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A MATHEMATICAL APPROACH TO ESTIMATE THE ERROR DURING CALCULATING THE SMOKE LAYER HEIGHT IN INDUSTRIAL FACILITIES

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Research article

Abstract:	Engineering based calculation procedures in fire safety science often consist of unknown or uncertain input data which are to be estimated by the engineer using appropriate and plausible assumptions. Thereby, errors in this data are induced in the calculation and thus, impact the number as well as the reliability of the results. In this paper a procedure is presented to directly quantify and consider unknown input properties in the process of calculation using distribution functions and Monte-Carlo Simulations. A sensitivity analysis reveals the properties which have a major impact on the calculation reliability. Furthermore, the results are compared to the numerical models of CFAST and FDS.
Keywords:	Error propagation, Monte-Carlo Simulation, smoke layer height, CFAST, FDS.

Introduction

Engineering based calculations and CFD-modeling are latterly integrative components of the fire protection proof (Wiese, et al., 2013). Based on the calculated results, exceptions as well as deviations from the regulations can be justified and potential risks can be quantified. Since the calculation methods and the CFD-programs are validated as well as verified to model the problem, their results offer a suited basement to e.g. design exit routes, predict the activation behavior of smoke and sprinkler systems and model smoke dispersion in atria and high facilities (Krause, et al., 2013) (Münch, 2012) (Knaust, 2010).

A general problem in these calculations is the assumption of an appropriate fire scenario. CFD-tools need qualified initial and boundary data which are a priori often totally or at least partially unknown or are connected to a high level of uncertainty. Therefore, the results are restricted to the quality and accessibility of input data (Hosser, et al., 2008). Hence, conservative or plausible estimates of the expected fire scenario should face the problem of uncertainty. From that approach further problems arise:

1. The conservative estimation is often limited to the evaluation of the input data. But the relevant criteria for human safety are conservative calculation results.



Fig. 1 Different kinds of approaches for modeling in fire safety engineering

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- 2. The term "conservative" is not well defined at all. The quantified risk which is modeled by the conservative assumption is not apparent.
- 3. Generally, only a discrete fire scenario is modeled. The possibility that there are many fire scenarios resulting in a spectrum of outcomes as well as the influence of calculation errors and their impact on the results are often neglected.

The different kinds of approaches in fire safety engineering are shown in Fig. 1.

The consideration of these uncertainties as well as the examination of possible fire scenarios should be integrative components in the quality management in fire safety engineering.

The possibility to integrate uncertainties and errors in the calculation depends on the structure of the used model.

- 1. In algebraic models one can use Monte-Carlo Simulation, different probability functions and sensitivity analysis.
- 2. In CFD models it is possible to perform parameter variations based on a previous data analysis.

The consideration of stochastically distributed input data in the model allows the examination of different kinds of development potentialities. Hence, in regard to human safety it is possible to quantify the critical fire scenario which directly increases the plausibility and the acceptance of the results.

Since a building fire is a very rare event, it is not appropriate to only consider the expected mean fire (Wallace, 1952). Because the consequences of a real fire could be much more disastrous, the long-term, medium fire scenario could be an inappropriate estimator for the real event (Seekamp, 1965). Hence, the input data should be represented on a statistically based and limited treshold which adequately represents the expected fire scenario.

In structural fire protection it is common to test building components on a 90 % reliability. This 0.9-quantile also could be regarded as an adequate safety value for CFD models as well as engineering based calculations.

Materials and methods

In algebraic models the deviation in the results can be directly calculated with the error propagation law based on Gauss. Therein the error $\Delta \overline{f}$ can be calculated with eq. (1). This law includes the possibility that uncertainties can be compensated by each other. Hence, this equation provides the most probable error which is likely to occur.

$$\overline{\Delta f} = \sqrt{\sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i} \Big|_{\overline{x}_i} \Delta x_i \right)^2}$$
(1)

The impact of a single deviation Δx_i on the total error Δf can be calculated by eq. (2). The sensitivity parameter $\psi_{i \to \Delta f}$ indicates the fraction of impact from one arbitrary calculated error i on Δf . Based on that sensitivity analysis one can identify the most important input variables and quantify their magnitude of influence on the results.

$$\psi_{i \to \Delta f} = \frac{\left(\frac{\partial f}{\partial x_i}\Big|_{\bar{x}_i} \Delta x_i\right)^2}{\left(\Delta f\right)^2}$$
(2)

Calculation example

The above mentioned solution approach shall now be applied to a working example. In an arbitrary industrial facility the smoke layer height as well as the associated error shall be calculated comparing three different approaches using an (i) algebraic model, (ii) a numerical two-zonal model (CFAST) and (iii) a CFD model (FDS).

