Numerical Simulation and Validation of Pyrotechnic Smoke Emissions

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Abstract: *This paper aims at evaluating the practicability of an alternative strategy for the classical assessment of possible hazards aligned with the use of theatrical pyrotechnics especially at indoor venues, where the emission of solid reaction products (aerosols) is an important factor for permission for the use of pyrotechnics at stage shows. A CFD model was used to calculate the respective aerosol liberation and dispersion in a specific indoor facility. The results from these numerical simulations were compared with respective aerosol number concentration measurements carried out before, during, and after the burn-off of theatrical pyrotechnic fountains in an examination room, representing a small stage or theatre. The simulation results reveal a fair agreement with the experimental results in general, with the trend to conservatively over-predict the aerosol concentrations at close range to the pyrotechnic article. The time dependent increase and decline of the aerosol concentrations due to the ventilation conditions as observed in the preceding experimental studies could be reproduced in the simulations.*

Keywords: *Theatrical pyrotechnic articles, aerosols, CFD*

Introduction and background

The use of pyrotechnics, such as theatrical articles, for numerous stage and television productions, is globally increasing. New effects and further developments widen this field of application almost every week. Due to this challenging evolution, effective measures are necessary in order to assess the possible risks aligned with the use of such articles, especially during indoor productions, where the audience and the production staff involved are exposed to potentially harmful reaction products of relevant concentrations. Enforcement bodies, e.g. those responsible for the permission for shows including the use of various pyrotechnic articles, are often overwhelmed by the large variety of different special effects and the impacts of the reaction products associated with them. This leads in many cases to a complete rejection of the use of pyrotechnics at a specific venue, just to avoid a situation where the enforcers could be blamed for not acknowledging all possible hazards.

In general, pyrotechnic articles to be placed on the European market fall under the scope of the Directive 2007/23/EC.[1] Theatrical pyrotechnic articles are categorized in the following categories:

- T1: pyrotechnic articles for stage use which present a low hazard, with a further sub-categorization T1 "for outdoor use only", if considered necessary.
- T2: pyrotechnic articles for stage use which are intended for use only by persons with specialist knowledge.

The provisions of that directive assure that these articles are first introduced to a notified body in order to get them appropriately type tested and to demonstrate that all essential safety requirements of this Directive are fulfilled. Furthermore, the articles produced after that EC type-examination must also be in conformity to the initial type. This is usually guaranteed by applying sufficient quality systems for production and/or end product testing (e.g. batch testing), which are subject to regular

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inspections by notified bodies, as well.

However, the technical requirements for certification purposes as given in the applicable standard series prEN 16256[2] cover only performance parameters (such as effect dimensions, burning rate and sound pressure level etc.), net explosive content (NEC) and properties of the articles before, during, and after functioning (integrity, stability, unintended explosions, burning matter on ground etc.). Explicit requirements on gaseous or solid reaction products are not included in this standard. The categorization into T1 "for outdoor use only" may only be based on subjective observations of aerosol emissions during the EC type-examination tests by the staff, if all other requirements are met. Furthermore, how does a parallel use of numerous articles, in which all single articles have an indoor use permission, change the authorization of the use of such articles in a theatrical show? A reliable forecast of possible hazards due to the parallel firing of diverse articles is almost impossible for the pyrotechnicians and the enforcement bodies. Confident permission for an envisaged use of theatrical pyrotechnic articles can only be given if all relevant boundary conditions, such as ventilation systems, room geometry or any other protective measures of the affected persons are considered.

Numerical simulations, e.g. computational fluid dynamics (CFD), may play a major key role in future evaluations of such cases, as they can be considered as a possible alternative in this application field to estimate the potential hazard of the use of specific pyrotechnics under defined conditions. CFD is an effective and powerful tool, especially when considering the increasing development of computational processing power in the recent past. In addition, the results from CFD calculations might be integrated in quantified risk assessments (QRA), as well, in order to get a more reliable statement.

The objective of this work was to investigate the practicability of CFD in terms of accuracy of results, time and effort, compared to conventional estimations of the impacts of solid reaction products (aerosols) on a possible indoor use of the respective pyrotechnic articles. This has to be seen in the context of making the authorization process easier for the involved parties: applicants (pyrotechnicians or manufacturers) and enforcement bodies.

For model validation purposes, the respective CFD calculations of this work, using ANSYS CFX V14.0, were compared with the results obtained from previous aerosol measurements during the burn-off of theatrical pyrotechnic articles at an

Figure 1. *Examination room for the measurements carried out by Dutschke et al.*[3]

indoor venue by Dutschke *et al*.[3]

Previous experimental setup – overview

In order to get a reliable validation of the applied numerical model, a case study was chosen in which aerosol emissions during the burn-off of theatrical pyrotechnic articles in a venue-like environment were investigated. These results were previously published by Dutschke *et al*.[3] In this work the authors measured particle number concentrations in the indoor air during and after the burn-off of fountains (amongst others) under defined ventilation conditions. The experiments were performed in a lecture hall with several seating rows, depicting a theatre or stage, see Figure 1.

The room had an overall volume of approximately 718 m^3, offering the following ventilation conditions:

- Outlet – integral: 4400 $m^3\,h^{-1}$ (directly through openings at the room ceiling), and
- Inlet – integral: 4200 $m^3\,h^{-1}$ (directly through circular openings underneath each seat and implicitly through the clearance between both door frames and door panels due to the dominating outlet ventilation conditions).

The theatrical fountains were burned off centered between both laboratory benches, see Figure 1, with the following average properties: burning time 10 s, effect height 3 m, net explosive content (NEC) 32 g.

The local particle number concentrations were measured over minimum 30 minutes at three defined measuring points. The experiments were carried out for each measuring point separately with identical fountains, since only one measuring device (Scanning Mobility Particle Sizer, SMPS) was available. The measuring points in the examination room are shown in Figure 2. The exact same points were also used as validation references

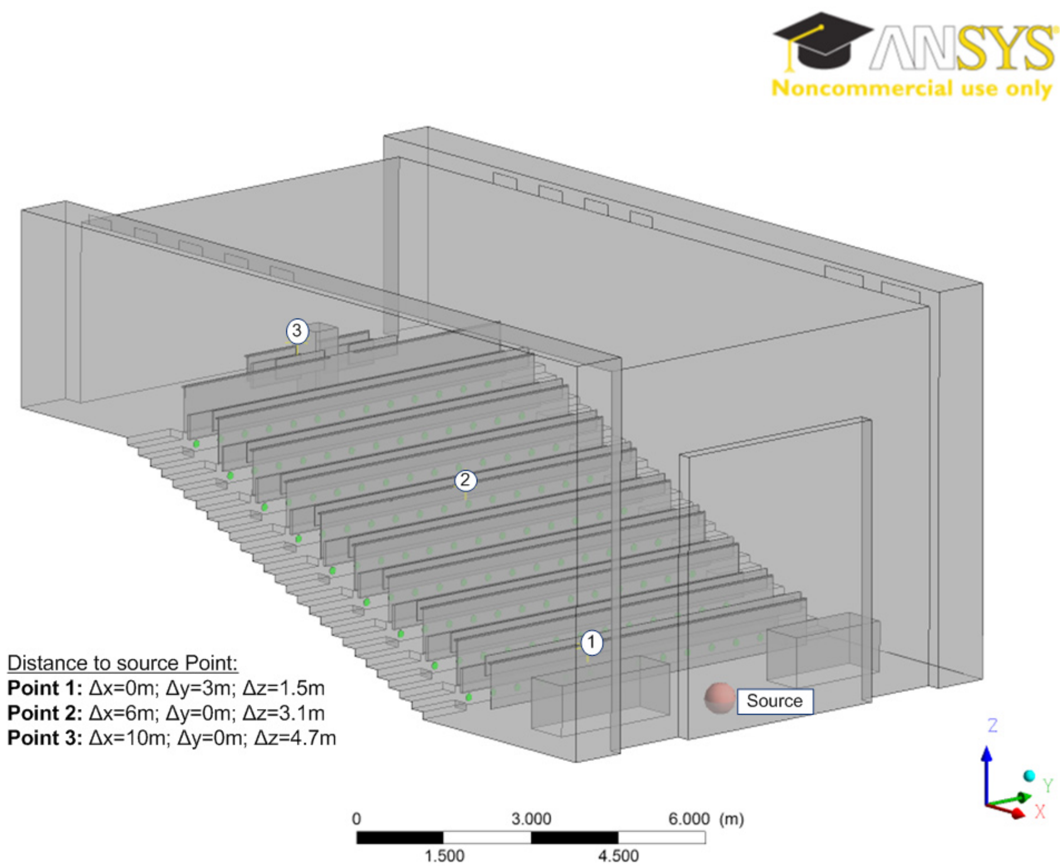

Figure 2. *CAD model of the examination room.*

(monitor points) for the CFD simulations described as follows.

Numerical modeling

The overall goal of the simulations with ANSYS CFX V14.0 was to calculate the liberation of smoke due to the burn-off of a theatrical pyrotechnic fountain and the following transport and dispersion of that smoke in the examination room.

Governing transport equations

The following equations for the conservation of mass, momentum and energy generally apply for three-dimensional, transient, compressible, laminar Newton fluid flows (in Cartesian tensor notation):

Continuity equation (conservation of mass):

$$\frac{\partial \rho}{\partial t}+\frac{\partial\left(\rho u_i\right)}{\partial x_i}=0$$

Momentum equation: Navier–Stokes (conservation of momentum):

$$\frac{\partial \rho u_i}{\partial t}+\frac{\partial\left(\rho u_i u_j\right)}{\partial x_j}=-\frac{\partial p}{\partial x_i}+\frac{\partial \tau_{ij}}{\partial x_j}+\rho g_i$$

and

$$\tau_{ij}=\eta\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\eta\frac{\partial u_i}{\partial x_i}\delta_{ij}$$

Species transport

$$\frac{\partial \rho \mu_k}{\partial t}+\frac{\partial \rho u_i \mu_k}{\partial x_i}=\frac{\partial J_{k,i}}{\partial x_i}+S_{\mu k}$$

and

$$J_{k,i}=-\rho D_k\frac{\partial \mu_k}{\partial x_i}$$

and

$$\mu_k=\frac{m_k}{\sum_{k=1}^{K} m_k}$$

Heat equation (conservation of energy):

$$\frac{\partial \rho h}{\partial t}+\frac{\partial \rho u_i h}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\lambda\frac{\partial T}{\partial x_i}\right)-\frac{\partial}{\partial x_i}\sum_{k=1}^{K} J_k h_k+\frac{\partial p}{\partial t}+u_i\frac{\partial p}{\partial x_i}+\tau_{ij}\frac{\partial u_i}{\partial x_j}+S_h$$

and

$$h=\sum_{k=1}^{K}\mu_k h_k$$

and

$$h_k=h_{0,k}+\int_{(T)} c_{p_k}\,\mathrm{d}T$$

Nomenclature

Latin letters	Greek letters
c_p: specific heat capacity	δ_{ij}: Kronecker–Delta
g: gravity	η: dynamic viscosity
h: specific enthalpy	λ: thermal conductivity
i: tensor index (1, 2, 3)	μ_k: mass fraction
j: tensor index (1, 2, 3)	ρ: density
k: species	τ_{ij}: shear stress tensor
m_k: mass	
p: pressure	
S_h: volumic heat flow	
t: time	
T: temperature	
u: velocity	
x: Cartesian coordinate	

Turbulence closure model

Within the numerical simulations of this work, a transient turbulent flow was considered by applying the method of Scale-Adaptive-Simulation (SAS). This approach uses a dynamic function for the turbulent length scale to switch between Reynolds-averaged Navier–Stokes equations (RANS) and the more sophisticated Large-Eddy-Simulation (LES). In contrast to RANS, where all turbulent scales are modeled, LES resolves the large scales ("eddies") and models only small scales. The final resolution of the turbulence is influenced by the mesh size and the time step. SAS basically combines the advantages of both approaches: reasonable CPU times (in case of RANS) and an increased turbulence resolution and accuracy (in case of LES). Further details are given in the ANSYS CFX-Solver Modeling Guide.[5]

Geometry and numerical grid

The examination room which was used in the investigations of Dutschke *et al.*[3] was implemented into the ANSYS-workbench as a ".x_t"-file (parasolid), generated with a common computer-aided design (CAD) tool. The red sphere in Figure 2 indicates the location of the source point simulating the theatrical pyrotechnic fountain. The relevant ventilation openings are located near the ceiling and close to the ground. Eleven outflow ventilation openings are located in the ceiling. Below each bench a row of circular

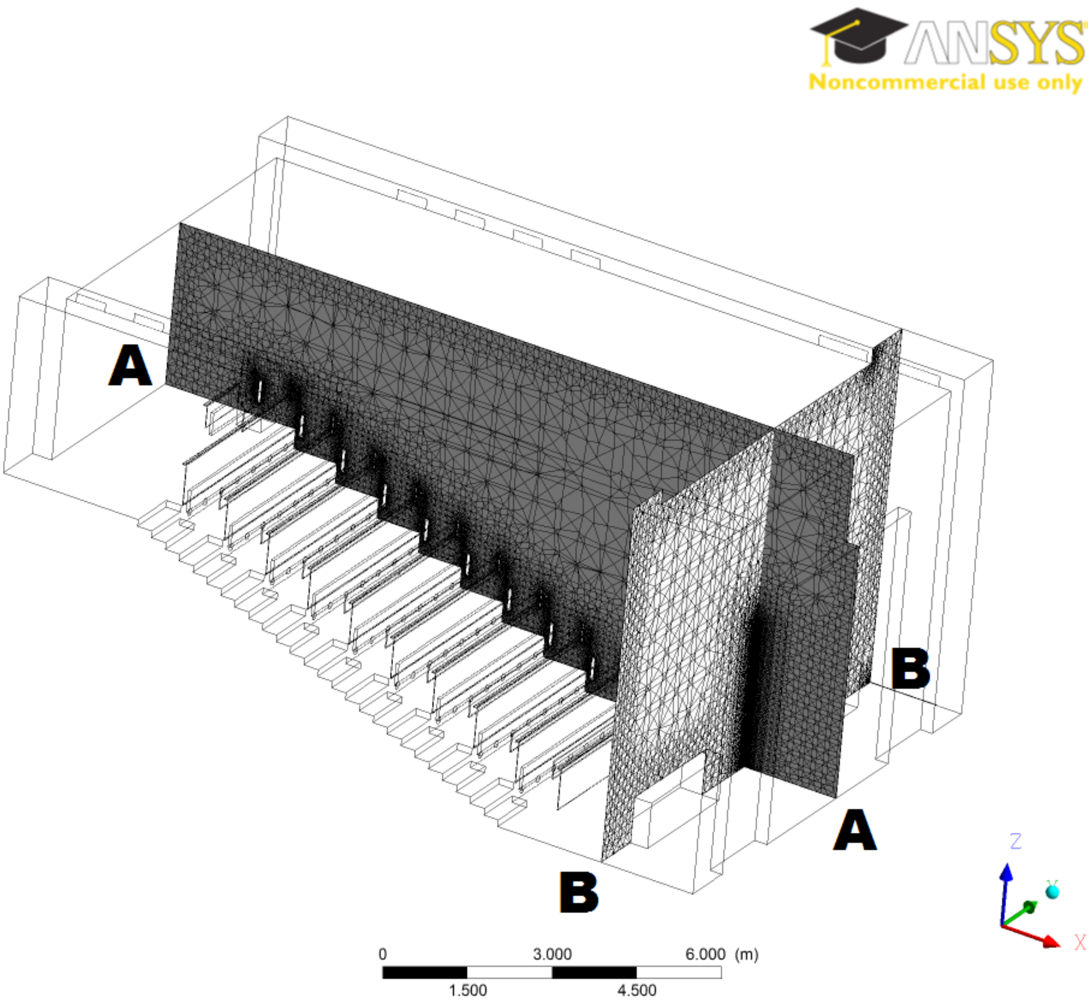

Figure 3. *General view of the domain with two cut planes visualizing the mesh.*

inflow ventilation openings are located. And, thus difficult to visualize in Figure 2 because of its small size, two door clearances with a height of 1 cm and a width of 1 m are respectively placed on the upper floor and the ground floor intersection with the wall on the back right side (in the positive *y*-direction) when looking at Figure 2.

The entire geometry was internally meshed with tetrahedrons (unstructured) and prisms for an appropriate wall boundary layer resolution, resulting in a total number of approximately 3.7×10^6 nodes and 12.77×10^6 elements (consisting of 8.73×10^6 tetrahedrons and 4.04×10^6 prisms).

In Figure 3 a general view of the fluid domain is illustrated with two planes AA and BB showing the mesh. In Figure 4 a detailed view of the AA and BB planes details the refinement in relevant areas. The mesh was refined around the source point (up to the maximum effect height of 3 m), since there were high velocity, temperature and concentration gradients expected, as well as around the inlet and outlet areas. In the same way refinements were made in areas with smaller geometry length scales, as for example around the tables and benches. These refinements related to length scale changes around the tables and benches and the prism layers for the near wall resolution are shown in Figure 5.

Material properties

Air as an ideal gas was defined as the existing ambient material. The density of the air was calculated by the ideal gas law, whereas fixed values of 28.96 kg kmol^{-1} for the molar mass and 1004.4 J (kg K)$^{-1}$ for the heat capacity at constant pressure were used. The smoke has been accounted for as an additional variable with a density of 1.3 kg m^{-3}. The advantage of using an additional variable is that no other physical properties have to be defined, although a dispersion of the substance is simulated.

Simplifying model assumptions

To keep the simulations as simple as possible in a first step, physical aerosol effects such as coagulation (particles collide and coalesce with each other, resulting in decreasing particle number concentrations), condensation of vapor phase on particle surfaces (directly affecting the aerosol particle size distribution) and nucleation were neglected. Further details on the numerical simulation of these effects are given amongst others by Hussein *et al*.[4]

The body of the fountain consisting of a cylindrical shape of around 3 cm diameter and 10 cm height was not explicitly resolved by the CAD model. Due to the small size of the fountain body compared to the dimensions of the room, neglecting that object seemed possible without significant effects on the flow in the room aligned with the advantage of simplifying the mesh generation and saving CPU time. Therefore, instead of modeling the body of the fountain, the smoke source was considered as a source point situated at the height corresponding

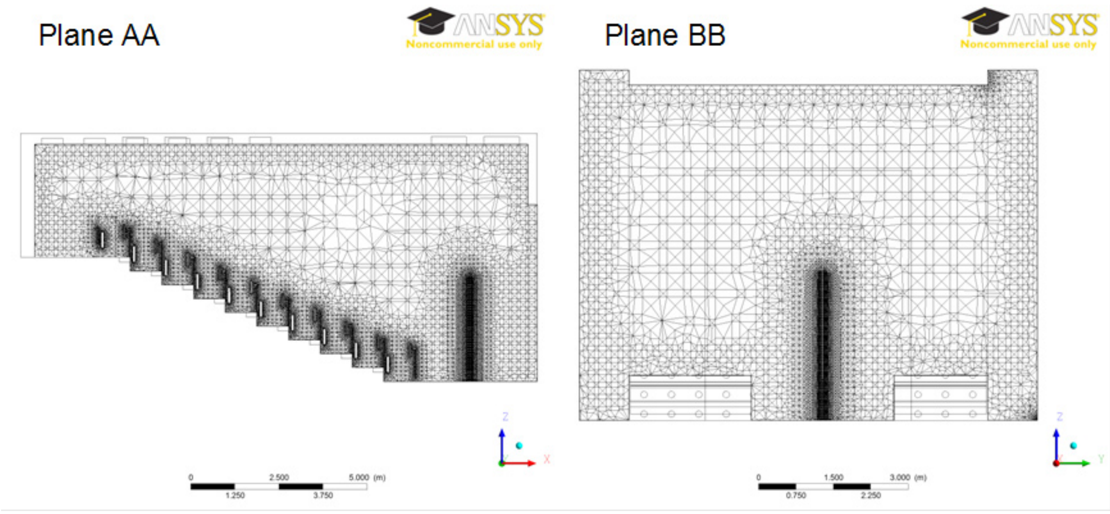

Figure 4. *Cut planes AA and BB for detailed view of the mesh.*

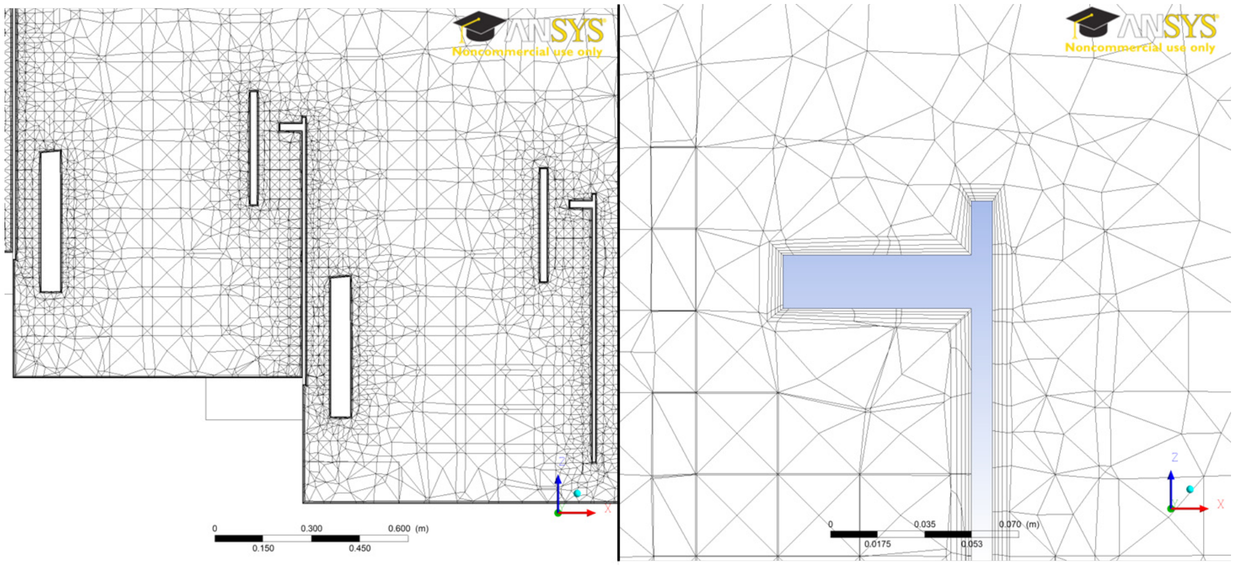

Figure 5. *Detail side view of the mesh around tables and benches with length scale dependent refinement and prism layers.*

to the length of the real fountain.

Furthermore, other minor simplifications of the room geometry were performed for the same reasons of making the mesh generation easier and saving significant CPU time.

Boundary and initial conditions

As the boundary conditions during the experiments did not vary much and were therefore highly reproducible, mean values were used for the simulations. Walls, floor, ceiling, tables and benches were modeled as "wall" boundaries with a "no slip" condition. The source point was defined for releasing a mass fraction of smoke = 1 with a release velocity oriented in the *z*-direction (normal to the ground in direction of the ceiling) of 1.5 m s^{-1}. The latter value corresponds to the measured velocity during the test runs. The mass flow of smoke released was calculated from the known values of released volume and release duration. 8 L of smoke were released during 10 s, corresponding to a volumetric flow of 0.8 L s^{-1}. With an assumed smoke density of 1.3 kg m^{-3}, a mass flow of 0.001 043 kg s^{-1} was determined. The release duration was limited to 10 s according to the real functioning time of the fountain. The air inlet surfaces were modeled as "inlet" boundary conditions, with 0.75 m s^{-1} flow velocity at the circular inlets on the ground and 1.39 m s^{-1} at the door clearances. The air oulet surfaces on the ceiling were set as "outlet" boundary conditions with an outflow velocity of 0.87 m s^{-1}. The velocity values were also calculated from known ventilation and geometric conditions.

As the released smoke is initially at a much higher temperature than the ambient air, the heat transport has been taken into account using the Total Energy model of CFX (see also ANSYS CFX-Solver Modeling Guide[5] for further details).

The simulation was set up as a transient simulation with a total duration of 1860 s. In the first 60 s only the flow in the domain was calculated without any release of smoke, to obtain a flow field in the domain. After that the release was activated for 10 s and during the last 1790 s the dispersion of the smoke was calculated. The time steps used were manually preset as a time step list, with variable time steps varying from 10^{-2} s up to 2.5 10^{-1} s.

Processor properties and software

All CFD simulations were carried out on a high-performance cluster consisting of several nodes. The relevant node contains of 32 cores in total (4 × Magny-Core [8 cores]; AMD Opteron 2.6 GHz/256 GB RAM), of which 24 cores were actually used for the calculations of this work. The program ANSYS 14.0 with its workbench platform was chosen for the CFD simulations of this work.

The total wall clock time of one case calculation (simulated time of 30 minutes) was around 14 days.

Results and discussion

Although the experimental values were determined in three separate experiments, the simulated values originate from one simulation run. The results shown in the following originate from a simulation with the above described mesh of nearly 13 million cells. Preceding short estimations of the grid influence showed that a highly refined mesh is needed. Unfortunately, further refinements were in principle possible but not on the available hardware. As mentioned before, the concentration of smoke during the experiments was measured at three different locations in the theatre. In Figure 6 the measured time dependent concentrations of smoke are plotted against the simulated values for all three locations.

Although a perfect match of the transient concentrations between the experimental values and the simulations is not reached, it can be seen that the transient dispersion is reproduced quite accurately by the simulations. With only small deviations in time, the simulations predict the rise of the smoke concentration in good agreement with the experimental data. In addition to that, the simulation results detailed in Figure 6 also reveal the decline of the aerosol concentrations due to the comparatively short functioning time of the fountain in combination with the existing ventilation (boundary) conditions. The overall trend is in fair agreement with the experimental results.

Table 1 gives detailed information about the maximum aerosol concentrations and the corresponding time values of the simulations in comparison with the experimental results (see also Figure 6).

The simulations generally tend to over-predict the aerosol concentrations in point 1 and 2 by a factor of roughly 6 and 9, whereas in point 3 an under-prediction by a factor of 5 was observed. However, the simulated times to the respective maximum aerosol concentration peaks correspond very well with the experimental results (Table 1).

In terms of labor protection aspects the time dependent dose information of a certain aerosol exposure of the persons involved is a major key factor when assessing the potential hazards of the burn-off of indoor pyrotechnics. Therefore, the simulated time averaged concentration values over 30 minutes were compared at all three points with the corresponding experimental results published by Dutschke *et al*.[3] As shown in Table 2 the agreement of the time averaged concentration values between simulations and experiments for the points 1 and 2 is better than for the single time dependent maximum values presented in Table 1. However, for point 3 slightly less good agreement on that matter was observed.

The general trend of over-predicting the aerosol concentrations in the close range and under-estimating the concentrations further away from the fountain was not influenced by the time averaging.

The fact that the general prediction type changes from a conservative character at close range to the pyrotechnic article to an optimistic quality further downstream in the examination room may be due to the constant summation of calculation uncertainties, implicitly included in

Table 1 *Transient aerosol concentration characteristics*

Points	Maximum aerosol concentration [mg m^{-3}]		Time to maximum concentration [s]	
	Experiments[a]	Simulations	Experiments[a]	Simulations
1	1.6	9.4	480	436
2 (1st relevant peak)	0.11	1.2	480	481
2 (2nd relevant peak)	0.13	0.8	720	700
3	0.14	0.028	840	870

[a] Values taken from Dutschke *et al.*[3]

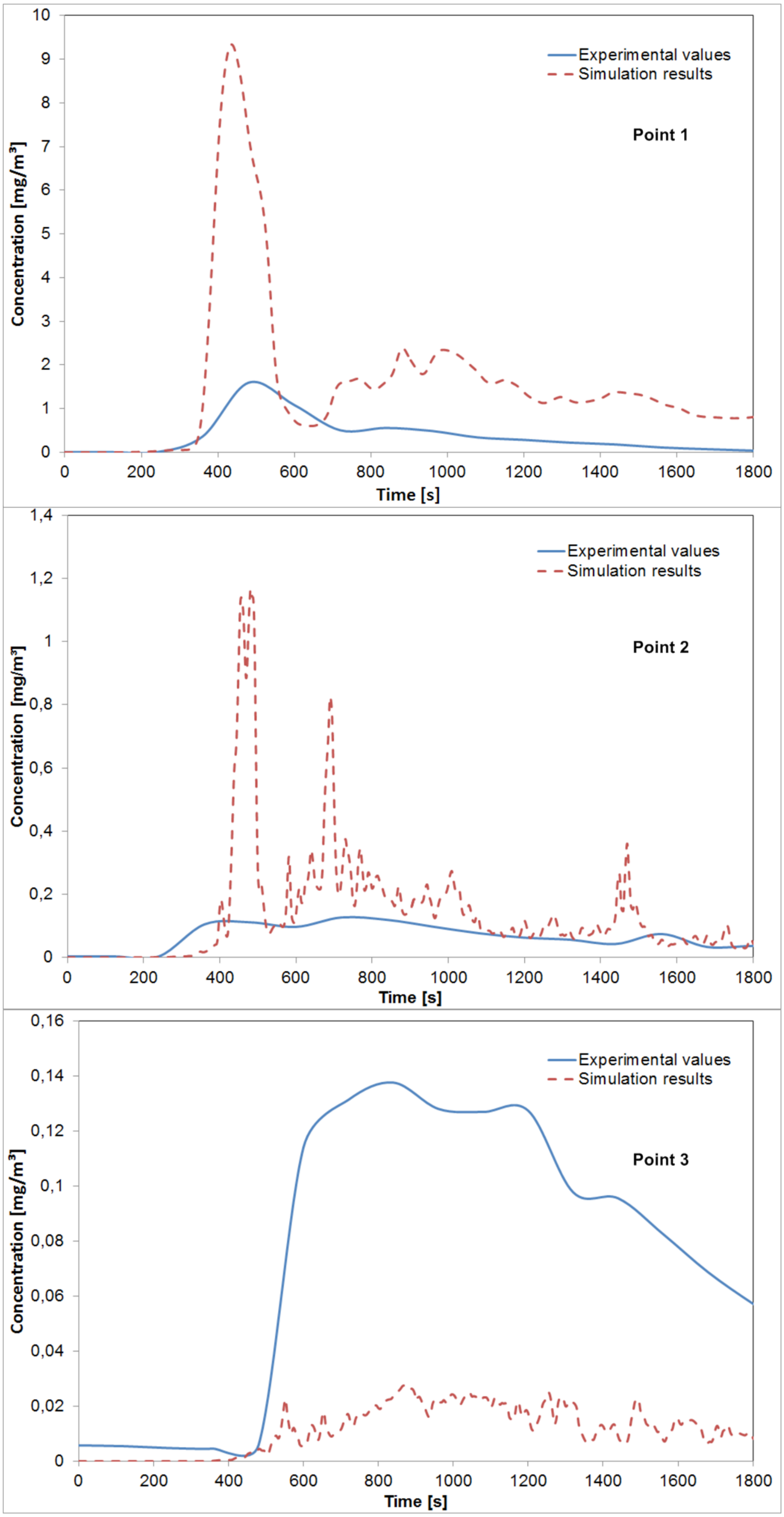

Figure 6. *Measured and simulated aerosol concentrations vs. time at all three measuring/monitor points.*

Table 2. *Time averaged smoke concentrations*

Points	Experimental time averaged concentration (over 30 min) [mg m^{-3}][a]	Simulated time averaged concentration (over 30 min) [mg m^{-3}]
1	0.39	1.62
2	0.07	0.141
3	0.09	0.0115

[a] Values taken from Dutschke *et al.*[3]

the grid refinement, boundary conditions settings and other simplifying model assumptions as mentioned earlier in the text. Using mean values for the boundary conditions instead of the exact values during the experiments could have led to differences in the flow and concentration fields. Furthermore, although the experimental venue was a closed room with regulated ventilation conditions, the simulation omits the fact that one half of the walls of the room consisted of windows. These certainly had an influence on the air and aerosol flow conditions inside the room due to possible effects of sun radiation. In addition to that, the windows might act as heat bridges to the outside, leading to differences in the temperature field influencing the buoyancy and therefore the flow field.

Figure 7 shows the flow vectors during the burn-off of the theatrical fountain 5 seconds after ignition on the centerline cross-section area of the simulated room.

The flow inside the room strongly depends on several aspects like constructional details (e.g. arrangement and dimensions of the chairs and tables) and ventilation conditions etc. Three-

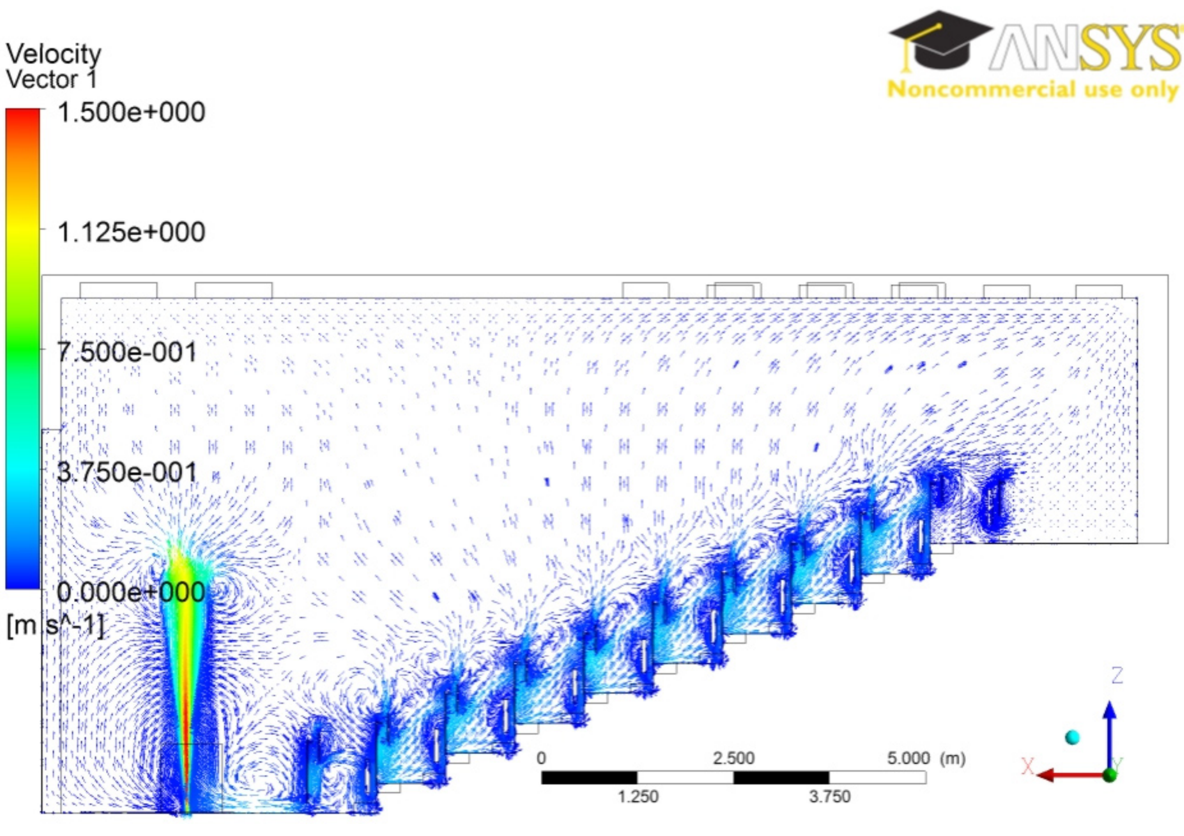

Figure 7. *Flow field in the simulated theatre during the burn-off of a theatrical fountain 5 seconds after ignition.*

dimensional flow measurements inside the room (e.g. with hot-wire anemometry instruments) during the experiments might have given precise flow information in order to improve the estimation of possible calculation uncertainties.

The expansion of the aerosol cloud (for a concentration of 1 mg m^{-3} and higher) due to the dispersion inside the room, as well as the contraction due to the short functioning time of the fountain and the existing ventilation conditions, is displayed in Figure 8.

Summary

This study presents results of the investigations to evaluate the possibility of using common CFD tools for the assessment of possible hazards aligned with the liberation of smoke during the burn-off of pyrotechnic articles in indoor venues. Therefore, a CFD model from ANSYS CFX was taken to simulate the dispersion of aerosols released by the functioning of a typical theatrical pyrotechnic fountain. The calculations were afterwards compared with corresponding preceding experiments.

As a general evaluation it can be stated that the chosen CFD model assumptions led to overall satisfying results compared with the experimental values. The calculations over-predicted the maximum aerosol concentrations in the close range to the pyrotechnic fountain, which corresponds to a conservative hazard estimation. The close range to the aerosol source point plays an important role from the safety point of view, since actors and audience are often in very close proximity to the pyrotechnic effects used in theaters and stage shows. However, a different situation was observed in the far range. With increasing distance from the source point the maximum aerosol concentration values were under-estimated by the simulations in this case, likely due to the summation of calculation uncertainties corresponding to the chosen model assumptions.

In comparison with the accuracy of the maximum concentration values, the transient behavior of the aerosol liberation was much better reproduced by the simulations. The times at which the respective maximum concentration values appeared at all three measuring/monitor points matched the experimental values very well.

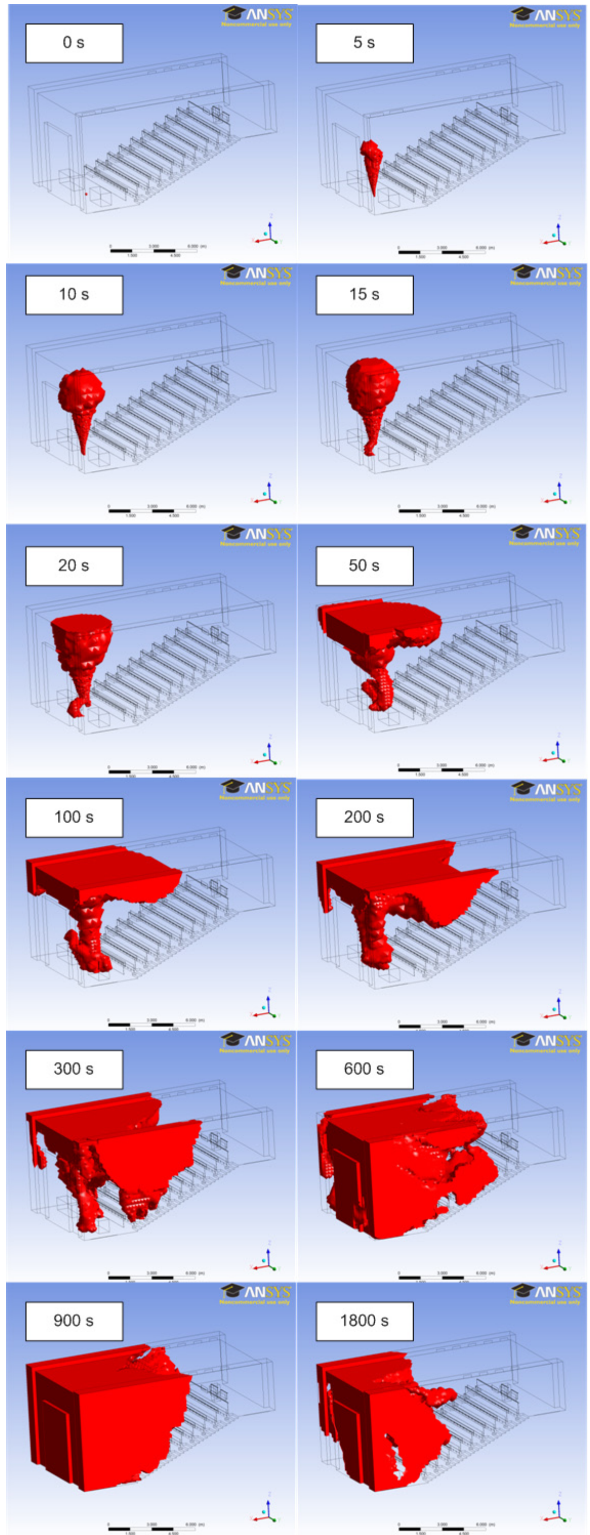

Figure 8. *Time dependent dispersion of the aerosol cloud visualized for a concentration of 1 mg m^{-3} and higher.*

Future simulations might even get better agreements with experimental results, when:

- they are in addition validated with flow measurements,
- more sophisticated numerical methods and approaches are applied,
- physical aerosol effects such as coagulation, condensation of vapor phase on particle surfaces and nucleation are taken into account, and
- a more refined grid is used.

Conclusions

In spite of the high numerical efforts, combined with comparatively long computation times, an application of CFD to estimate potential hazards during the use of pyrotechnics with regards to the liberation of solid reaction products appears to be possible and reasonable. Especially when considering the fast development of computational processing power in the recent years, the application of CFD in this field will become more and more feasible in the future.

CFD results may also play an important role in countries where quantified risk assessments (QRA) are taken into account prior to the permission of the use of pyrotechnics in stage and theatre shows, as they can give information not only on absolute concentration values, but also on transient dispersion effects, basically for every desired venue. These maximum or time averaged concentration values could be compared with national threshold values with regards to labor protection regulations. In particular when using several pyrotechnic articles in parallel during a show, the advantages of CFD may dominate the long computation times.

Another benefit of CFD is the fact that this tool offers the possibility of receiving relevant information, such as concentration, temperature, velocity etc. for every desired location within the 3D fluid domain.

However, several disadvantages of CFD simulations will still exist in the future, regardless of the promising CPU development. These include amongst others the problem or challenge of adequately modeling the flow domain (e.g. construction and import of CAD files), and setting boundary conditions and material properties realistically.

References

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