Summary, research project:

Quantification of smoke as a basis for fire safety concepts and concepts for smoke reduction in the case of fire

funded by the research initiative „Zukunft Bau“

Our refernce number	VII.39 / VH 7340
Copy	1/2
Client	BBR Deichmanns Aue 31-37 53179 Bonn
Date of allocation note	10.09.2009
Allocation number	SF-10.0818.7-09.20
Head of project	Dr. -Ing. Anja Hofmann
Editor	Nils Monreal, M. Eng.

Der Forschungsbericht wurde mit Mitteln der Forschungsinitiative Zukunft Bau des Bundesinstitutes für Bau-, Stadt-, und Raumforschung gefördert.
Die Verantwortung für den Inhalt des Berichtes liegt beim Autor.

Contents

Summary contains pages 1 to 7

Aim of the research project

The research project aimed on the quantitative analysis of smoke of building and consumer materials under different ventilation and temperature conditions. In literature often only qualitative information is given which is either focused on the toxicity or the smoke density. Quantitative characterization of smoke is difficult because smoke production and some gas components depend not only on the material but on ventilation conditions and temperature and on the ignition source. Experimental data therefore depend significantly on the test setup. So it was necessary to use different test setups in which ventilation and temperature conditions could be varied. Different test apparatuses were used with different ignition sources. Experiments under under-ventilated conditions were performed in the Smoke Density Chamber (SDC) and in the DIN tube. Experiments were performed under well ventilated conditions in the Single Burning Item (SBI) apparatus. All experiments were performed with controlled air supply.
The experimental data were used to establish empirical correlations for the influence of temperature and oxygen on smoke production and generation of smoke gas components. These correlations were used to establish a numerical smoke model.
The CFD (Computational Fluid Dynamics) programs ANSYS-CFX and FDS (NIST) were used. Three typical scenarios with smoke development in residential and non-residential buildings were investigated. A sub-model was developed which takes the smoke gas components into account and correlates them with the smoke density. This provides a quantitative significant leap in the use of CFD software to predict smoke free areas for escape routes or routes for the fire service. The influence of the high toxic carbon monoxide is taken into account. Models which are used up to now, e.g. in FDS, do not provide these possibilities. To show the difference in the smoke models two of three fire scenarios were calculated with the normal smoke model in FDS and one scenario shows the new smoke model – implemented in CFX.

Realisation of the research project

The identification of representative fire scenarios showed the importance of fire scenarios in which as well the influence of the materials, the temperatures as the ventilation conditions can be investigated. The temperatures and ventilation conditions must be variable and adjustable. The smoke production should be measured as attenuation and also as a function of particle number and size. Therefore the Smoke Density Chamber (SDC), the DIN tube and a calorimeter were chosen for the experiments. SDC, DIN tube and calorimeter must be modified so the required data for the numerical model could be generated. The first two apparatuses were modified in a way that a variable oxygen supply is possible. After the modification data for the smoke production and the smoke gas components under different temperature and ventilation conditions can be measured. The time-dependent rates of smoke production and production of smoke components can be identified with the given temperature and ventilation conditions. Experiments were performed several times with the same materials but different heat sources and ignition sources to quantify the influences.
The smoke production was measured through the incoming and outgoing mass flows. Additionally the mass losses of the specimens were measured on a scale during the tests.
With Fourier-Transformed-Infrared-Spectroscopy the volume concentrations of smoke gas components were measured online. Also the smoke density was measured with infrared transmission as well as the number and size of smoke particles with a gravimetric method.
The SDC is the standardized test for tests with a transition of well ventilated conditions to under ventilated conditions because normally the chamber is closed and there is no oxygen supply. The SDC has been used to adjust the conditions for smoke production for different materials. As representative materials