The geometry of the facility is given in Tab. 1.

Tab. 1 Geometry of the calculation example

Length	Height	Inlet	Outlet	Flow
X Width		area	area	coefficient
20 m X 50 m	10 m	52 m ²	30 m ²	0.7

Algebraic model

Based on an energy and a momentum balance as well as the perfect gas law, the mass flow through natural vents can be directly calculated using an algebraic two-zonal model, eq. (3). The model assumes quasi-steady-state conditions between inflow and outflow. The driving force of ventilation is induced by the pressure difference between the upper and the lower layer. A general description of the model can be found in (Schneider, 2007). Fig. 2 illustrates the basic concept of the model.

$$\dot{M}_{out} = A_{out} C_{out} \rho_{low} \sqrt{2 g h_{up} \frac{T_{low}}{T_{up}} \frac{1 - \frac{T_{low}}{T_{up}}}{\left(\frac{A_{out} C_{out}}{A_{in} C_{in}}\right)^2 \frac{T_{low}}{T_{up}} + 1}}$$
(3)

To calculate the upper layer height, eq. (3) will be solved for h_{uv} , see eq. (4).



Fig. 2 Mass and pressure balances in the algebraic two-zonal model

For steady-state conditions the mass flow through the vents is equal to the mass flow of the fire plume $\dot{M}_{out} = \dot{M}_{Pl}$. Based on the formulation of Heskestad the plume mass flow is given by eq. (5) (Quintiere, 2006).

$$\dot{M}_{Pl} = 0.071 \dot{Q}_C^{1/3} z^{5/3} + 0.001846 \dot{Q}_C$$
 (5)

The convective part of the total heat release rate is assumed to follow the relation $\dot{Q}_c = 0.7 \ \dot{Q}$. To consider the time dependency of the heat release rate, a point-shaped fire origin is assumed with a uniform and constant velocity of fire spread in all direction that follows the t^2 - law.

$$\dot{Q}(t) = \alpha t^2 \tag{6}$$

The coefficient α is a constant that governs the speed of fire spread and is given for different kinds of fire scenarios by (92B, 2000).

Concluding the density of the lower layer is represented by the perfect gas law.

$$\rho_{low} = \frac{p_{low}}{R_{low}T_{low}} \tag{7}$$

The upper layer height can now be calculated under the condition of a variable rate of heat release using the linear system of equations (4-7).

In this set of equations the following properties are assumed to be totally or at least partially unknown:

- a) the coefficient of fire spread α ,
- b) the time of fire spread *t*,
- c) the temperature of the lower layer (ambient temperature) T_{low} and
- d) the temperature of the upper layer T_{uv} .

Depending on the assumptions for these unknown properties, an error for the upper layer will be invoked in the calculation. Hence, the scope of the modeling process is to find plausible and reasonable estimations for these parameters as well as to quantify the expected error for the smoke layer height.

Coefficient of fire spread

The coefficient α characterizes the speed of fire spread. One can distinguish between four situations, low, medium, fast and ultra fast fire spread (92B, 2000). For this example a medium fire spread is considered. Since this assumption can both over- and underestimate the real situation and no further information on this property is known, a fast and slow fire spread are also considered. Hence, the coefficient α will be modeled with as a random number following a uniform distribution in the interval of [0.002931 kW/m²; 0.04689 kW/m²]. This distribution takes into account, that no information on α are available and thus, models it with the highest uncertainty possible.

Time of fire spread

In between the moment the fire starts until the point of effective fire fighting, the fire can spread unhindered. This period can be subdivided into several single intervals, e.g. period until fire detection, period of dispose the fire brigade, period until fire brigade arrives as well as the period until effective fire fighting starts. Generally, this time is unknown, a random parameter and case sensitive, respectively. Since we do not consider a special building, a general estimation for a broader spectrum of facilities has to found. In Germany this time is regulated by law and should not exceed 12 minutes (2013).

The time of fire spread is evaluated in (Brening, et al., 1985) as a random number following a log-normal distribution and the mean deviation is estimated with 5 minutes.

Based on eqn. (8) and (9) the parameters of a log-normal variable can be calculated from normal distributed variables.

$$\mu_L = \ln \mu - \frac{\sigma_L^2}{2} \tag{8}$$

$$\sigma_L = \sqrt{\ln\left(\frac{\sigma^2}{\mu^2} + 1\right)} \tag{9}$$

Lower layer temperature

The moment of fire outbreak is totally unknown and thus, also the time of day and the season as well. Consequently, the lower layer temperature (ambient temperature) is a random variable.

Basedonthemeanseasonal temperature connected with a statistical assessment, the distribution of the expected lower layer temperature can be estimated. For the city of Magdeburg the seasonal temperature distribution of 2012 was evaluated and the data set was fitted with a distribution function. According to (Nadarajah, 2003), the Gumbel-distribution is a suitable function to model weather phenomena. The calculated parameters are $\mu = 286.9$ K and $\sigma = 6.9$ K.

Upper layer temperature

The upper layer temperature is an input data that only can be calculated with appropriate numerical models. Best suited models are CFD-programs in which the governing equations of mass, momentum and energy are solved. For the present situation this temperature is unknown and hence, must be estimated by plausible assumptions.

Based on the Heskestad plume model (Quintiere, 2006), the maximum temperature rise in the plume was experimentally determined with $\Delta T = 900$ K. Typically the upper layer temperature is greater than the lower layer temperature. From the data set of the ambient temperature, a maximum value of $T_{low,max} = 302.5$ K could be evaluated which is therefore the minimum threshold value for the upper layer temperature. Thus, the maximum upper layer temperature is $T_{up,max} = 302.5$ K + 900 K = 1,202.5 K. Since no further information on the distribution are known, the upper layer temperature is modeled by a uniform distribution. The parameters are $\mu = 752.25$ K and $\sigma = 450$ K.

In a first order of approximation all random numbers are assumed to be stochastically uncorrelated. The stochastic properties as well as their distributions and parameters are summarized in Tab. 2. These data as well as the algebraic model are integrated in a Monte-Carlo Simulation with 10^6 cycles.

Tab. 2 Stochastically distributed input data for the calculation

Input data for the numerical models

The results of the Monte-Carlo Simulation shall be compared to the numerical calculations of CFAST and FDS. By comparing the results, statements concerning the reliability and validity of these models can be given. With respect to the heat release rate, two simulations are carried out for each model:

- a) The heat release rate is quantified according eq.
 (6). Therein, the mean values for *α* and *t* are used, resulting in a mean heat release rate. This value is used as the input data for CFAST and FDS.
- b) Based on eq. (6) and the distributions for α and *t*, the distribution of the heat release rate is calculated by a Monte-Carlo Simulation. Following, the 0.9-quantile for the heat release rate is used as the conservative input value for CFAST and FDS.

The relevant heat release rates used for the numerical models are summarized in Tab. 3. Fig. 3 shows the distribution of the heat release rate as a result of the Monte-Carlo Simulation.

Tab. 3 Calculated input data for the numerical models based on Monte-Carlo Simulation

Simulation 2

Simulation 1

Ĺ	y = 12,913 kW	$Q_{0.9} = 33,60$	60 kW
1	conservative threshold	ſ	
0.9		\square	
0.8-			-
lity			
iqpaq			-
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0.2			-
0	15,000 30,00	₩ . 00 45,000	60,000
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Fig. 3 Calculated distribution of the heat release rate based on the stochastic input data and Monte-Carlo Simulation

Property	μ	σ	Distribution	Parameter
α	0.02491 kW/s ²	0.02198 kW/s ²	uniform	U(0.002931;0.04689)
t	720 s	300 s	log-normal	LN(6.5;0.4)
T _{low}	286.9 K	6.9 K	Gumbel	G(286.9;6.9)
T _{up}	752.25 K	450 K	uniform	U(302.25;1,202.25)

Results and Discussion

In Tab. 4 the results of the Monte-Carlo Simulation are summarized. The interface layer height between upper and lower layer is calculated by means of the ceiling height and the upper layer height using eq. (10).

$$h_{int} = 10 \, m - h_{up} \tag{10}$$

For the exemplary industrial facility considered above, a mean interface layer height of 7.80 m can be expected. The mean calculation error is 2.20 m. This deviation is caused by the partially unknown and stochastically distributed input parameters that impact the quality and reliability of the calculation.

Tab. 4 Calculated interface layer height as well as the associated error based on Monte-Carlo Simulation

\overline{h}_{int}	$\Delta \overline{h}_{int}$	h _{int,0.9}
7.80 m	2.20 m	5.10 m

In Tab. 5 the unknown and stochastically distributed parameters are shown and their respective impact on the calculated interface layer height error. It turns out that the parameters α and *t* are the most important properties with respect to the calculation reliability with a combined impact of 98.40 %. Since reliable calculations for the interface layer height are requested, suitable and precise estimations for α and *t* should be carried out.

Although the upper layer temperature was characterized by a wide range of numbers due to the uniform distribution, their impact on $\Delta \overline{h}_{int}$ is quite moderate.

Tab. 5 Calculated results of the sensitivity analysis

α	t	T	$T_{\mu p}$
52.00 %	46.40 %	0.14 %	1.46 %

Furthermore, the distribution of the calculated interface layer height is given in Fig. 4. Since a conservative calculation scenario is the relevant criterion for human safety, an interface layer height of 5.10 m can be ensured. This layer height can be expected in at least 90 % of all fire scenarios. In other word, since a minimum lower layer height of 2.50 % is often requested by the authorities, this layer height can be guaranteed with a probability of > 95 %. Concluding, the above presented calculation procedure effectively provides conservative results.



Fig. 4 Cumulative distribution of the interface layer height based on Monte-Carlo Simulation. The figure includes the results of the numerical models CFAST and FDS

The results of the numerical models are shown in Fig. 4 and Tab. 6. An interface layer height of nearly 3 m for FDS and 7.50 m for CFAST is calculated. It is obvious that the results only show a low dependency on the heat release rate. Although the input variable was almost tripled, the calculated interface layer heights were almost constant. Since larger heat release rates cause an effective thermal flow in the facility, the layer height is almost constant.

It is remarkable to note that FDS calculates results which are in between the conservative criterion and the layer heights of CFAST only represent nearly 70 % of all scenarios. The results show, that FDS is an appropriate model to reliably predict the interface layer height in industrial facilities compared to CFAST which significantly underestimates the potential risk of fire spread and smoke dispersion.¹ This is essentially caused due to the simplicity of model structure of CFAST that solves an oversimplified set of equations.

Tab. 6 Comparison of the interface layer height between the different numerical models and heat release rates

Model	\bar{Q} = 12,913 kW	$\dot{Q}_{0.9} = 33,660 \text{ kW}$
FDS	$\overline{h}_{int} = 3.54 \text{ m}$	$h_{int,0.9} = 2.95 \text{ m}$
CFAST	$\overline{h}_{int} = 7.50 \text{ m}$	$h_{int 0.9} = 7.10 \text{ m}$

In that demonstrated example above, the impact of the chosen fire scenarios on the results could be shown. Consequently, two basic conclusions and recommendations can be given.

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The results of FDS converging for mesh cells < 20 cm.

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Engineering based calculation procedures containing unknown input data or properties that are connected to a significant level of uncertainty should be evaluated a priori by data analysis. Subsequently, the results of the data analysis provide the mean and the 0.9-quantile as the conservative threshold criterion for the calculation procedure. Furthermore, these kinds of statistics can be integrated in databases to make them accessible for quantitative risk assessment. Calculated results that are based on these statistics represent a broad spectrum of scenarios and thus, directly improve the reliability and acceptance of the conclusions.

The 0.9-quantile, as a suitable number for the conservative threshold risk, allows directly the quantification and differentiation between the situations of safety and danger.

Conclusion

Since unknown and uncertain input data can have a significant influence on the reliability of calculating results, it is necessary to evaluate the sensitivity of the results with respect that input variables. To shift the model sensitivity from the totally unknown parameters to the partially unknown data, which can be predicted by comparatively reliable statistics should be the major scope in ensuring the quality of calculations. Concerning the example shown in that paper, a suitable procedure could be presented to solve problems in fire safety engineering with the aid of statistics, distributions functions as well as Monte-Carlo Simulations.

Symbols

Symbol	Description	Unit
A_{in}	Inlet vent area	m^2
A_{out}	Outlet vent area	m^2
C_{in}	Flow coefficient of inlet	-
C_{out}	Flow coefficient of outlet	-
g	Gravity acceleration	m/s^2
$h_{_{int}}$	Interface layer height	m
h_{up}	Upper layer height	m
<i>M</i> _{out} −	Mass flux of outflow	kg/s
$\dot{M}_{_{Pl}}$	Plume mass flow	kg/s
p_{low}	Ambient pressure	Ра
Ż	Heat release rate	kW
\dot{Q}_{c}	Convective heat release rate	kW
R_{low}	Gas constant of air	J/kg K
t	Time	S
T_{low}	Lower layer temperature	Κ
T_{up}	Upper layer temperature	Κ
α	Coefficient of fire spread	kW/s^2
Δx_i	Uncertainty of input variable i	$[\Delta x_i]$
Δf	Uncertainty of calculated result	$[\Delta f]$
$\psi_{i \to \Delta f}$	Sensitivity parameter of variable <i>i</i>	-
$ ho_{low}$	Density of ambient air	kg/m ³

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