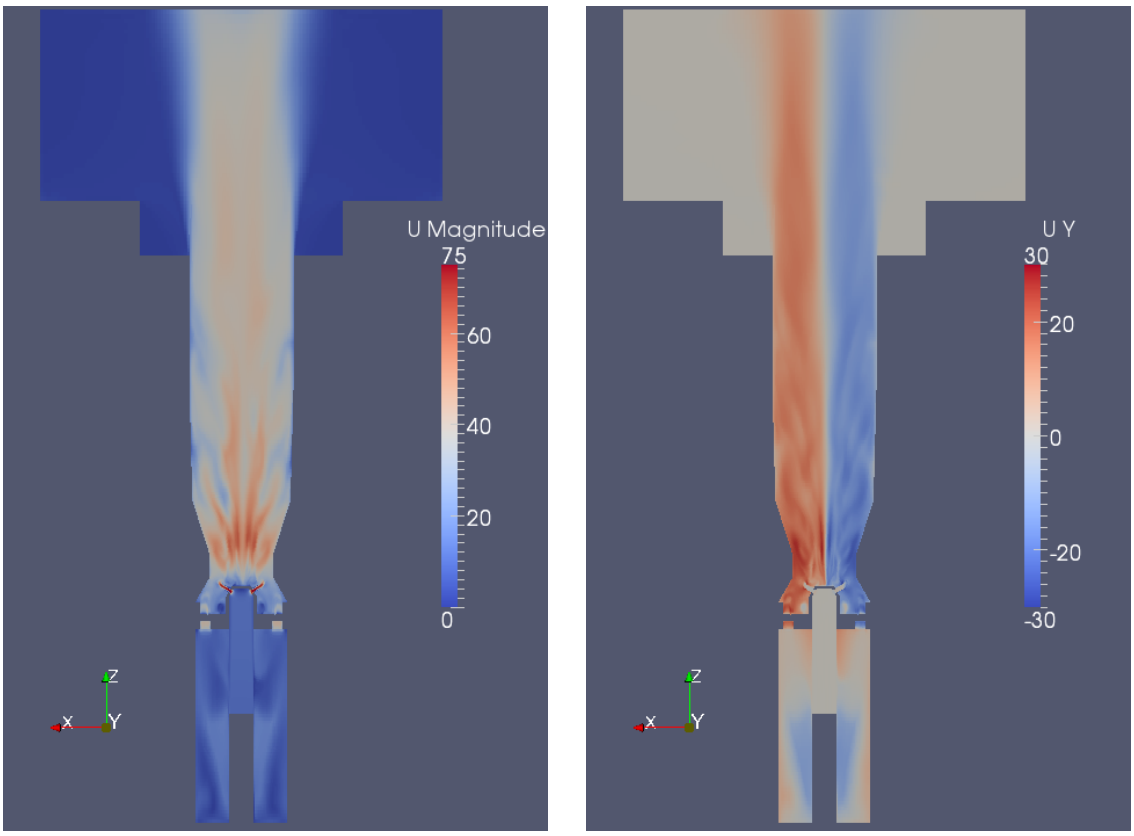


Figure 1: left: velocity magnitude ($m/s$), right: y-velocity ($m/s$).