- Material A: PUR3554 (represents consumer products, e.g. mattresses, upholstery)
- Material B: PUR3045SE (less flammable, building product)

were chosen.
In the SDC different irradiance levels were used. Additionally the SDC was modified in a way that air / oxygen can be supplied accurately. The influence of the irradiance levels and the air supply were investigated for the different materials. An opening to sample smoke was added in the test set up to measure the number and size of smoke particles during the tests. The modifications of the SDC were extensive – so not all of the planned experiments could be performed during the project. The modifications are still usable – so additional tests can be performed during further studies. Additionally tests in the DIN tube were performed. The DIN tube also had to be modified to allow an adjustable air / oxygen supply. During the modifications it became clear that the DIN tube allowed the adjustment of the air supply better than the SDC. Therefore the DIN tube data were used as input for the numerical model. The influence of bigger specimen sizes on the results was investigated with calorimeter tests (modified Single Burning Item apparatus). The DIN tube and the calorimeter were modified that the smoke gas composition as well could be measured. The planned measurement of the mass loss in the DIN tube could not be realized because of the small specimen weight in relation to the weight of the apparatus. A scale inside the tube also was impossible to realize. The mass loss during the tests was realized in the SDC and the calorimeter measurements.

Tests were performed in the modified SDC, the Single Burning Item test apparatus (according to DIN EN 13823) and in the calorimeter (modified SBI test apparatus) (work packages AP 2.1, 2.2, 2.3) and in the modified DIN tube. All data are described in the final report. Examples are given in the next section.

The experimental data were used as a basis for empirical correlations between temperature and oxygen concentration with smoke production and smoke gas components. The empirical correlations are the basis for the numerical model which can be used in state of the art CFD programs.

Mixture fraction
The mixture fraction model is the basis for the implementation of the new smoke model. The mixture fraction model uses a kinetic reaction. The stoichiometric coefficients have to be chosen. Therefore the CO_2 to CO ratio or the CO_2 to C ratio is fixed for a kinetic reaction or set of reactions. A methane oxygen reaction could be as follows:

$$6CH_4 + 10O_2 \rightarrow 3CO_2 + 2CO + 1C + 12H_2O$$

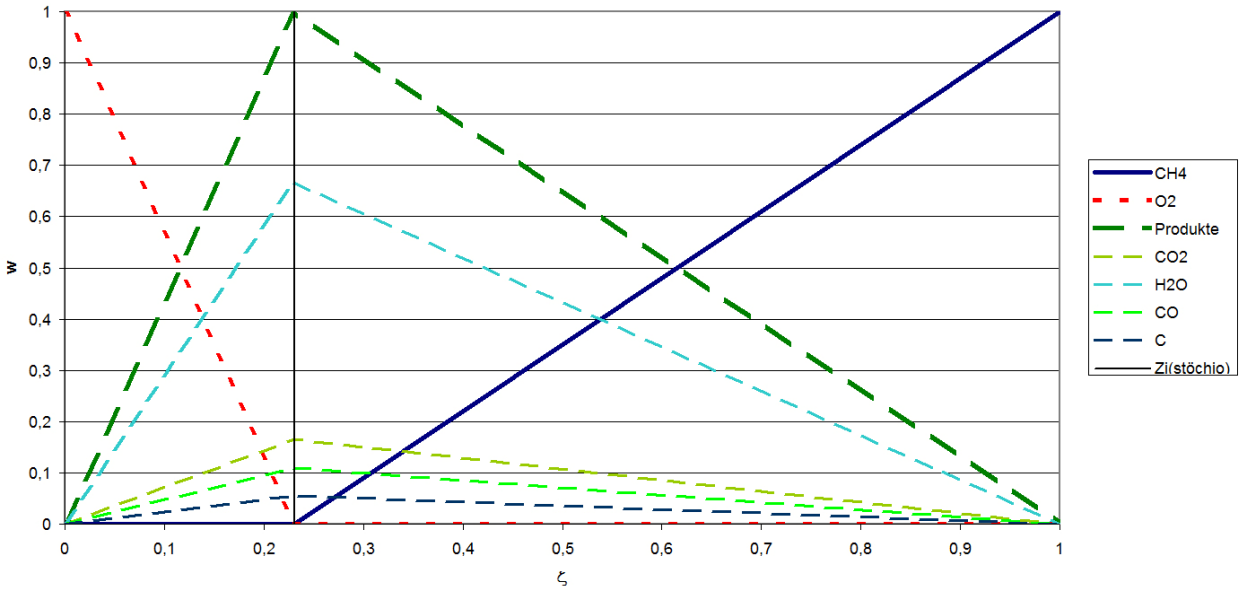

Figure 1: Mixture fraction example: methane-oxygen reaction

The mixture fractions are shown in figure 1. The left hand side represents 100 % oxygen, the right hand side 100 % fuel. At 0.23 a stoichiometric mixture is given where fuel and oxygen are fully consumed and transformed to products (CO_2, CO, C and H_2O).

An example for the analysis of the experimental data and the implementation to the numerical smoke model for one investigated material is given in the next section. An electronic analysis tool was developed to generate the kinetic equation for the numerical model with the experimental data. The kinetic equation depends on the temperature and the oxygen concentration.

Summary of results

For the investigated materials empirical correlations were found which represent the influences of temperature and oxygen concentration on smoke production and smoke gas components. All experimental data are in the final report. For example the influence of temperature and oxygen concentration on CO to CO_2 ratio could be shown.
On the basis of the experimental data which were generated under varied ventilation and temperature conditions the numerical model was developed. The new developed analysis tool allows the easy generation of kinetic equations for the numerical model.
To generate the kinetic equations the experimental data of the DIN tube experiments were used. The concentration of the toxic products were used for 25-95% of the test time during a quasi-steady-state period. The analysis tool creates a file with the mean values of the toxic products. The mean values can be plotted in diagrams, using the open source software Gnuplot. For all experimental data the analysis tool creates diagrams within a “Latex” document which are numbered and labeled automatically. Documents of this type were created for all experiments.

