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# ON THE APPLICATION OF CFD IN FIRE SAFETY. BETWEEN THEORY AND PRACTICE OR THE USER'S ROLE

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**Abstract.** *Over the last few years computational fluid dynamics (CFD) has steadily gained attractiveness for fire engineers as a prediction tool for flame propagation, smoke spreading, and other safety-related issues. Compared to other engineering fields, e.g. the automotive industry, with a lot of experience in the application of CFD, the practical application of CFD techniques to fire protection problems is still a major challenge. This lack of experience is caused by complicated – sometimes even unknown – initial and boundary conditions, the conjunction of many computationally expensive physical effects (e.g., radiation, turbulence, and combustion), and the necessity of using very high resolutions and large uncertainties in the input data and model parameters. As a consequence, for a competent and responsible application of CFD techniques the user require in-depth knowledge of fire safety in relation to the possibilities and limits of the CFD codes.*

*Nevertheless, CFD programs for computing fire safety related issues are meanwhile available for all interested users. In the case of the Fire Dynamics Simulator (FDS) program even free of charge [1]. Moreover, advertisements and simple user interfaces suggest easy use of such tools. In contrast, the preconditions to be satisfied in order to obtain reliable results from CFD models are rarely discussed. A frequently asked question reads: "How trustworthy are the results generated by a CFD program?"*

*Yet, even with the best available code at hand, a user lacking sufficient knowledge regarding the implemented physics, adopted model simplifications, and numerical schemes employed in the CFD program will not succeed in producing reliable results and interpreting of them. Such knowledge is, therefore, just as important for trustworthy simulations as the availability of a well-tested CFD program. This article aims at clarifying some important issues in this context. Using the well documented and freely available program Fire Dynamics Simulator (FDS) the paper explains some aspects of the model assumptions, the implemented numerical scheme and discusses their importance for the application in fire safety for rolling stock. It is beyond the scope of the paper to provide more than a rough overview of related correlations but some basics are necessary to understand what is at stake.*

## 1 INTRODUCTION

Modern trains become more comfortable and faster, railway stations and tracks are moved into the subsurface to use the valuable space in the cities, e.g. the German Stuttgart 21 project. A trouble-free and efficient train service is an important component of a functioning economic cycle. In addition to economic aspects, safety aspects play a major role during the development and operation of passenger railway transport systems. In combination with long tunnel systems the relocation of rail traffic into the underground resulting in additional fire safety problems.

A key issue is the prevention and evacuation of heat and smoke. Smoke spreading can lead to dangerous situations very quickly. Fire brigades and rescue teams are not able to get large crowds out of confused smoke-filled railway stations and tunnels. Passengers and staff must be able to move themselves out of dangerous situations.

Another aspect is the damage to the trains and buildings by fire. Even small fires can produce a lot of toxic smoke and heat. The damage to central control units can lead to failure of important functions in the railway system. As a result, e.g., trains cannot approach the next emergency station or important system functions may fail. Furthermore, severe disabilities or even the failure of the railways can lead to a full breakdown of the traffic with significant economic losses. Therefore smoke and heat control is an important issue for fire safety engineering for railway systems.

With the increasing availability of computational power and lower-priced computers, computational fluid dynamics (CFD) is steadily gaining attractiveness for fire engineers who employ numerical CFD programs as a prediction tools for fire safety issues. The use of this technology, however, requires new skills from other scientific disciplines like numerical fluid dynamics, combustion modelling, numerics, and computer sciences. In particular, many problems in these areas are still not resolved conclusively. The use of CFD in fire protection can therefore in no way be regarded as state of the art. It calls for a multidisciplinary approach and the consideration of other scientific facts. Although CFD programs for fire safety related issues are easily available for all interested users, the ability to formally operate and run such programs is not a sufficient criterion for creating trustworthy results and – equally important more – competent interpretation.

This article is organized as follows: After a general description of the fundamental problems and open issues in fire modeling, the article gives a brief introduction to the task of turbulence modeling. Turbulence modeling is an important aspect in the calculation of turbulent combustion reactions. Therefore, the next section discusses some issues between turbulence and combustion modeling process. Against this background, in the last section, the problems become apparent, which occur in connection with the modeling of combustion in practical fire protection.

## 2 OPEN ISSUES

Over the last few years computational fluid dynamics (CFD) gained more and more attractiveness for fire engineers as a prediction tool for flame spreading, smoke movement and other safety-related issues. While in other engineering fields a lot of experience in the application of CFD is established, the practical application to solving fire protection problems is still a major challenge. This difference is caused by the specific practical requirements of fire protection issues. On the contrary to well established fields of CFD applications (e.g. combustion engines or areoplanes) used materials, geometry scales and the dominant physical effects can change rapidly in and between fire safety problems. Even more, there are large uncertainties in the input data. In difference to engineers of e.g. gasoline or diesel engines, fire engineers: i) did not know many chemical reaction details about the combustible materials, ii) boundary conditions changes during the simulation (e.g. if window glasses broken or a construction failed) and iii) simplistic modeling approaches often failed at changing physical regimes.

Even more, fire modelling include many of open research areas with computationally expensive physical effects (e.g. radiation, turbulence, and combustion) and the necessity of very high resolution. For this reason, CFD users require in-depth knowledge of fire safety in relation to the possibilities and limits of the CFD codes and used numerical models.

An important prerequisite for a proper application of any model is a good solution of the specific scale problems in fire protection engineering. These are the different spatial scales: arising from i) the representation of the rolling stock geometry, ii) the relevant scales of the fluid dynamics within and outside this geometry, and iii) the combustion processes. While building structures have spatial scales ranging up to 100 meters, e.g. train station platforms or tunnels, doors and other ventilation openings are in the range of meters and geometrical scales of seats and inventory are in the range of centimeters. For comparison, the necessary spatial resolution to describe the gradients in a diffusion flame are in the range of millimeters.

Figure 1: Example for different spatial scales of a diffusion flame and a wagon.

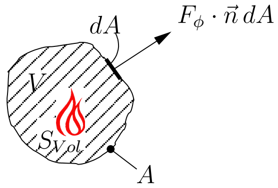
In connection with the spatial scales to be resolved by the model are the time scales of the observed physical and chemical processes. The numerical resolution of the time scale depends on the fastest propagation speed, e.g. the sound speed. It is currently impossible to resolve all relevant scales with the highest possible precision in the CFD models for practical applications in fire protection engineering.

In fact, fire safety engineers are often interested in more common statements as to specific flow information. As a consequence flow models on which fire simulation codes are based rely on a number of simplifications that are justified in most applications. As an example, for fire-induced flows fire protection engineers are normally not interested in resolving sound waves. Instead they may completely filter out their influence by considering the asymptotic limit equations that arise as the Mach number vanishes ($Ma \to 0$). The remaining zero-Mach number equations describe the advection of entropy and vorticity and the influence of the various source terms on these quantities (e.g. [2, 3, 9]). Yet, there are practically relevant situations in which such simplifications may fail and lead to erroneous results, e.g. simulation of explosions.

In the next sections the article discuss some aspects of turbulence and fire modelling using the world-wide used CFD program Fire Dynamics Simulator (FDS) to demonstrate the current problems.

## 3 SCALE PROBLEM AND TURBULENCE MODELLING

In practical problems we are usually not able to resolve all scales within a CFD simulation. What does it mean, when temporal and spatial scales can not be completely resolved, because the available computing capacity is not sufficient? The fundamental equations are able to fully describe the transport processes of the fluid. For example, equation (1) describes the rate of change of the quantity $\phi$ within an arbitrary control volume $V$. The required resolution is determined by physics but the numerical discretization determines the computational cost. What are the consequences if the problem must be represented for computational cost reasons by a lower resolution than required by physics?




$$\int_V \frac{\partial \phi}{\partial t}\, dV + \oint_A F_\phi \cdot \vec{n}\, dA = \int_V S_{Vol}\,(\phi)\; dV \qquad (1)$$

$\phi$ : Variable of control volume

Figure 2: Basic equation for a control-volume approach of $\phi$.

The vast majority of fluid flows in fire protection applications are turbulent. In the conceptual model of turbulence, turbulent flows are composed by eddies of different sizes. The large eddies are unstable and break apart into smaller ones. At the smallest eddies the kinetic energy disappeared and is fully converted into thermal energy of the flow through viscous effects. The full resolution of this process over all scales and dependencies is called Direct Numerical Simulation (DNS). Such simulations are possible only for a few centimeters of volume size.

The main idea of turbulence modeling is to replace the computation of the effects of smaller eddies with a subgrid model. A so-called energy cascade describes the transport of kinetic energy from the largest to the smallest eddies (Kolmogorov's theory [4, 5]). This cascade starts at the system-dependend integral length scale $l_{max}$ and ends at the Kolmogorov scale $l_\eta$, where the kinetic energy dissipate due to viscous forces. Using this theory, turbulence models approximate the net-effect of the neglected part of the cascade. Therefore a coarser numerical resolution is possible. Unfortunately there is no common valid turbulence model available.

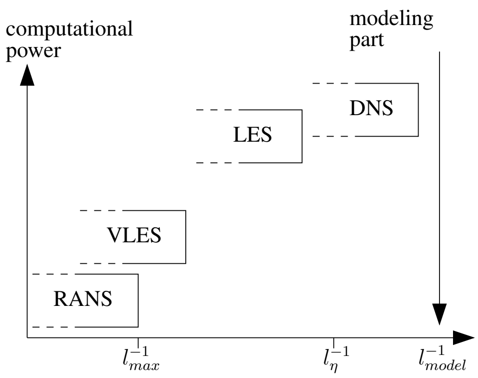



Figure 3: Resolved length scales of different turbulence models.

Therefore different turbulence modelling approaches exist, more or less useful for a limited range of applications. For practical fire simulations we have to use one of these turbulence models. Through the use of under-resolved representations of the basic equations, we cut off a part of this cascade. The location of this cut depends on the turbulence model. Older and most common turbulence models are Reynolds-averaged Navier-Stokes (RANS) models. This RANS-models cut off the complete part of the cascade beginning from the integral length scale $l_{max}$. The integral scale of turbulence, which is roughly the largest scale within the cascade.

With increasing computational power Very Large Eddy Simulation (VLES) or Large Eddy Simulation (LES) models provides the resolution of a part of the cascade. Nevertheless, a common problem of all turbulence models are i) the use of more or less problem-dependent empirical parameters and ii) difficulties in reproducing the fundamental mathematical concept of smaller truncation errors with decreasing grid spacing. For more details see [8].

In connection with this problem, however, we are interested in another subject. For simplification we consider a discretization using a Cartesian grid as shown in figure 4.

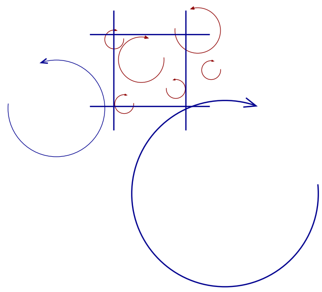


Figure 4: Resolved (blue) and unresolved (red) vorticies in a cartesian grid.

Vortex structures with length scales smaller than the grid length scale can no longer be represented by the discretization. The net-effect of this filtered eddies must be taken into account by a turbulence model. Furthermore, equation (1) changes to a representation of a numerical resolved mean value of $\widehat{\phi}$

$$\int_V \frac{\partial \widehat{\phi}}{\partial t} \, dV + \oint_A F_{\widehat{\phi}} \cdot \vec{n} \, dA = \int_V S_{Vol} \left( \widehat{\phi} \right) \, dV. \tag{2}$$

Depending on the turbulence model and the grid spacing, equation (2) represents now the behavior of turbulence model averaged values. Both, the closure terms of the turbulence model approach, as well the source term $S_{Vol} \left( \widehat{\phi} \right)$ require model and material parameters as turbulence model averaged values. Using this modeling approach and appropriate turbulence models, it is possible to use larger mesh sizes to reduce the computational costs. In practice of fire safety engineers, a grid spacing of 10 cm or more is used.

### 3.1 Turbulence modelling and combustion

Up to this point we have not considered the influence averaging to the modelling of combustion. In the energy equation the source term $S_{Vol} \left( \widehat{\phi} \right)$ includes the modelling of the combustion process. Combustion processes are strongly influenced by local temperature-dependent quantities. But with practical grid spacing of 10 cm and more the temperature profile within the combustion zone can not be resolved with such averaged turbulent quantities.

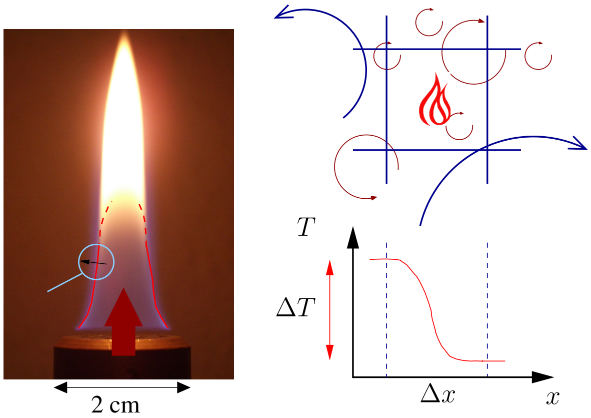



Figure 5: Dimension of a diffusion flame (left) and unresolved temperature profile in a grid cell because of numerical turbulent averaging (right).

As seen in figure 5, it is not possible to reproduce the local temperatur profile with the averaged temperatur $\widehat{T}$ of the grid cell provided by equation (2). In this case the combustion zone is completely unresolved. What does that mean for modelling of practical fire safety problems?

## 4 SOME ASPECTS OF FIRE MODELLING

Fire modelling is a important source term for CFD simulations in fire protection. Fire protection engineers distinguish between different types of fires: e.g. pre-flashover and post-flashover fires, hydrocarbon, wood or smouldering fires. However, in the scientific discipline of numerical combustion modeling, a different classification is used. Figure 6 gives a simplified overview.

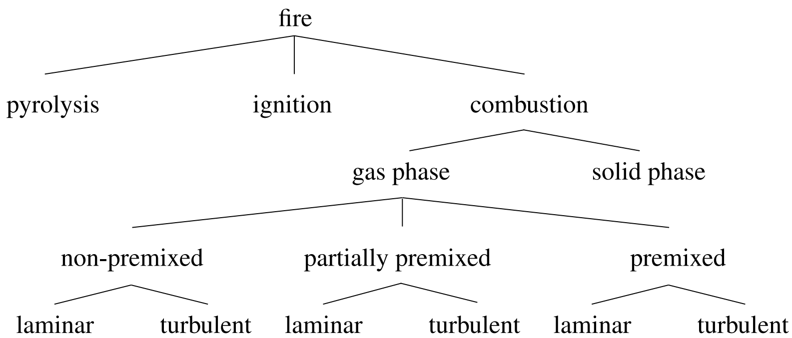



Figure 6: Subdivision of fire into different model regimes.

Combustion modeling is a still very active research area, far from providing general models. In the following discussion we limit our description here to combustion in the gas phase. As shown in figure 6, combustion in the gas phase can be divided in three different modes.

In the non-preximed combustion mode fuel and oxygen are not mixed and separated by the combustion zone. In the premixed mode fuel and oxygen are mixed and the flame moves from the burned to the unburned area. Between these two modes partially premixed combustion takes place. While there are well-functioning model approaches for premixed and non-premixed combustion, partially premixed combustion is an open research area and only a few model approaches with limited range of applications are available. However, it is a quite important regime for fire protection application.

Detailed combustion calculations requires high resolution in space and time. One reason is the mutual influence of combustion reaction and flow. For example, vortices inside the combustion zone affects the species concentrations of fuel and oxygen. The species concentration determines the chemical reaction kinetics and thus the products of combustion. Conversely, the combustion energy generated during combustion leads to local changes of densities and other variables. As a consequence of the modeling difficulties and the immense computational requirements, CFD programs for fire protection are often limited to simplified combustion models.

In the case of the Fire Dynamics Simulator (FDS) a mixture fraction model based on a global step reaction model is implemented. The model is based on the assumption, that the reaction takes place on an infinitely thin flame sheet. This thin flame sheet separates fuel and oxygen in the grid cell. Than a mixture fraction $Z$ can be defined as the ratio of the mass of a subset of the burnable species to the total mass present in the volume [6]. With the assumption "mixed is burned" combustion takes place where oxygen and fuel exist in a grid cell. The combustion process itself is described by a global one step reaction. e.g. for methane

$$\mathrm{CH_4} + 2\,\mathrm{O_2} = 2\,\mathrm{H_2O} + \mathrm{CO_2}. \tag{3}$$

This mixture-fraction approach dispense with a detailed analysis of combustion, in favor of computational efficiency. However, in this way, no detailed chemical kinetics can be modeled. The production of soot and toxic gases must therefore be specified by the user. This is done via specific yield parameters in FDS.

The question remains how the fuel comes into the flow domain. The most common way is a user-defined time-dependent heat release function, called heat release rate per unit area (HRRPUA). Hence FDS calculates with the given heat of combustion value a fuel mass flow through user pre-defined surfaces. These kind of pyrolysis approximation is totally independent from the physical interaction between the reaction flow field and the pyrolysis process in the solid. To be precise, there is even another, more or less simplified pyrolysis model in FDS, but because of many unknown model parameters not widely used for practical applications.

Figure 7 demonstrates a mixture fraction combustion simulation in FDS. Defined by a time-dependent HRRPUA function fuel ($Z = 1$) flows through the surface of a user-defined object into the flow field ($Z = 0$). This results in a separating surface between fuel and fluid. In each grid cell with this separating surface, where fuel mixed with oxygen from the initial fluid ($1 < Z < 0$), the combustion process (mixed is burned) is computed based on the simple global one-step reaction.

In fact, this kind of fire modelling is far away from the detailed combustion modelling of e.g. gasoline or diesel engines. On the other hand, it is a possibility to estimate the effects of pre-defined worst-case fire scenarios in larger geometries. However, the users must be aware, that all these simulations based on strong simplifications. Neither explosions nor re-ignition of premixed fuel-oxygen smoke situations covered by this kind of a mixture fraction model.

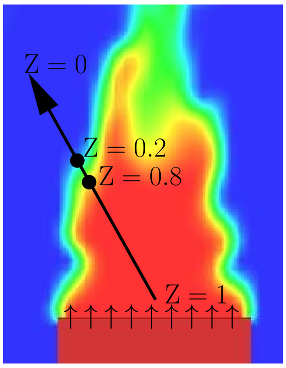



Figure 7: Local mixture-fraction combustion over a fuel-emitting surface.

## 5 CONCLUSIONS

Computational fluid dynamics codes are complex and the user's knowledge regarding the implemented physics, additional model simplifications, and numerical schemes employed in a CFD program is just as important for trustworthy results as the code itself [7].

The vast majority of fluid flows in fire protection engineering are turbulent. As described above for CFD simulations it is generally impossible to resolve all details of the turbulent fluctuations. Therefore, turbulent flow CFD simulations are notoriously under-resolved and describes the net effects of turbulent flows in the form of more or less empirical closure terms. Consequently, further assumptions are necessary to resolve this conflict. Because the combustion process is the driving force of the fire-induced flow, the understanding of these issues is quite important.

In simplified terms, the user should know that the grid size affects more than just the computational speed of his program but also the underlying physics. Therefore, engineers performing CFD simulations of safety-related fire protection issues need not only an in-depth knowledge about the underlying physics and the used numerics but also about the interaction between both.

Taking into account the specific constraints, computational fluid dynamics (CFD) is a valuable tool for safety analysis in fire protection. Its application requires a lot of experience in a multidisciplinary field of fire protection, fluid dynamics, combustion dynamics and especially scientific computing and numerics. Computational fire modeling is far away from being state of the art – not to speak about putting it into a normative standard.

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