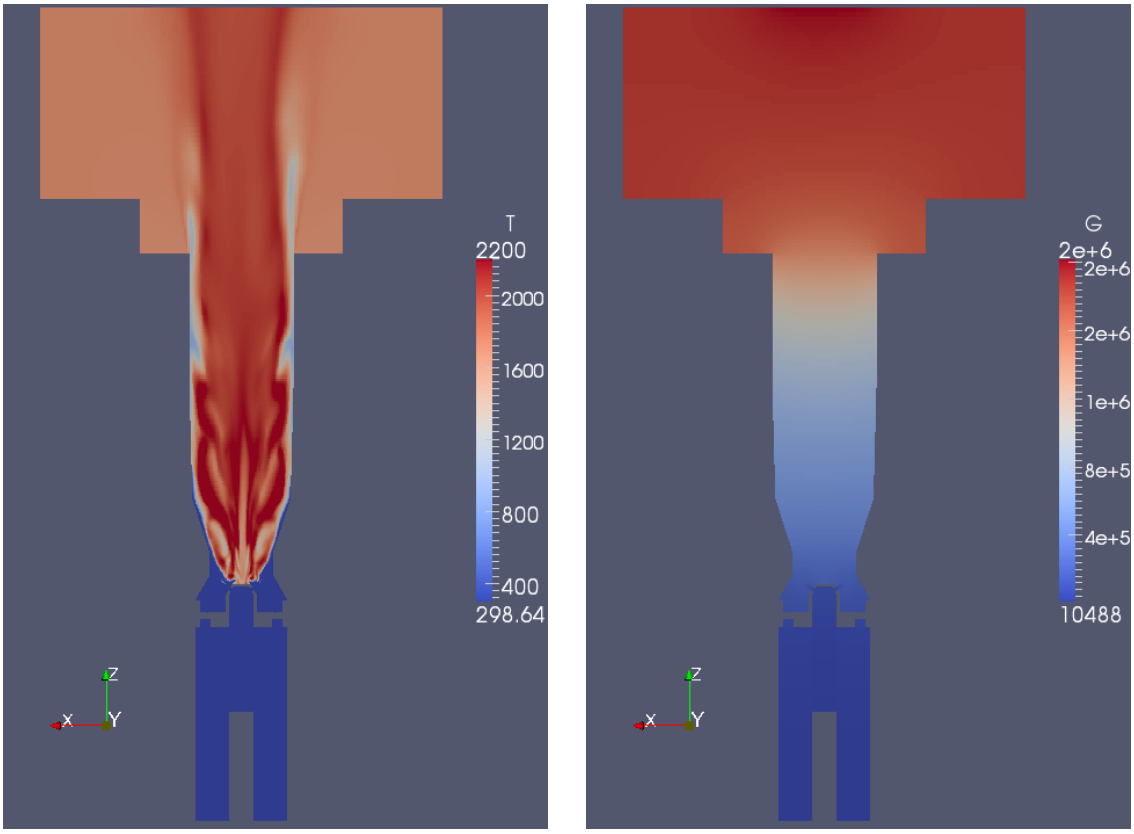


Figure 2: left: temperature ($K$), right: radiation intensity ($W/m^2$).

The contour plots in Fig. 1 show the effect of the expansion of the hot flue gases that accelerate the flow inside the burner. The right part of Fig. 1 shows the highly swirling flow (swirl number S=0.9) created by the swirl generator in the bottom of the burner. The swirl enhances mixing of air and fuel and also stabilises the flame at high gas velocities.

In Fig. 2 the cooling effect of the air on the burner walls and the temperature distribution in the flame are shown. Due to the relatively cool walls of the burner and comparably low emissivity of the flue gases the radiation intensity inside the burner is much lower than in the oven volume.

Fig. 3 shows an uninterrupted layer of air close to the burner walls which doesn't mix with fuel and provides cooling for the refractory material of the burner walls.

It is clearly seen in Fig. 4, showing species mass fractions, that due to incomplete mixing and reaction only approx. 60 % of the available methane reacts inside the computational domain. The rest will react and release heat inside the high temperature oven.

The next steps of the research will include the examination of more sophisticated turbulence and radiation models (RSM and FvDOM respectively) as well as multiple gas phase reactions applied to the notorious Tecflam case in order to validate simulation results with highly reliable and detailed measurements.

## Benchmark for parallel performance on VSC2

To evaluate parallel performance benchmark cases were set up on the Vienna Science Cluster 2 (see `http://vsc.ac.at/`) showing excellent speed-up down to very small domain sizes of 9000 cells and less. The reference case uses 16 CPUs. At the time of writing this is

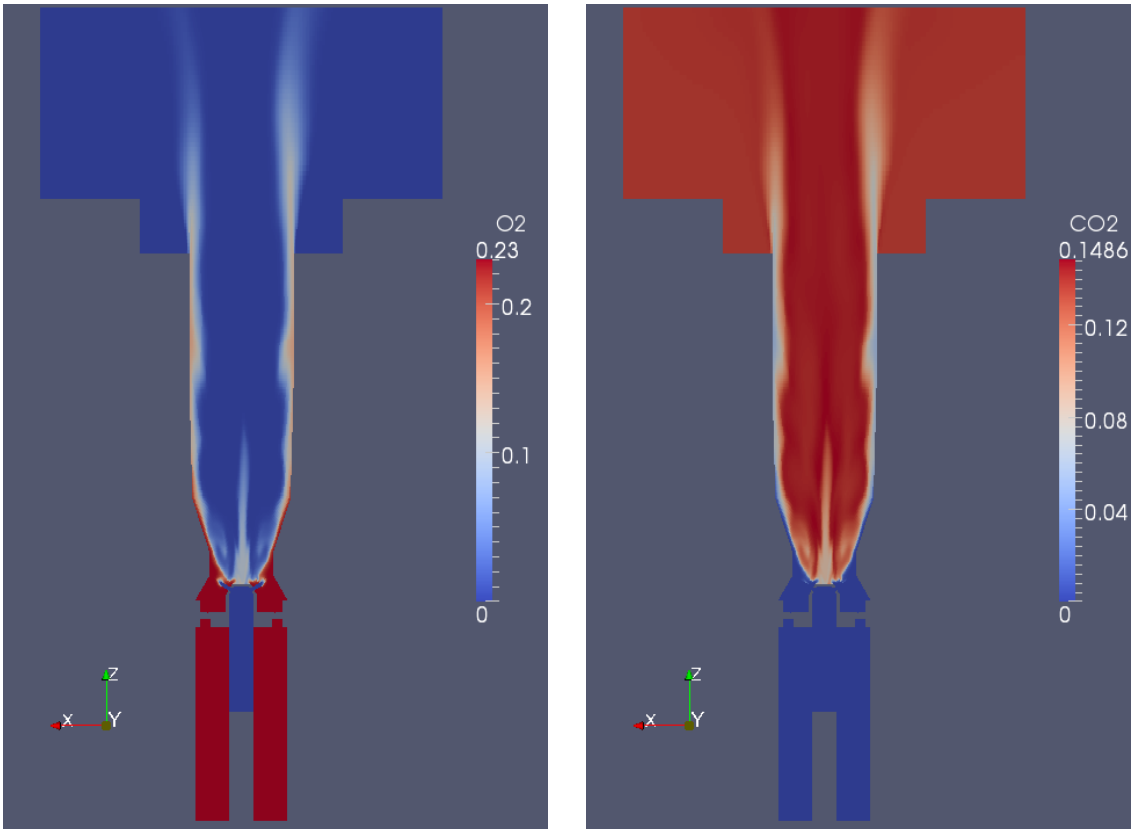


Figure 3: left: species mass fraction of $O_2$ (1), species mass fraction of $CO_2$ (1).

the smallest requestable slot in the batch-queue environment on VSC2. The cluster goes into production in 2012. The benchmarks were performed with a test account.

```
Solver:     edcSimpleFoam (OF-1.7.1) (useBinaryTree off)
Model:      EDC/PSR (single reaction)
Mesh:       4718216 cells (pure hex)
Iterations: 200 (no disk writes except log-file)

Decomposer: scotch-5.1
Compiler:   gcc-4.5.1
MPI:        OpenMPI-1.4.1
```

| par | cells/core(1) | wall time(s) | speed-up(1) |
|---|---|---|---|
| 1x | 4718216 | | |
| 2x | 2359108 | | |
| 4x | 1179554 | 54251 | |
| 8x | 589777 | 31855 | |
| 16x | 294888 | 22203 | 1.0 |
| 32x | 147444 | 11666 | 1.9 |
| 64x | 73722 | 5812 | 3.8 |
| 128x | 36861 | 2749 | 8.0 |
| 256x | 18430 | 1117 | 19.8 |
| 512x | 9215 | 558 | 39.8 |
| 768x | 6143 | 520 | 42.7 |
| 1024x | 4607 | 431 | 51.5 |