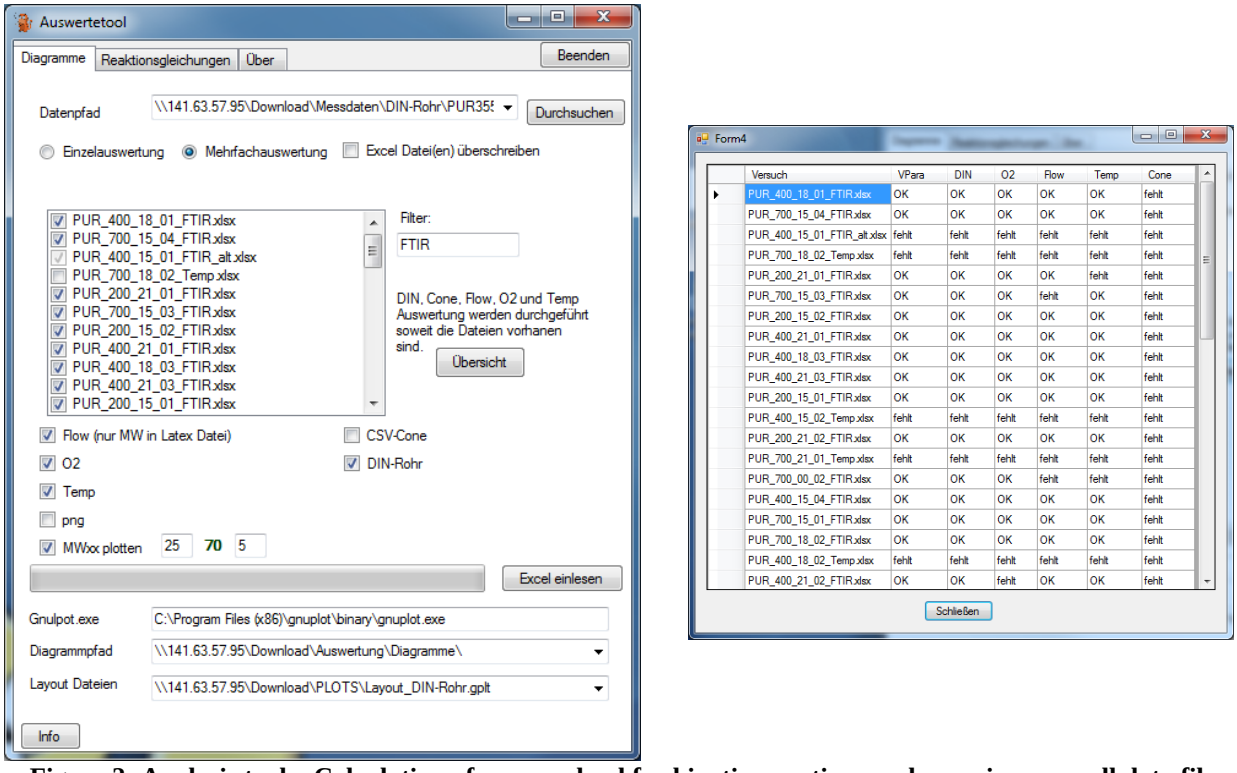

Figure 2: Analysis tool – Calculation of mean valued for kinetic equations and overview over all data files provided by the analysis tool

Figure 2 gives an example of the analysis tool (left hand side) for the calculation of the mean values and the generation of the diagrams. The test time which is used to calculate the mean values are adjusted automatically. The analysis tool provides an overview over the test data files and shows for which ventilation and temperature conditions test data exist.
In the next section the way forward for one material is given as an example.

Kinetic equation for PUR
As a basis for the calculations a total formula for the material must be chosen. For polyurethane (PUR) the total formula for polyurethane of the SFPE handbook was picked.

$$1C_{6,3}H_{7,1}N_1O_{2,1} + xO_2 \rightarrow x_1CO_2 + x_2CO + x_3C + x_4HCN + x_5H_2O + x_6N_2$$

The concentrations of the products depend on the experimental conditions and the fraction varies with temperature and oxygen concentration. To provide the data for the numerical model the tests were performed under varied temperature and ventilation conditions. The experiments were performed several times and the results are the mean values of the quasi steady state test time. The mean values (ppm) are used to generate the stoichiometric coefficients for the kinetic equations. The analysis is straight forward with the new developed analysis tool.

