

# On the Influence of Mesh Generation and Manipulation Methods on the Quality of RANS-based Turbulent Combustion Simulations

D. Christ<sup>\*1</sup>, D. Toporov, R. Kneer

Institute of Heat and Mass Transfer (WSA), RWTH Aachen University

## Abstract

A large number of approaches for the generation and manipulation of grids used in numerical simulations are available which differ substantially in the required amount of manual input and operation experience. This study applies the method of "Design of Experiments" (DoE) to evaluate the influence of various parameters on turbulent combustion simulations. Thus, it becomes possible not only to determine the influence of individual parameters but also to quantify the impact of mutual interactions. Several parameters have been studied, including manually built structured and automatically created unstructured grids. Meshes consisting of hexahedral, tetrahedral and polyhedral elements are discussed. Additionally, different grid refinement methods in combination with various discretization schemes for the convection term have been analyzed. The influence of these parameters on the quality of predictions was assessed by comparison with experimental data.

## Introduction

Although a great number of literature especially on various aspects of numerical discretization schemes exist, e.g. Waterson (2007), the influence of mesh type on the numerical results is usually studied on very simple systems including only one or a few transport equations and structured, uniformly spaced meshes. Turbulent combustion in contrary consists of numerous transport equations, meshes are often unstructured in order to fit a certain geometry. Further influence arises from different models for turbulence/chemistry interaction, radiation, turbulence etc. Therefore this study focuses on evaluating the response of this complex system to changes in individual parameters. For a quantification of these responses, the method of Design of Experiments (DoE) is used. The following sections first describe the test case which was simulated, then the mesh generation and refinement procedures applied as well as the details of the solver software used for the simulation. The DoE method is briefly described and the planning and evaluation of the realized "numerical experiments" is discussed.

## Turbulent combustion test case

A turbulent non-premixed methane-air flame has been simulated to study the influence of different mesh generation and manipulation methods on the quality of numerical results. The experimental setup and the measured data were published by Lewis (1981). A sketch of the setup is shown in Figure 1. The turbulent reacting flow includes a recirculation zone so the flow is not aligned with an orthogonal mesh at several locations. Furthermore, since the furnace is relatively narrow the heat transfer from the flame to the furnace walls occurs not only through radiation but also through convective heat transfer. Therefore the gradient of the gas temperature near the furnace wall has a major influence on the resulting temperature inside the flame. For proper velocity profiles in the gases entering the furnace a segment of the pipe flow before the burner was included

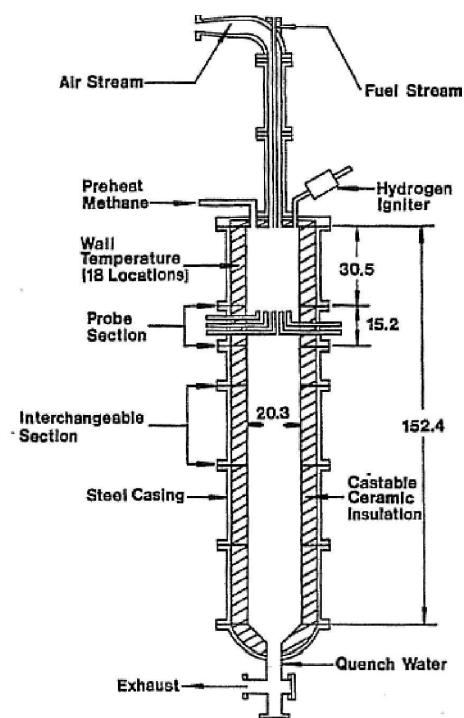


Figure 1: Sketch of the test case in Lewis (1981)

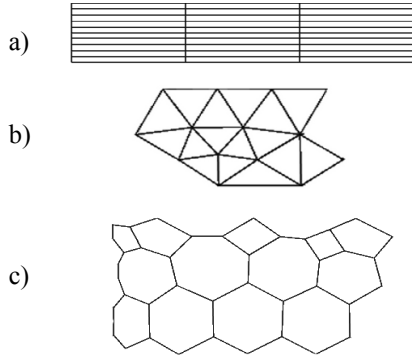
into the simulated domain.

## Generating the mesh

The meshes for this study were generated with the program Salome, version 3.2.6. This software is published as open source and can be used for mesh generation and post-processing of CFD cases. It allows the creation of tetrahedral and hexahedral meshes. Hexahedral meshes yield the advantage that they can be aligned with the main flow direction. As flow through the border of a cell is assumed to be perpendicular to it, aligning the cell borders with the flow minimizes the error induced with this assumption. Tetrahedral meshes are in principle not aligned with the flow and the resulting error is reduced by

<sup>1\*</sup>Corresponding author: christ@wsa.rwth-aachen.de  
Proceedings of the European Combustion Meeting 2009

increasing the cell number similar to increasing the number of pixels in a photograph. An interesting option can be the polyhedral mesh which summarizes several tetrahedral cells into one polyhedron. Thus a high number of cell borders for a better resolution is maintained while the number of cells which determines calculation time is reduced. Examples for meshes consisting of hexahedral, tetrahedral and polyhedral cells are illustrated in Figure 2.



**Figure 2:** Examples of a) hexahedral, b) tetrahedral and c) polyhedral meshes

Preliminary trials showed that refining polyhedral meshes can cause corruption and therefore these were not included in this study. Hence the meshes deployed consist of hexahedral elements. They are two dimensional and the distribution of cells was done either automatically or manually.

Commonly meshes are generated manually, i.e. the distribution of cells along the geometrical object is defined by the user. Thus it is possible to create a mesh that has higher resolution in regions of interest, like the expected position of a flame, or regions containing high gradients, like pipes or inlets, that need fine meshes to resolve important flow details. This approach has the advantage that the mesh can be optimized for the known flow direction and the number of cells can be used more efficiently. Manual mesh generation has to follow certain rules and guidelines as shown in Table 2. However, strictly following these rules does not guarantee a mesh which can lead to stable calculation. Thus creating a suitable mesh for a certain case is to a certain extent a matter of trial and error. In the given case e.g. any mesh grading worsened computational

stability so the cell distribution was kept uniform along each axis.

**Table 2:** Mesh generation guidelines by Casey (2000)

aspect ratio	< 20..100
angle between edges	40°-140°, uniform 90° best
warping angle	< 75°
cell grading	depending on software

In case of automatic mesh generation, the only required user input is the geometry as well as the requested cell type, i.e. tetrahedra, hexahedra or polyhedra. The program Salome offers a further parameter for automatic mesh generation which specifies the mesh resolution as a number from 0 to 1. The automatically generated meshes used in this study were created as coarse as possible with a parameter value 0. As the rest of the mesh generation process proceeds automatically, the time required is significantly shorter than in case of manual grid generation. This advantage has the drawback that the resulting mesh is not necessarily aligned with the main flow direction, the cell resolution is equally high in both more and less relevant regions and in case of complex geometries it may lead to a low quality of the generated mesh. This can cause a necessary mesh inspection and repair.

### Refining the mesh

In order to show that the chosen mesh resolution is sufficient for a given case, the cell size of the existing case was increased and the new results were tested for consistency. This procedure is called mesh refinement study and is also recommended by Casey (2000). The automatically generated mesh in this study has been intentionally designed to be too coarse so that various refinement steps would be necessary before the mesh was fine enough for the solution to become mesh independent. Two different strategies for increasing the number of cells in the mesh were applied: refinement of all cells and refinement of only a fraction of the cells contained in the mesh.

Global refinement of the mesh means simply to double the number of points in each direction. For a

**Table 1:** Applied boundary conditions

	<b>methane inlet</b>	<b>air inlet</b>	<b>furnace wall</b>
<b>velocity [m/s ]</b>	21.3	34.3	wall function
<b>temperature [K]</b>	300	589	1140
<b>k [m<sup>2</sup>/s<sup>2</sup>]</b>	6.8	17.64	zero gradient
<b>omega [1/s]</b>	595	219	zero gradient

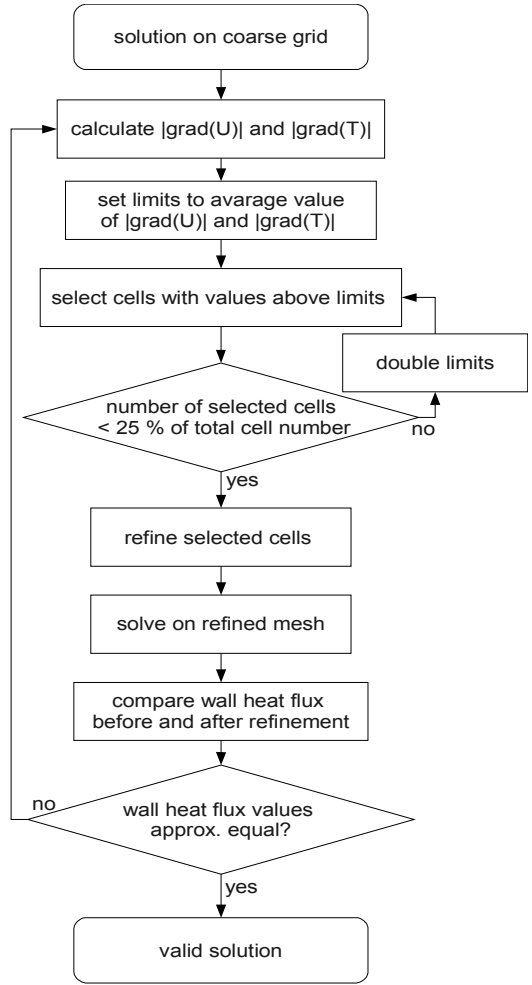
two-dimensional case this results in a quadrupled number of cells. As the refinement is uniform throughout the mesh, the mesh topology is unchanged and characteristic numbers such as orthogonality or warping angle remain unchanged. Global refinement is therefore without influence on the numerical stability of the calculation. A drawback is the resulting high number of cells which includes also cells in regions with minor importance. In this study a converged solution was globally refined until the value for heat flux over the furnace wall stabilized.

During selective refinement, cells are inserted only in regions of interest. This requires the definition of a "region of interest" through numerical parameters which can be chosen arbitrarily. In general, high gradients in pressure, velocity or temperature as well as certain values of temperature, reaction rate or intermediate species may be a suitable indicator for a given case. The increased number of cells in such a region then leads to improved spatial resolution and yields a higher accuracy. The case used in this study consists of a furnace with a flame zone and a pipe flow before the furnace inlets. Consequently, two parameters were chosen, the gradients of velocity and temperature, so that both the velocity profile near the pipe wall and the heat transfer from the flame zone to the furnace wall would be affected by refinement. The algorithm of determining threshold values, selecting cells, mesh refinement and determining the appropriate level of refinement is given in Figure 3. In contrast to global mesh refinement, selective refinement changes the grid topology especially when a single cell to cell connection is replaced by a connection of multiple cells to a single one thus leading to a "hanging node".

### Simulating reacting flow

The simulations were conducted using OpenFOAM, version 1.5. As it is a modular set of tools rather than a monolithic application, creating custom applications for a specific purpose is a common practice. For turbulent reacting flow simulation it was necessary to add a model for turbulent gaseous combustion and for gas radiation. Furthermore a model for calculating the local absorption coefficient was included. The boundary conditions are summarized in Table 1.

The RANS equations are solved by applying the  $k-\omega$ -SST model by Menter (1994). The transport equations for five species, namely  $\text{CH}_4$ ,  $\text{O}_2$ ,  $\text{CO}$ ,  $\text{CO}_2$  and  $\text{H}_2\text{O}$  were implemented containing a source term for volumetric reaction.



**Figure 3:** Algorithm of the automatic mesh refinement procedure

The chemical reactions for the combustion of methane with air were modeled using two global reactions:



The chemical kinetics of these reactions were calculated according to Arrhenius-type reaction rate equations as described in Oksanen (1997). The pre-exponential factor was converted for the use of concentrations instead of mass fractions. The resulting equations are

$$\bar{R}_{kin,1} = 7.18e+10 * e^{-\frac{\bar{T}}{24444K}} [\bar{C}_{CH4}]^{-0.3} [\bar{C}_{O2}]^{-1.3} \left[ \frac{kmol}{m^3 s} \right] \quad (3)$$

$$\bar{R}_{kin,2} = 1.93e+11 * e^{-\frac{\bar{T}}{15152K}} [\bar{C}_{CO}]^1 [\bar{C}_{O2}]^{0.25} [\bar{C}_{H2O}]^{0.5} \left[ \frac{kmol}{m^3 s} \right] \quad (4)$$

These reaction rates, however, are valid for kinetically controlled regions. For regions controlled by turbulent mixing, the Eddy-Dissipation Model (EDM)

**Table 3:** Design of Experiments matrices

design variables and corresponding factor levels (low/high):				effect matrix contains:										
"1": refinement method (selective/global)				main effects ("1","2","3")										
"2": numerical scheme (linear upwind/limited linear)				interaction effects of two design variables ("1&2", "1&3", "2&3")										
"3": mesh generation method (automatic/manual)				interaction effect of three design variables ("1&2&3")										
design matrix				matrix of independent variables							response matrix			
exp.#	design variables			mean value	1	2	1&2	3	1&3	2&3	1&2&3	accuracy	solution time	number of iterations
	1	2	3											
1	low	low	low	+	-	-	+	-	+	+	-	0.6667	0.0305	0.2034
2	high	low	low	+	+	-	-	-	-	+	+	0.3333	0.8527	0.3966
3	low	high	low	+	-	+	-	-	+	-	+	0.6667	0.0224	0.1586
4	high	high	low	+	+	+	+	-	-	-	-	0.3333	1	0.3267
5	low	low	high	+	-	-	+	+	-	-	+	0.4167	0.0723	0.8966
6	high	low	high	+	+	-	-	+	+	-	-	0.5	0.1561	1
7	low	high	high	+	-	+	-	+	-	+	-	0.4167	0.0349	0.4828
8	high	high	high	+	+	+	+	+	+	+	+	0.4167	0.0957	0.6897
effect matrix				0.4688	<b>-0.0729</b>	-0.0104	-0.0104	<b>-0.0313</b>	<b>0.0938</b>	-0.0104	-0.0104	←		
				0.2831	<b>0.243</b>	0.0052	0.0166	<b>-0.1933</b>	<b>-0.2069</b>	-0.0296	-0.0223		←	
				0.5193	0.0839	<b>-0.1049</b>	0.0098	<b>0.248</b>	-0.0064	-0.0762	0.0161			←

from Magnussen (1976) was used.

The basic assumption of the model is that turbulent eddies are homogeneously filled with a single reactant. A reaction can therefore only take place if two eddies, of which one contains methane and the other air, dissolve and both reactants mix. The mean reaction rate of reaction  $j$  for a specie  $i$  according to the Eddy-Dissipation Model is

$$\bar{R}_{EDM,j,i} = v_{j,i} M_i A \frac{\bar{\epsilon}}{K} \rho \min_R \left\{ \frac{\bar{Y}_R}{v_R M_R} \right\} \left[ \frac{kmol}{m^3 s} \right] \quad (5)$$

Here,  $A=4$  is a model constant,  $v_i$  is the stoichiometric coefficient of specie  $i$  and  $M_i$  is the molecular weight. From all reactants of reaction  $j$ , the minimal mean mass fraction  $\bar{Y}_R$  divided by the stoichiometric coefficient  $v_i$  and molecular weight  $M_R$  is used.

The reaction rates from chemical kinetics and the Eddy-Dissipation Model are coupled by the harmonic mean of both values. The total mean reaction rate of reaction  $j$  for specie  $i$  therefore results in

$$\bar{R}_j = \frac{(v_i \bar{R}_{kin,j}) \cdot \bar{R}_{EDM,j,i}}{(v_i \bar{R}_{kin,j}) + \bar{R}_{EDM,j,i}} \left[ \frac{kmol}{m^3 s} \right] \quad (6)$$

Although this is a simplified way of modeling combustion the model shows stable behavior and is computationally inexpensive. Hence the calculation time will be dominated by solving transport equations rather than calculating complex schemes for chemical reaction rates.

Radiative heat transfer was calculated using the P1 model which is included in the recent OpenFOAM release. This model is considered well suited for

combustion applications. In gaseous combustion heat radiation is emitted not only by walls but also by hot gases. The emission coefficient of the gas is therefore non-zero and depends on gas temperature and composition. In addition to a model for radiative heat transfer a formulation for the local emission and absorption coefficient of the gas is needed. Since the current OpenFOAM implementation only offers constant emission coefficients a new model was included into the program core. The weighted-sum-of-gray-gases model (WSGGM) by Smith (1982) treats the gas as a combination of various gray gases with different emission and absorption coefficients. The model assumes, that the local absorption and emission coefficients depend on the temperature as well as the mass fractions of  $CO_2$  and  $H_2O$ . The WSGGM was developed for zonal approaches so it is not directly implementable into mesh based CFD-software. The implementation of the solver used in this study therefore calculates the emission coefficient for each cell according to Smith (1982) and then applies Kirchhoff's law  $\alpha = \epsilon$ .

### Numerical schemes

Two different discretization schemes for the convective term in the transport equations were employed to examine the interaction between the spatial resolution of the discretization schemes and the spatial resolution of the mesh. A general discussion of the classification, derivation and performance for a great number of discretization schemes is given in Waterson (2007). Only a very brief description is included here. The convective transport of a scalar from one cell to its neighbor is calculated using the velocity at the cell

boundary. Velocity values however are given at the cell centers. Applying the arithmetic mean of the cell center values for the cell boundary yields severe numerical instabilities. As a consequence many approaches have been developed which differ in spatial accuracy, calculation effort and numerical stability.

The "linear-upwind" scheme (LUD) extrapolates the value at the cell boundary from the values of the two cells located in the backward direction of the flow. This scheme is widely used, however it can lead to oscillations which result in unphysical values. Here it was used for transport equations discretization. The mass fractions transport equations, however were discretized using the first-order upwind scheme as LUD was unavailable in OpenFOAM for such scalars.

The other utilized discretization scheme was the "limited-linear" scheme. It uses the Total Variation Diminishing (TVD) approach, see OpenFOAM (2008). It contains a non-linear function  $\Psi(r)$  which depends on the ratio  $r$  of the gradients at the boundaries between the cell and its upwind and downwind neighbors. For the limited-linear scheme it is defined as

$$\Psi(r) = \max\left(0, \min\left(\frac{2}{k}r, 1\right)\right) \quad \text{with} \quad (7)$$

$$r = \left(\frac{\partial \Phi}{\partial x}\right)_{\text{downwind}} / \left(\frac{\partial \Phi}{\partial x}\right)_{\text{upwind}}$$

This corresponds to the Chakravarthy-Osher scheme in Waterson (2007). The coefficient  $k$ , with  $0 \leq k \leq 1$ , in (7) corresponds to better accuracy with  $k \rightarrow 0$  and better numerical stability with  $k \rightarrow 1$ , according to OpenFOAM (2008).

### Applying the Design of Experiments

The DoE method distinguishes so called design variables which are varied throughout individual experiments and response values which are measured and are supposed to be influenced by different design variables. For a basic application, each design variable has two factor levels (low and high) and its influence on a response value is denominated "main effect" while the influence of a combination of two or more design variables is called "interaction effect". The DoE method allows to evaluate statistically the significance of the obtained results. This permits to determine if an identified effect is substantial or if it is the product of the cumulation of measurement errors. The study applies the Design of Experiments to a computer performed calculation. As the calculation result is reproducible, the variance is zero which causes all obtained results to be statistically significant, cf. Scheffler (1973).

The following design variables and corresponding factor levels (low/high) were chosen:

1. refinement method (selective/global)
2. numerical scheme (linear upwind/limited linear)
3. mesh generation method (automatic/manual)

These factors are varied systematically within a "design matrix" which is part of Table 3. A number of three factors leads to  $2^3=8$  individual experiments which are realized in a random order to minimize systematical errors.

As response variables were selected: The accuracy of the calculated results, the solution time and the number of iterations necessary until the calculation converges. Both solution time and number of iterations were normalized by division through the largest measured value. The accuracy was determined by comparing the simulated results to experimental data in Lewis (1981). For a representative comparison radial profiles of temperature as well as radial profiles of oxygen mass fraction at several axial distances from the burner were evaluated. The correlation between simulated and experimental data was judged qualitatively since reproducing characteristic details of a profile such as peak values or gradients yields more information about the quality of the obtained results than the residual of an overall curve fit that is calculated quantitatively. For a numerical evaluation the DoE method suggests to use an empirical scale for qualitative data. The accuracy was therefore assigned a value from 0 to 3 from worse to best accuracy respectively. It has to be noted however, that all individual experiments yielded physically realistic solutions, e.g. the peak temperature varied only within  $1884 \pm 56$  K. Therefore the accordance of the results to the experimental data was rated relative to each other. The response value for accuracy was also normalized to the maximum value of 3.

### Discussions

Each individual experiment was carried out as a parallel computation on two processor cores of a SUN X4440 computer. The obtained results are listed in the response matrix contained in Table 3. Main and interaction effects are calculated using the sign from the the matrix of independent variables which corresponds to one particular effect and one experiment and applying it to the response variables of the same experiment. The sum of the values for one column in the matrix of independent variables divided by the total number of experiments is the resulting value for an effect. For example the main effect (ME) of the refinement method on the solution time is calculated according to Scheffler (1973) from the values in the column "solution time" with the signs from column "1" in the matrix of independent variables:

$$ME_{1, sol.time} = (-0.0305 + 0.8527 - 0.0224 + 1 - 0.0723 + 0.1561 - 0.0349 + 0.0957) / 8 = 0.243 \quad (8)$$

The first column in the matrix of independent variables is a unit vector so the resulting "effect" is actually the mean value. It provides a measure when evaluating the importance of main and interaction effects. The values contained in the effect matrix show the influence when changing a factor from low to high. Therefore a negative value means that the response value will decrease when e.g. the limited-linear scheme (high) is applied instead of the linear-upwind scheme (low).

The effect matrix shows that the use of selective mesh refinement leads to an improvement of accuracy of the calculation, having the highest impact on the accuracy from all deployed design variables. Furthermore the time needed for calculation is 24,3 % shorter compared to global mesh refinement. Less iterations were required indicating that the selectively refined mesh contains less cells and as a result the time necessary for one iteration step is shorter. The numerical schemes have only minor influence on accuracy and solution time. However, the solution procedure with the linear-upwind scheme needs approximately 10 % more iterations to converge than with the limited-linear scheme. As the solution time is the same for both schemes, the smaller number of iterations for the limited linear scheme is equalized by its increased computational requirements. The mesh generation approach influences all studied response variables. The automatically generated mesh yields a marginal advantage in accuracy while reducing simultaneously the number of iterations necessary for convergence. The average solution time is 19,3 % increased and 24,8% more iterations are required for an automatically generated mesh than for a manually generated mesh. When taking into consideration the interaction effect

between mesh generation approach and refinement procedure, two possible interpretations are possible. Either the solution time is considerably shorter when a manually generated mesh is employed together with selective mesh refinement (low/high) or the solution time is dramatically increased when an automatically generated mesh is utilized together with global mesh refinement (high/low). Since the individual experiments #2 and #4 took a long time to solve, the second interpretation is regarded favorable.

## Conclusion

This study applied the Design of Experiments method to examine the influence of mesh refinement procedure, numerical scheme and mesh generation method on the accuracy, solution time and required iterations for the convergence of a turbulent combustion simulation. Applying the DoE method leads to a reliable quantitative assessment of the numerical results. It was found that for an accurate solution with low computational effort, automatically generated meshes can be used but only in combination with selective mesh refinement. Manually generated meshes perform well with both selective and global mesh refinement strategies having slight advantages with selective mesh refinement. However, manual mesh generation requires significantly more effort during the design process. The numerical scheme used for calculating turbulent combustion has shown little influence both in required time and accuracy. Based on the obtained results the combination of automatically generated meshes with selective mesh refinement can be used for solving more complex problems in turbulent combustion with advantages in grid generation and calculation time.

## References

- Casey (2000): Casey, M., Wintergerste, T., Best Practice Guidelines, published by ERCOFTAC Special Interest Group on "Quality and Trust in Industrial CFD"
- Lewis (1981): Lewis, M.H., Smoot, L.D., Turbulent Gaseous Combustion Part I: Local Species Concentration Measurements, *Combustion and Flame* 42, pp. 183-196
- Magnussen (1976): Magnussen, B., Hjertager, B., On the Mathematical Modeling of Turbulent Combustion with the Emphasis on Soot Formation and Combustion, 16th Symposium (Int.) on Combustion, pp. 719-729
- Menter (1994): Menter, F.R., Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications, *AIAA Journal* 32(8), pp. 1598-1605
- Oksanen (1997): Oksanen, A., Detailed Application of EDC-Reactor Technique with Extinction in Gas-Fired Furnace, 4th International Conference on Technologies and Combustion for a Clean Environment, pp. 45-50
- OpenFOAM (2008): , OpenFOAM User Guide, Version 1.5, OpenCFD Ltd.
- Scheffler (1973): Scheffler, E., Einführung in die Praxis der Statistischen Versuchsplanung, VEB Deutscher Verlag für Grundstoffindustrie, Leipzig
- Smith (1982): Smith, T.F., Shen, Z.F., Friedman, J.N., Evaluation of Coefficients for the Weighted Sum of Grey Gases Model, *Journal of Heat Transfer* 104, pp. 602-608
- Waterson (2007): Waterson, N.P., Deconinck, H., Design principles for bounded higher-order convection schemes – a unified approach, *Journal of Computational Physics* 224, pp. 182–207