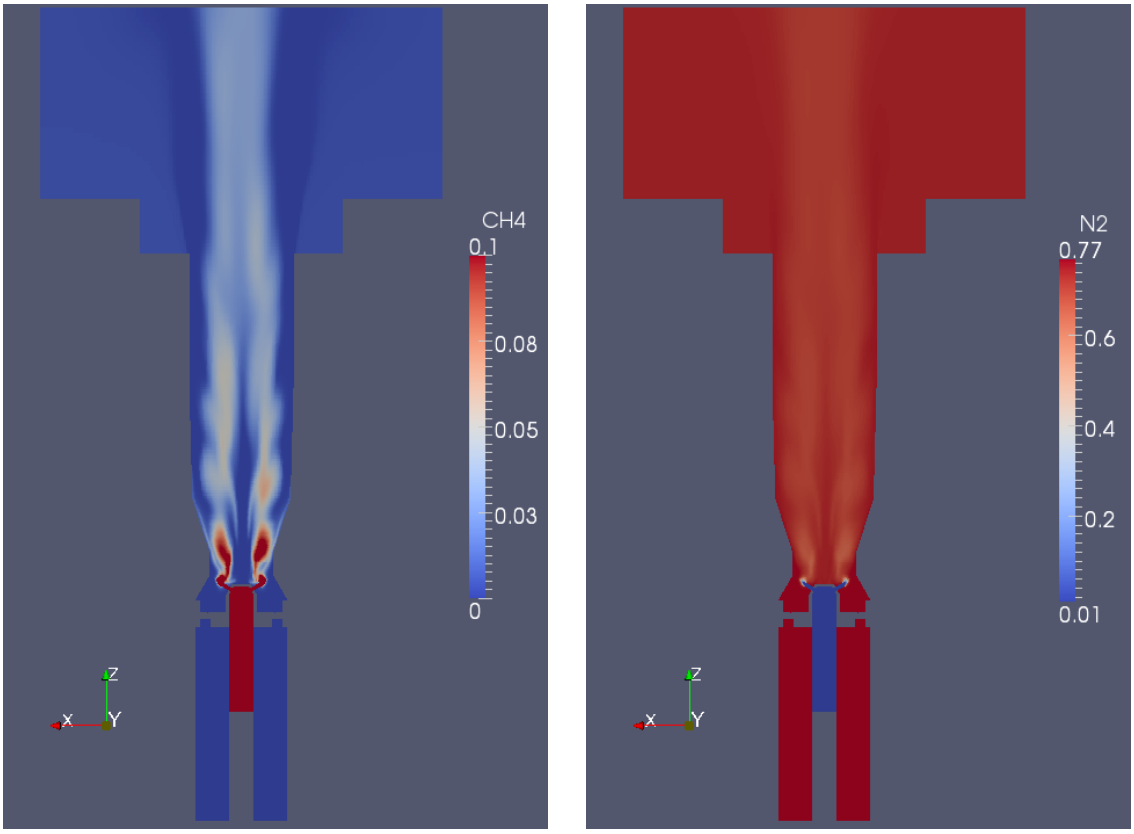


Figure 4: left: species mass fraction of $CH_4$ (1), species mass fraction of $N_2$ (1).

### Acknowledgements

Heartfelt thanks to Dominik Christ from RWTH-Aachen for the publication of the edcSimpleFoam code and also for the kind support and giving the author pointers in the right directions. (The cake was not a lie.)

Thanks also go out to the partners in the FFG-funded "EDAB" project enabling this research in the first place.

## References and further reading

[1] Saad A. Ahmed. Velocity measurements and turbulence statistics of a confined isothermal swirling flow. *Experimental Thermal and Fluid Science*, 17:256–264, 1998.

[2] Guillaume Albouze. *Simulation aux grandes échelles des écoulements réactifs non prémélangés*. PhD thesis, L' Université de Toulouse, 2009.

[3] Robert Barlow and Jonathan Frank. Piloted $CH_4$/air flames C, D, E and F - release 2.1. *Sandia National Laboratories*, 2007.

[4] Robert S. Barlow. Laser diagnostics and their interplay with computations to understand turbulent combustion. *Proceedings of the Combustion Institute*, 31:49–75, 2007.

[5] Dominik Christ. Simulating the combustion of gaseous fuels - 6th openfoam workshop training session. Technical report, RWTH Aachen, 2011.

[6] Ivar S. Ertesvag and Bkorn F. Magnussen. The eddy dissipation turbulence energy cascade model. *Combustion Science and Technology*, 1999.

[7] A. Frassoldati, S. Frigerio, E. Colombo, F. Inzoli, and T. Faravelli. Determination of NOx emissions from strong swirling confined flames with an integrated CFD-based procedure. *Chemical Engineering Science*, 60:2851 – 2869, 2005.

[8] Michael Harasek, András Horváth, Christian Jordan, Christian Maier, and József Nagy. Short notes on the numerical simulation of the effects of oxygen enrichment in a turbulent, non-premixed, swirling methane-air burner. `http://www.zid.tuwien.ac.at/fileadmin/files_zid/projekte/2010/10-166-1.pdf`.

[9] Peter A. M. Kalt, Yasir M. Al-Abdell, Assaad R. Masri, and Robert S. Barlow. Swirling turbulent non-premixed flames of methane: Flow field and compositional structure.

[10] Olaf Keck. *Untersuchungen zur Chemie-Turbulenz-Wechselwirkung an eingeschlossenen verdrallten Erdgas/Luft-Diffusionsflammen.* PhD thesis, Fakultät für Luft- und Raumfahrttechnik der Universität Stuttgart, 2001.

[11] T. Landenfeld, A. Kremer, E. P. Hassel, J. Janicka, T. Schäfer, J. Kazenwadel, C. Schulz, and J. Wolfrum. Laser-diagnostic and numerical study of strongly swirling natural gas flames. *$27^{th}$ International Symposium on Combustion / The Combustion Institute*, pages 1023–1029, 1998.

[12] Bjorn F. Magnussen. On the structure of turbulence and a generalized eddy dissipation concept for chemical reaction in turbulent flow. *$19^{th}$ American Institute of Aeronautics and Astronautics, Aerospace Science Meeting*, 1981.

[13] Bjorn F. Magnussen. The eddy dissipation concept - a bridge between science and technology. *ECCOMAS Thematic Conference on Computational Combustion, Lisbon*, 2005.

[14] A. R. Masri, P. A. M. Kalt, and R. S. Barlow. The compositional structure of swirl-stabilised turbulent nonpremixed flames. *Combustion and Flame*, 137:1–37, 2004.

[15] W. Meier, O. Keck, B. Noll, O. Kunz, and W. Stricker. Investigations in the tecflam swirling diffusion flame: Laser raman measurements and CFD calculations. *Appl. Phys.*, B71:725–731, 2000.

[16] Peter Theisen. *Meodellierung der Turbulenz-Chemie-Interaktion in technischen Brennkammern.* PhD thesis, Fakultät für Luft- und Raumfahrttechnik der Universität Stuttgart, 2000.

[17] Francieli Aparecida Vaz and A. L. De Bortoli. Analytical, numerical and experimental results for piloted jet diffusion flame (Sandia flame D).

[18] Weiping Yang and Jian Zhang. Simulation of swirling turbulent combustion in the tecflam combustor. *Computers and Chemical Engineering*, 32:2280–2289, 2008.