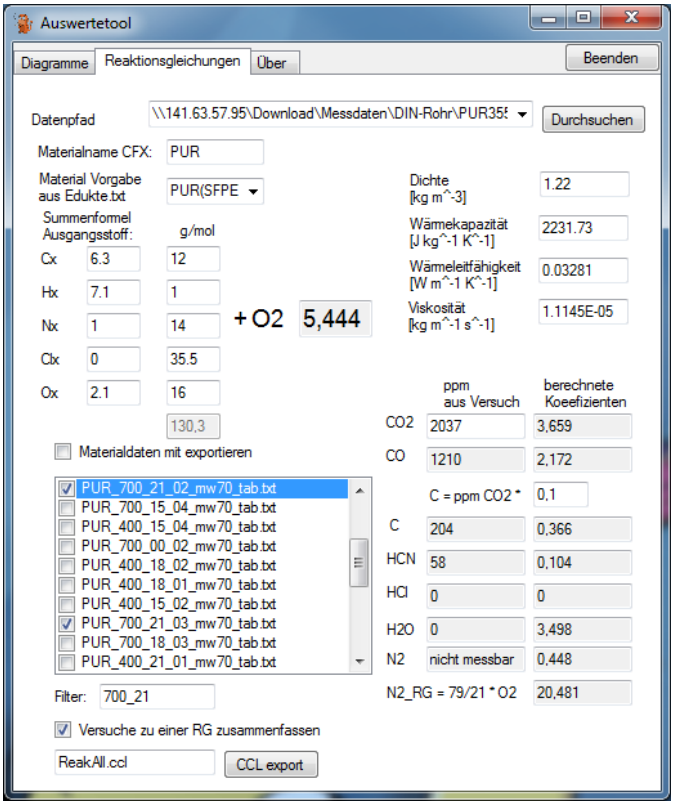

Figure 3: Analysis tool – Calculation of the kinetic equations

In Figure 3 the analysis tool is shown with the calculation of the kinetic equation for the material PUR3554 under the conditions: 700 °C and 21V% oxygen. In the upper part the coefficents for the educts are shown, on the right hand side below the mean values of the concentrations of the products and the calculated stoichiometric coefficients. The kinetic equation can be directly exported to ANSYS CFX. Also the material parameter can be exported for the use in CFX.
Tables 1 and 2 show the stoichiometric coefficients for the reactions of the materials PUR3554 and PUR3045SE with oxygen. The stoichiometric coefficients were generated for different temperature and ventilation conditions. The first number shows the temperature in °C the second number gives the oxygen concentration in volume%.

Table 1: Mean values (repeated experiments), stoichiometric coefficients for the products (x_1-x_4) fort he reaction of material PUR3554 with oxygen

Parameter	CO2	CO	C	HCN
400_15	4,1010	1,6782	0,4101	0,1111
400_18	4,8540	0,8848	0,4854	0,0758
400_21	4,9540	0,7988	0,4954	0,0524
700_15	3,6380	2,1673	0,3638	0,1309
700_18	3,7640	2,0371	0,3764	0,1226
700_21	3,6590	2,1723	0,3659	0,1037

Table 2: Mean values (repeated experiments), stoichiometric coefficients for the products (x_1-x_4) fort he reaction of material PUR3045SE with oxygen

Parameter	CO2	CO	C	HCN
400_15	5,0510	0,6380	0,5051	0,1063
400_18	5,6040	0,1261	0,5604	0,0104
400_21	4,3930	1,2985	0,4393	0,1697
700_15	4,5170	1,1743	0,4517	0,1571
700_18	4,5680	1,1191	0,4568	0,1558
700_21	4,8560	0,8736	0,4856	0,0855

For chosen materials the experiments under varied ventilation and temperature conditions were performed. The tests provide the data for the numerical calculation of the smoke production and some gas components. Experiments were performed in the modified SDC, the modified DIN tube and in intermediate scale in the calorimeter (SBI apparatus) with varied temperatures and oxygen concentrations. Only with these correlations the oxygen and temperature dependence of the smoke generation could be implemented in the numerical model. The DIN tube experiments were used to generate the kinetic equations for the numerical model. An analysis tool was developed which provides a user-friendly graphic interface and a straightforward method to generate the kinetic equations that can be directly used in available CFD programs.
The SDC was used to compare the numerical results with experimental results (validation). With the intermediate scale experiments the quality of the predictions which were done with small scale experimental data were assessed.
The experimental set ups to perform tests with other materials are now available. The modified DIN tube, the modified SDC and the SBI with the addition of the FTIR spectrometer are available for further experiments to generate a bigger data basis for the numerical calculations.

The developed analysis tool uses mean values of gas concentrations to create the kinetic equations for the numerical calculations. All diagrams are created automatically. Two freeware programs are used: Gnuplot and Latex. The kinetic equations are used as input for the numerical calculations. With the optimized numerical calculations gas concentrations of very toxic smoke gas components, e.g. CO, can be predicted within the calculated geometries. The next step is the calculation of visibility ranges. The investigated topics are under on-going research for which this project was the initial. Further research will be made available and published.

Bundesanstalt für Materialforschung und -prüfung (BAM)
12200 Berlin, 2010-05-25

VII.39 AG Brandszenarien und Brandanalytik

im Auftrag

Dr. Anja Hofmann
Arbeitsgruppenleiterin

im Auftrag

Nils Kersting

Verteiler:
1. Ausfertigung: <>
2. bis <> Ausfertigung: