

Measurement and simulation of fire smoke

BRANDFORSK PROJECT 702-041



Abstract

The arson fire at the Växjö psychiatric hospital in 2003, in a tragic way demonstrated the importance of knowing how materials will behave when ignited. The ignitability of a PUR-based mattress proved to be the initiator for a fast and intensive flash-over where the PVC floor carpet played an important part. This was shown in a reconstruction made at SP where the PVC-material also explained the very high smoke density reported. The findings were confirmed by soot samples taken at the hospital as they contained high amounts of chlorides.

As the PUR-material will produce isocyanates when heated, the soot samples taken were also analysed with regards to these substances but no trace of isocyanates were found. However, isocyanate-metabolites were found in lung-tissues from both death victims.

The reconstruction and another full-scale experiment where a mattress was burnt were in the project both compared to CFD-based simulations. In the mattress case, an advanced flamelet-model was used for calculating the chemical composition of the gas, where as in the reconstruction, small-scale data was used as input for gas composition.

The small-scale data was obtained using a suggested ISO-method for measuring smoke composition in various ventilation conditions. The method is based on a "Purser furnace", which was constructed as part of the project.

Key words: smoke, toxicity, particles, Purser furnace, building materials, CFD, flamelet

**SP Sveriges Provnings- och
Forskningsinstitut**
SP Rapport 2005:29
ISBN 91-85303-60-7
ISSN 0284-5172
Borås 2005

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SP Report 2005:29

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Preface

In fire accidents, the major threat to human life and health is the produced smoke. Smoke from a local room fire might spread to an entire building through corridors and ventilation systems, thereby menacing people also far from the fire itself. This was tragically demonstrated in a hospital fire in Växjö, Sweden, in August 2003. In spite of the fact that combustion only took place in a single room and further that it was of a relatively short duration (~13 min), two people were killed and three others were severely injured by the fire smoke, even though several of the victims were located quite far from the fire room. Sixteen people in total were intoxicated by the fire smoke.

There is a need to be able to estimate toxicity in fire smoke from burning materials of different sorts and from different kind of fire scenarios. Such knowledge admits to minimize toxicity in fire smoke by choosing appropriate materials from the beginning and provides the possibility of a correct estimation of the fire hazard. Practically no drug therapy of fire victims with severe lung and respiration injuries exist today. A better knowledge of the fire smoke content at least provides the opportunity for treatment of fire victims.

In the reported project, small-scale and large-scale fire experiments, using well-defined building materials, have been performed and used as input and/or comparison for smoke generation and simulation. The newly suggested small-scale experimental method (ISO/CD 19700⁵) based on a “Purser furnace” were used in order to obtain small-scale smoke data under different ventilation conditions.

In the project we have also ”reproduced” the fire scenario from the tragic hospital fire in Växjö. A major difficulty for the fire brigade in Växjö was the very dense smoke produced and we have through our experiments been able to find a likely explanation for this heavy smoke production.

Other basic questions asked as we started the project were:

- Is it possible to simulate a room fire and the smoke spread in a room/corridor scenario using CFD and gas production data obtained from small-scale experiments?
- Can CFD and an existing flamelet model for nitrogen containing fuels (BRANDFORSK project 321-011) be used to simulate with a reasonable precision the gas concentrations and smoke spread from a room fire?

Summary

This project was initiated in order to:

1. Study a new small-scale toxicity test method for fire smoke
2. Reconstruct a the severe fire accident at the Växjö psychiatric clinic in 2003
3. Make simulations of smoke spread from full-scale fires and calculate gas composition based on small-scale test data or a chemical kinetics model.

The result of the project has shown that the small-scale test method is usable and provides interesting techniques for smoke generation testing under various ventilation conditions, but we also found some difficulties that need to be considered. One such difficulty is that not all materials will exhibit a flaming combustion during the experiment, even though large amount of toxic gases are being produced. A complete small-scale toxicity test method obviously must be able to handle such materials too.

The reconstruction clearly demonstrated that the PVC-based floor carpet was responsible for the heavy smoke and the reported high intensity of the fire. The reconstruction pointed at the often neglected importance of the floor and the flooring material for the development of an enclosure fire.

The simulations gave further explanations for the graveness of the Växjö hospital fire. It indicated that the hot smoke leaving the fire room out to the corridor had enough time and space to cool down and sink to the floor level before reaching the rooms at the end of the hospital corridor, which made the situation very difficult for anybody being stuck in this region. Simulations also showed a good agreement with experimental data when the advanced chemical kinetics model was used, but also that a reasonably good agreement was obtained when small-scale toxicity data was used as input to the CFD-simulation.

1 Background

For many years the importance of material qualities with respect to fire and fire smoke has been in focus for research in Sweden and elsewhere. Internationally there has been an increasing interest in smoke toxicity, largely triggered by fire disasters such as the King's Cross underground fire in London and the more recent subway fire in South Koreaⁱ where the smoke played a key-role in the disaster. This interest can be traced to numerous reports but it is also mirrored in the international standardisation work, e.g. by ISO/TC 92/SC3: "Fire threat to people and the environment".

Risk evaluation, i.e. estimating egress time from burning buildings is the major interest. Fire safety engineering requires a design fire¹ but also knowledge about which fire gases that are generated, which in turn depends on the fire scenario and the materials involved. Some materials will produce very large amounts of particles and dangerous gaseous substances^{2,3,4} in a fire, and this information needs to be included in a risk evaluation. Knowledge of the fire smoke generating capability and the related toxicity from burning of different materials is further of importance from both an ecological and a health-related perspective.

Within the fire community, carbon monoxide, CO, has for a long time been considered as the sole explanation for fire smoke intoxication. However, other and much more toxic substances might be present in the smoke. Hydrogen cyanide, HCN, is produced when nitrogen containing material is burning. The substance is 35 times more toxic than carbon monoxideⁱⁱ. Already at a concentration of 20 ppm HCN in air, people start to show signs of intoxication after some time and at 120 ppm a 30 minute exposure might be lethal. The toxic effect of HCN is also synergistic with CO.

Another highly potent toxic group of substances, obtainable from fires in nitrogen containing materials is isocyanates. There are many different isocyanates but they are all considered to have approximately the same acute toxicity, which means more than ten times as toxic as HCN and 300-400 times as toxic as CO. It has further been demonstrated²⁻³ that isocyanates, contrary to CO and HCN might be found in high concentrations in fire smoke also when there is a surplus of oxygen, i.e. in well-ventilated fires.

There is an inherent difficulty in testing of smoke toxicity if the toxicity is to be related to a specific fire scenario, e.g. if a flaming or smouldering fire is considered, or if data from a well-ventilated or under-ventilated fire scenario is requested. At present, a subgroup within the International Standardisation Organisation, ISO/TC 92/SC3, is preparing a new small-scaled testing method for smoke toxicity from fires in materials⁵. The method is based on the "Purser furnace". The principle and experimental equipment suggested is already being used as an IEC-standard (IEC 60695-7-50) for cable materials. The suggested standard provides the ability for testing all different burning scenarios mentioned above and it has been used in this project in order to obtain small-scale data for simulating large-scale fires.

In a tragic arson fire at a psychiatric clinic in Växjö, Sweden, August 2003, two young women were killed and several others were severely injured. The fire was local (one room only), of a short duration (~13 minutes) but was very intense. The basic fire-"engine" was a polyurethane (PUR) based mattress. Since PUR will produce both HCN and isocyanates together with CO in a fire and since the events were quite well documented, the Växjö-fire was an interesting case-study for investigating smoke toxicity

ⁱ http://www.banverket.se/upload/6115/PM_Korea.pdf

ⁱⁱ Toxicity comparison is very difficult, even when speaking of substances that have similar effects on humans. In the above context, the American IDLH-values have been used for the comparison, see www.cdc.gov/niosh.

in a real fire. Also, the reports from the fire brigade pointed out a specific enigma in relation to the fire smoke as it was said that the smoke density was "exceptionally" high. Based on the initial information on what had been burning it seemed difficult to fully understand this and one of the quests for this project became therefore to try to find some plausible explanation for the dense fire smoke.

2 Project set-up

Prerequisites for the project, simulation tools and experimental equipment, will be described in this chapter. Most of these already existed prior to this project but it was also necessary to construct a new type of equipment, a “Purser furnace” for the small-scale experiments. This also provided an opportunity to study equipment that might very well be a corner stone in future tests of toxicity in fire smoke, and some critical aspects of using the furnace will be given in this report.

2.1 Small-scale tests

In the project 7 different materials were tested in a Purser furnace:

- Mattress
- Wood cribs
- Fluorinated polymer cable
- PUR (polyurethane), rigid
- PVC-floor carpet
- Polyethylene pellets
- PVC pellets

The experiments were performed according to the testing methodology suggested by ISO/CD 19700. The selection of material was based on a previous project² and on the need for information and data to be used in simulating the large-scale scenario.

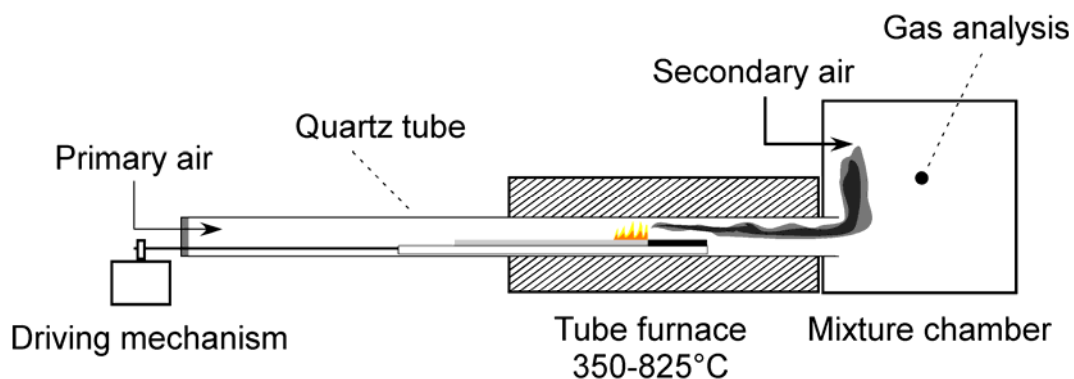


Figure 1 Schematic picture of a Purser furnace

The experimental set-up for a Purser furnace is based on a tubular furnace where a quartz tube is fixated in a non-moving furnace. The sample is placed in a sample vessel in the tube and it is slowly transferred into the furnace during the experiment. The oxygen flow in the tube is controlled by the primary air intake and the smoke is transported to a mixing chamber where secondary air is added.

In principle, the type of combustion is defined by the quotient fuel/oxygen. If the amount of oxygen molecules counterbalances the amount of fuel exactly, then the condition is said to be stoichiometric. Formally, this is expressed by saying that the equivalence ratio ϕ is equal to 1ⁱⁱⁱ. An under-ventilated combustion would imply that $\phi > 1$ and well-ventilated burning conditions that $\phi < 1$. In the Purser furnace, ϕ is easily changed by varying the flow rate of primary air or/and the fuel input rate.



Figure 2 The Purser furnace from the front end (left photo), showing the quartz tube and primary air intake (plastic tube) and the back side with the mixing chamber (right photo)

In these measurements an instrument capable of measuring the equivalence ratio, a “ ϕ -meter”⁶, was connected to the mixing chamber. As the flow of secondary air is known, the registered ϕ -value in the mixing chamber can be used to calculate the ϕ -value in the reaction zone, i.e. in the quartz tube enveloped by the furnace. Samples for measuring the smoke composition is easily obtained from the mixing chamber (see Figure 2).

Advantages with the method are:

- Small-scale implies low experimental costs
- The combustion is, due to a continuous inflow of fuel and oxygen during the experiment, more or less stationary.
- Different combustion conditions are easily studied by controlling ϕ .
- A well-controlled temperature environment is obtained from the enveloping furnace.
- The mixing chamber makes it easy to obtain samples at close to room temperature.

During the tests, particle size distribution from some of the experiments in the Purser furnace was measured. The main objective was to be able to compare them to previous tests² in other experimental set-ups and to the large-scale experiments performed during this project. Further was the smoke in the mixing chamber analysed with regards to its content of HCN, NO_x, CO, CO₂, O₂, halogens (all measured with FTIR analysis) and isocyanates (impinger analysis technique).

ⁱⁱⁱ Equivalence ratio $\phi = \{\text{real quotient [fuel/oxygen]}\} / \{\text{stoichiometric quotient [fuel/oxygen]}\}$.

2.2 Full-scale tests

Two full-scale tests were performed in the "Room-Corner" enclosure scenario (Figure 3). In one of them the enclosure was furnished similarly to the room involved in the Växjö hospital fire and in the other a plain mattress was burnt. In both experiments, the same measurement as in the small-scale tests were performed, i.e. HCN, NO_x, CO, CO₂, O₂, halogens and isocyanates were measured as well as the particle size distribution and the equivalence ratio ϕ . The experiment involving only a mattress was made in order to obtain comparison data for the CFD simulation. The Växjö hospital fire reconstruction, however, also had other objectives than doing a simulation comparison, as explained below.

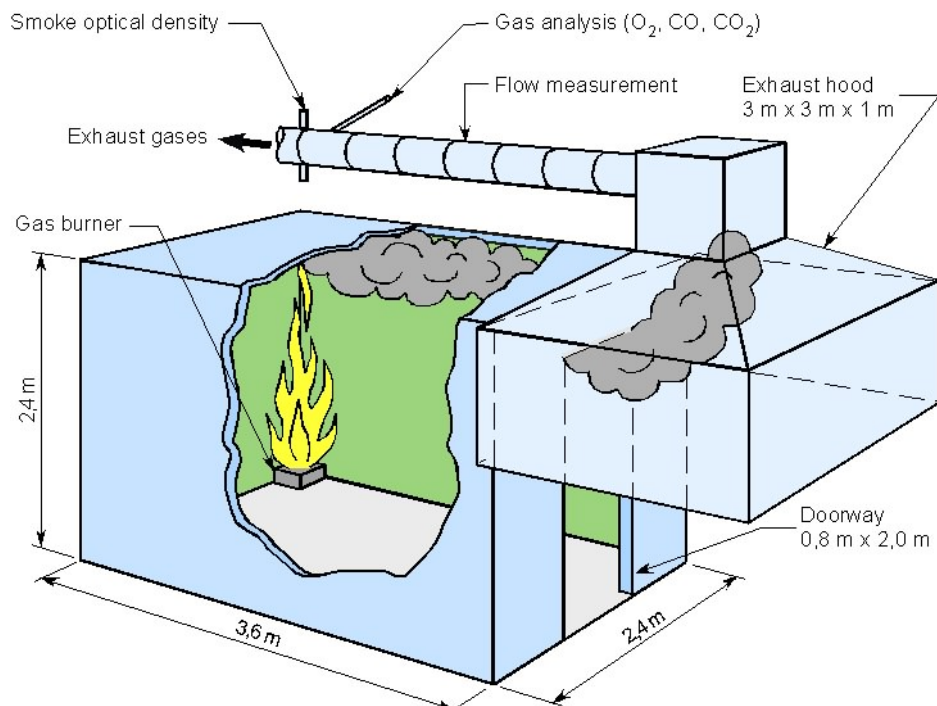


Figure 3 Room-Corner fire scenario, according to ISO 9705

2.2.1 The Växjö hospital fire

In the fire at the psychiatric clinic in Växjö, Sweden, August 2003, the main reason for the very fast and intense fire was most likely a PUR-based mattress. The mattress quality with respect to fire was said to be based on the Swedish Standard SS 876 00 01, which stipulates a glowing cigarette or a small gas flame (equal in effect to a cigarette lighter) as ignition sources. Obviously, a test based on such ignition sources has, in terms of fire safety, nothing to do with an environment where there is a high risk for arson fires. A mattress of the same type as in the fire was tested at SP according to the more severe standard SS 876 00 10, where a 30 kW gas burner (approximately equivalent to a few burning sheets of paper) is situated close to the mattress surface for 2 minutes. The tested object is not allowed to contribute more than 55 kW in fire effect in order to pass the test and as can be seen in Figure 4, the mattress was very far from the criterion; within 2 minutes the mattress produced more than 1 MW, enough to cause a flashover in a room of the same size as the hospital fire room.

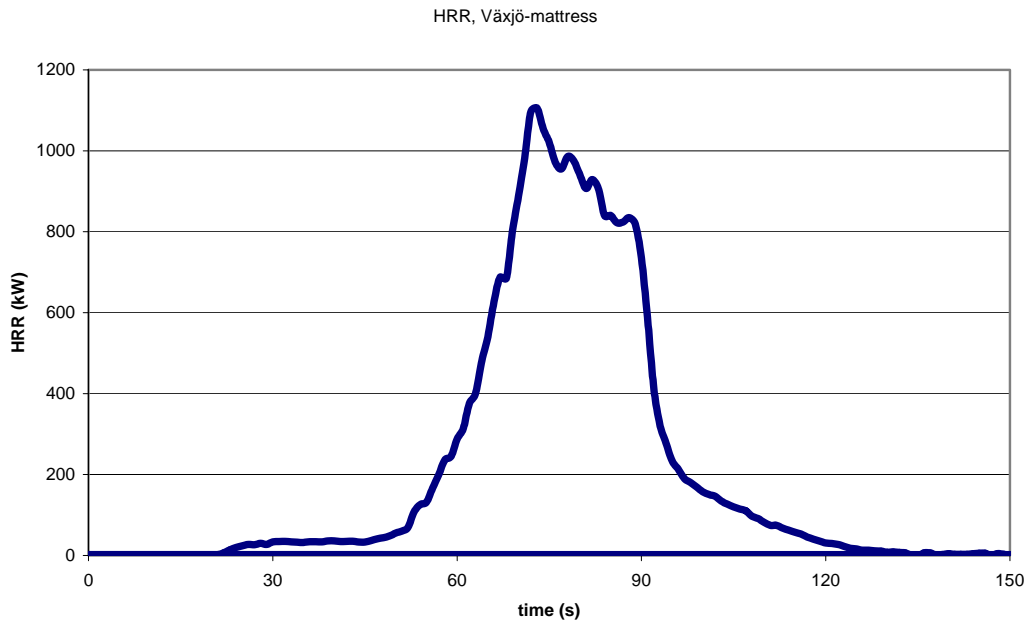


Figure 4 HRR for a mattress of the same type as in the Växjö hospital fire

In the hospital room there was also other objects involved in the fire, notably a TV-set, an armchair, desks, wardrobes, personal belongings and a wood based desk and chest.

However, due to the short period of time before the fire brigade was able to extinguish the fire (~13 min) much of the wooden based furniture was, if not intact, so at least left with a lot of combustible material after the extinguishment.

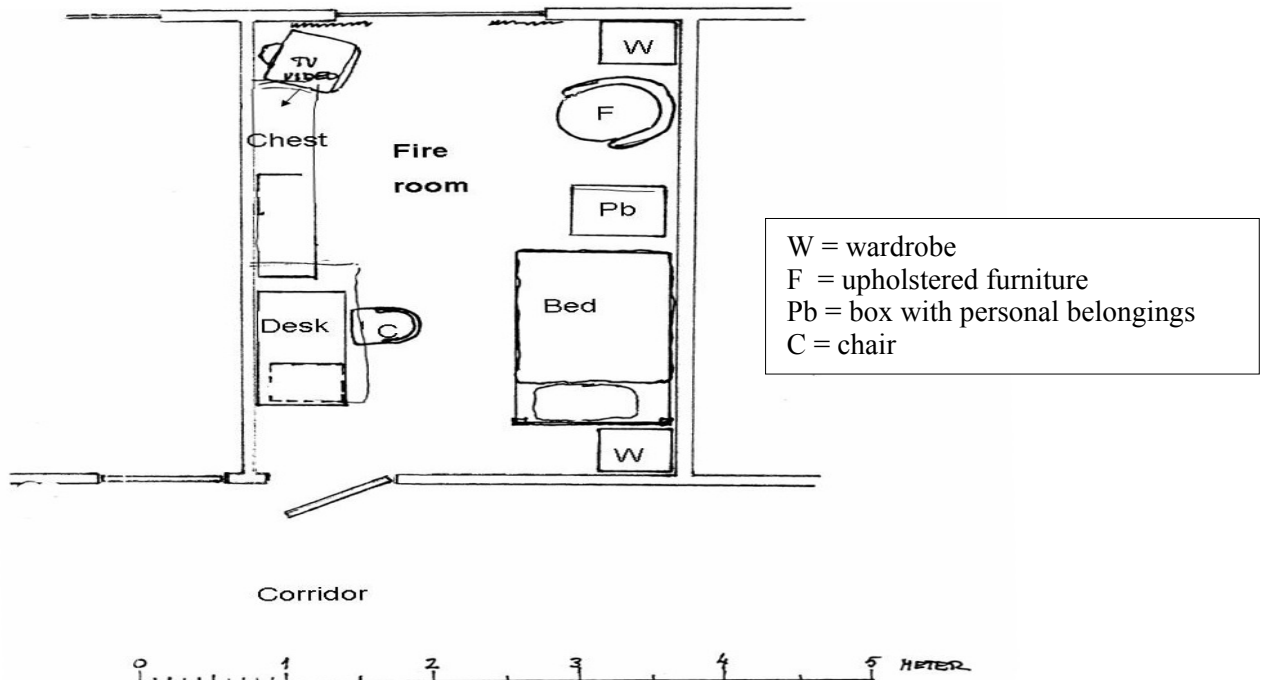


Figure 5 Schematic picture of the Växjö hospital fire room

As the hospital was a psychiatric detention clinic where most of the patients had criminal record, doors were locked and the windows were unbreakable, so even if the drama took

place at the first floor, it was necessary for smoke divers to rescue several patients. This was found to be very difficult mainly due to a heavy smoke.

Even though it is well known that PUR might produce a lot of smoke and that a TV-set was burnt, which also is a typical “smoke producer”, it seemed difficult to explain the very high amount of smoke reported. When studying photos of the post-fire remnants, it was seen that the front side of the wooden desk in the fire room was evenly burnt. This indicated that something on the floor level must have been burning, since otherwise, the furniture would have been burnt mainly on top due to the hot smoke gas layer. When this was investigated further, it was discovered that a PVC-carpet indeed had been in place in the fire room and that virtually nothing at all was left of the carpet after the fire. In the Room-Corner experiment, a PVC-carpet was therefore put on the floor and it was to be seen that this had a major impact on the fire development.



Figure 6 Photo of a desk from the fire room

Apart from the floor carpet, a bed with a mattress from the clinic was used together with a TV-set, a desk, upholstered furniture of the same kind as was used in Växjö and finally low energy containing, but easily ignitable, curtains. The experimental set-up can be seen from the photo in Figure 7. It should be noted that the real fire room contained more combustible objects but it was decided to mainly use what was supposed to have been major sources for fire and smoke. Another important difference between the experiment and the real fire was that the window was broken after a while due to the heat and since the door was open, the fire was able to develop without any lack of oxygen. In the experiment, only one inlet/outlet for oxygen and fire gases was available. Basically, reproducing a fire is inherently difficult but the main objective for the investigation made was to try to understand the heavy smoke produced as well as the intensity and fast evolution of the fire.



Figure 7 Photo of furniture etc used in the Växjö fire reconstruction

In the experiment, the mattress and TV-set were ignited simultaneously using wood-crib that produced an effect of 10-15 kW.

2.2.2 Measurements

2.2.2.1 Inorganic gases

Time resolved measurements of the concentration levels of various inorganic gases in the mixing box of the Purser furnace (small-scale) or the Room-Corner door opening (full-scale, see Figure 8), close to the maximum height of the opening, were obtained using a BOMEM MB 100 FTIR spectrometer. The analyser was equipped with a heated gas cell (volume = 0.92 l, path-length = 4.8 m, temperature = 150°C). A spectral resolution of 4 cm^{-1} was used, with 4 averaged spectra (based on 3 full scans) recorded per minute. The smoke gases were continuously drawn to the FTIR with a sampling rate of 4 l min^{-1} using a stainless steel probe with a ceramic filter. Both the filter and gas sampling lines (4 mm i.d. PTFE) were heated to 180 °C. The proper function of the FTIR equipment was verified by measurement of a calibration gas. The FTIR data (spectra) was quantitatively evaluated for a selected number of gas species. These gases were: carbon monoxide (CO), hydrogen chloride (HCl), hydrogen bromide (HBr), hydrogen fluoride (HF), hydrogen cyanide (HCN), nitrogen monoxide (NO), nitrogen dioxide (NO₂), ammonia (NH₃) and sulphur dioxide (SO₂). In the full-scale experiments, measurements were also made in the exhaust duct of O₂, CO and CO₂ in accordance with the ISO 9705 instrumentation.

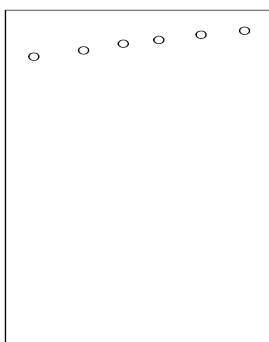


Figure 8 Sketch of the measuring points across the door opening. The opening height is 2.0 m.

2.2.2.2 Particles

Particles were sampled and size determined using a *DEKATI* low pressure impactor^{iv}. A sub-flow of the smoke gases was led to the impactor from the mixing chamber of the Purser furnace (and from the exhaust duct in the full-scale experiments). The sub-flow had a flow rate was 10 l min^{-1} . The low pressure impactor measures airborne particles, size distribution in the size range $0.03 - 10 \text{ }\mu\text{m}$, with 13 channels by the means of pre-weighed impactor plates. Airborne particles are size classified according to their aerodynamic diameter in the cascade low pressure impactor. The sampled mass distribution within the 13 size ranges was determined gravimetrically after each test. The gravimetric determination was made using a calibrated analytical balance with a mass error less than $4 \text{ }\mu\text{g}$. The impactor plates were stored in a desiccator before weighing. The sampling of particles covered the complete test-period

2.2.2.3 Isocyanates

Isocyanates and amines were sampled using an impinger-filter sampling system⁷. This system samples airborne isocyanates in a 30 ml midget impinger bottle containing 10 ml reagent solution of 0.01 mol dm^{-3} DBA (D-n-butylamine) in toluene. A 13 mm glass fibre filter with a pore size of $0.3 \text{ }\mu\text{m}$ was placed in series after the impinger. After sampling, the filter was immediately placed in a test tube containing together with the impinger flask solution. It has been shown⁷ that large particles ($> 1.5 \text{ }\mu\text{m}$) are retained in the impinger solution, whereas smaller particles pass through the impinger solution and are collected by the filter. The filter is continuously impregnated by the reagent solution during sampling (the DBA/toluene solution is rather volatile), and particles in the size range $0.01 - 1.5 \text{ }\mu\text{m}$ are collected^v.

The isocyanate sampling probe was positioned on the Purser furnace mixing box in the small-scale experiments and in the full-scale experiments, samples were taken isokinetically from the exhaust duct. The total flow rate for sampling of isocyanates was 1.0 l min^{-1} . The smoke gases were drawn through a 1.5 m heated sampling tube (4 mm i.d. PTFE, 150°C) by means of a calibrated sampling pump (1 l min^{-1}). Approximately 0.2 m of the sampling tubing, closest to the impinger-filter sampler, was left unheated to cool the smoke gases somewhat before entering the impinger bottle, in order to avoid too great losses of the volatile absorption solution.

The collected isocyanate samples were subsequently analysed for isocyanates and amines. The analysis method was based on LC-MS technique and has previously been described by Karlsson et al.⁷.

The sampling of isocyanates from the small-scale experiments normally covered the complete test-period. However, sometimes the pressure drop became too large due to a too high amount of particles in the filter system which stopped the sampling pumps.

In the full-scale experiments, three samples were taken from each experiment in order to obtain a somewhat “time resolved” measurement. This was particularly interesting for the Växjö fire reproduction experiment since this was likely to provide a flash-over situation and the isocyanate production could therefore be expected to vary a lot over time.

2.2.2.4 Equivalence ratio

The equivalence ratio, ϕ , in the combustion zone can be calculated in a Purser furnace experiment. Such calculations require, however, detailed knowledge of the chemical composition of the sample. A coarse step by step method to introduce well-ventilated

^{iv} www.dekati.com/dlpi.shtml

^v This is the size of particles that will pass the impinger flask.

respective under ventilated conditions, based on data on oxygen reduction in the mixing chamber, is described in ISO/CD 19700⁵.

The equivalence ratio, ϕ , can actually be measured/estimated using a phi-meter⁸. The instrument is based on making a mass-balance around a catalytic reactor where a total oxidation of unreacted hydrocarbons from the combustion zone is being made, using a surplus of added oxygen. The instrument is schematically pictured in Figure 9.

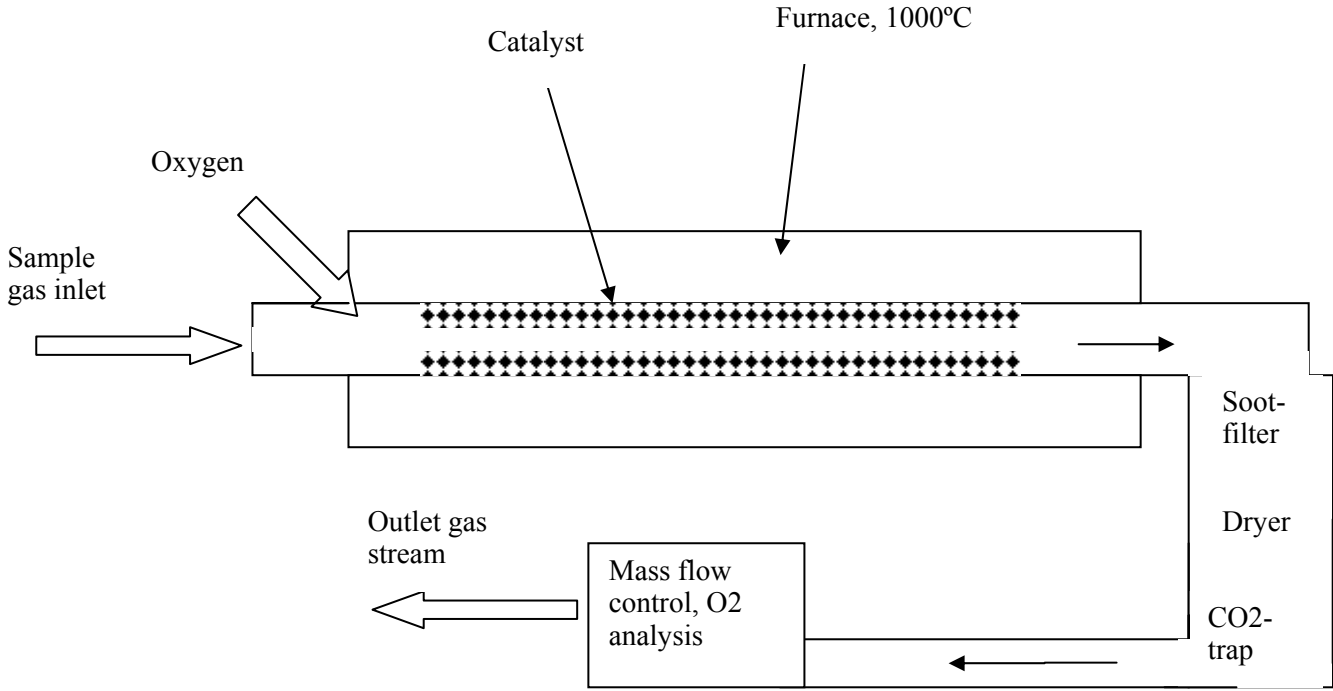


Figure 9 Schematic picture of the ϕ -meter

The equivalence ratio is obtained according to the expression:

$$\phi = \frac{x_{O_2}^i - x_{O_2}}{x_{O_2}^a (1 - x_{O_2})} \quad (1)$$

where $\{x_{O_2}^i, x_{O_2}^a, x_{O_2}\}$ represents phi-meter oxygen concentration with ambient air at the inlet, oxygen concentration of ambient air (~ 0.21) and -phi-meter oxygen concentration during the experiment respectively. The ϕ -meter is used in order to calculate ventilation conditions in the experimental set-up as a post process, i.e. it uses experimental exhaust gases as sample inflow to the ϕ -meter. For the full-scale experiments, equation (1) was used for estimating the value of ϕ , and the gas was sampled directly in the smoke coming from the room, 5-15 cm below the top of the door opening in the room-corner scenario (see Figure 3).

However, for the Purser furnace experiments, the gas was sampled in the mixing box and therefore diluted before the sample could be sent to the phi-meter. This means that x_{O_2} , the sample inlet gas oxygen concentration (see Figure 9) became too high and a corrected value must therefore be estimated in order to obtain a ϕ -value for the experiment.

A mass balance for oxygen in the phi-meter provides the following equation:

$$Q_3 x_{O_2} = Q_1 x_{O_2}^{in} + Q_2 + R \quad (2)$$

where $\{Q_1, Q_2, Q_3\}$ are the sample inflow, the pure oxygen inflow and the phi-meter outlet flow respectively. R is the reacting oxygen in the phi-meter and $x_{O_2}^{in}$ is the (diluted) gas sample oxygen inlet concentration from the Purser furnace to the phi-meter. The value we need is the corrected $x_{O_2} \equiv x_{O_2}^r$ that would be obtained if an undiluted inlet oxygen concentration was used, i.e. we want to solve the following oxygen mass balance:

$$Q_3 x_{O_2}^r = Q_1 \overline{x_{O_2}^{real}} + Q_2 + R \quad (2')$$

Subtracting (2) from (2') provides

$$Q_3 x_{O_2}^r = Q_3 x_{O_2} + Q_1 \overline{x_{O_2}^{real}} - Q_1 x_{O_2}^{in} \quad (3)$$

The following relation holds true⁶:

$$\frac{Q_2}{Q_3} = \frac{x_{O_2}^i - x_{O_2}^a}{1 - x_{O_2}^a} \quad (4)$$

Further, a total mass balance for the phi-meter, assuming that flow variations due to drying and CO₂ absorption can be neglected, provides:

$$Q_3 = Q_1 + Q_2 \quad (5)$$

The right-hand-side of (4) is obtained from measurements and if it is denominated "Y", equation (4) can be expressed:

$$Q_2 = Y Q_3 \quad (6)$$

Equation (5) and (6) provides:

$$Q_1 = Q_3 - Q_2 = Q_3(1 - Y) \quad (7)$$

Equation (7) in (3) leads to:

$$\begin{aligned} Q_3 x_{O_2}^r &= Q_3 x_{O_2} + Q_3(1 - Y)(\overline{x_{O_2}^{real}} - x_{O_2}^{in}) \\ &\Leftrightarrow \\ x_{O_2}^r &= x_{O_2} + (1 - Y)(\overline{x_{O_2}^{real}} - x_{O_2}^{in}) \end{aligned} \quad (8)$$

Based on equation (8), a corrected phi-meter oxygen outlet signal can be calculated from a known inlet concentration and measured data and used in equation (1), which will provide the corrected phi-value. However, the correct, un-diluted, oxygen inlet concentration has to be calculated first.

In the Purser furnace, the experimental exhaust gas flows (Z l/min) into the dilution/mixing box where samples are taken. Secondary air is added to the box in order to obtain 50 l/min total flow. An oxygen mass balance over the box provides:

$$x_{O_2}^{in} = \frac{\overline{x_{O_2}^{real}} Z + x_{O_2}^a (50 - Z)}{50} \quad (9)$$

i.e.

$$\overline{x_{O_2}^{real}} = \frac{50x_{O_2}^{in} - x_{O_2}^a (50 - Z)}{Z} \quad (10)$$

$x_{O_2}^{in}$ is measured in the experiments and Z is known.

The procedure for calculating the correct ϕ -value in the Purser furnace experiments is thus:

1. Calculate Y from equation (4) and (6)
2. Calculate the experimental exhaust gas concentration from equation (10)
3. Calculate the corrected phi-meter experimental oxygen value from equation (8)
4. Calculate the corrected phi-value from equation (1) using $x_{O_2}^r$ instead of x_{O_2} .

2.3 Simulation models

A model for HCN generation in fires was developed during the BRANDFORSK project 321-011⁹. The technique is based on using a laminar flamelet^{vi} model in a CFD-tool for making the simulations. The flamelet data have previously been calculated at Lund University for two different mixtures of ethylene and methyl-amine. These data were later implemented at SP into the CFD simulation tool SOFIE. The advanced combustion model makes it possible to semi-quantitatively simulate the gas phase chemistry for any nitrogen containing material and it is unique due to its capability of simulating hundreds of chemical reactions, including the reaction dependency of temperature *and* vitiation during the combustion. In this project, the simulation model has been used for comparison with full-scale data from a room-fire.

Another, simpler method for making a CFD-based fire gas simulation is to utilise data from small-scale experiments, and simply transfer the production rate information to the large-scale simulation. A difficult part is then to obtain and use appropriate data depending on if the combustion is taking place with a surplus of oxygen present or not. This kind of simulation has also been done during the project.

2.4 CFD simulation set-up

A Reynolds-Averaging Navier-Stoke (RANS) type CFD code, SOFIE (Simulation of Fires in Enclosures) was used. Two separate simulations were made using different combustion models:

- 1) Laminar flamelet model, which uses a detailed chemical kinetics scheme for the formation of chemical species as HCN and CO.
- 2) Eddy-break-up model, which uses a global chemical reaction converting the fuel and oxygen directly to main combustion products. In this model HCN and CO

^{vi} The chemical composition in "small flames" (flamelets) is pre-computed based on temperature chemistry and time step for the flamelet, and data is stored to be used in e.g. a CFD-model.

were treated as passive scalars. Input values for the CFD simulations were taken from the small-scale (yields) and full-scale experiments (HRR) respectively.

A transient mode of SOFIE was used in both simulations using a time step length of one second. The convergence of the solution was controlled keeping all solved variable's residuals (normalised) as low as possible, usually below 0.001. The under-relaxation parameters for the momentum equations were set to 0.3 at the beginning of the simulation and were reduced further to 0.2 at time $t=30$ s.

The flamelet model used in SOFIE is made for varying radiation. However, the model can be used in several different ways: As adiabatic flamelets (i.e. radiation switched off), non-adiabatic flamelets with fixed radiation and non-adiabatic flamelets with varying radiation. In this case the non-adiabatic flamelets with varying radiation was used.

The discrete transfer radiation model (DTRM) assuming 16 rays (default value) were used in the simulations¹⁰. A simple soot model was used. The soot was entered into calculation domain via fuel flow assuming that 2 % of fuel mass consisted of soot.

2.4.1 Case I: Single room scenario

The calculation domain was divided in 212 787 small control volumes (37, 71 and 81 cells in x , y and z directions, respectively). This corresponds to an average cell size of about 10 cm. The space was divided with a higher resolution in the combustion region, where the largest gradients in field parameters are expected. In the fire plume and in the vicinity of it, a typical cell size between 3 and 6 cm was used. Especially, in the vertical direction (y -coordinate) the space was divided finely, to be able to resolve the chemistry in the plume flow. In the other regions inside the room a typical cell size of 10 cm, and outside the room 15 to 25 cm, were used.

2.4.1.1 Fire source

In this test, the fire source was a bed and the only fuel was the polyurethane mattress. The computer model for the fuel was a mixture of methylamine and ethylene in the proportions of 1:3 implemented in the laminar flamelet model. The nitrogen content of this mixture is close to that of polyurethane, and hence the yield of nitrogen containing products of combustion is expected to be similar.

The computer model of the mattress was divided into three equal parts of 0.594 m² area. This was done in order to resemble the time development of the real fire behaviour during the test. In the simulation, the fire was started at the end of the bed, i.e. one of the 0.594 m² parts was ignited first. After 60 s the middle part was ignited and after 75 s the third part was ignited. The heat release rate (HRR) was increased smoothly from the three different parts of the fire source, so that the part that was ignited first also attained a high level of HRR first. At time 90 s all the parts had the same HRR, i.e. the whole mattress surface was burning. The HRR was given as input so that the total HRR would follow the curve taken from measurements (shown in Figure 22).

2.4.2 Case II: Hospital fire ground floor scenario

The scenario for the whole Växjö hospital ground floor was simulated using the eddy break-up combustion model; hence only calculation of main combustion products and CO was made. However, an additional parameter, a so called passive scalar, was included in the model, which makes it possible to calculate the spread of toxic substances, such as HCN, isocyanates, smoke, etc. The passive scalars are components assumed to be chemically stable, i.e. they are not destroyed once they are introduced into the computational domain. The primary reason for including the passive scalar option in

SOFIE is calculation of smoke spread. Indeed, many of the hazardous components in the smoke are stable once they have left the hot fire region, and can thus correctly be treated as passive scalars.

The calculation domain was divided in 308 425 control volumes (73, 25 and 169 cells in x , y and z directions, respectively). The cell sizes are thus larger in this case than in the single room scenario as the corridor and some adjacent rooms was included in the simulation. An average cell size of 0.4 m was used outside the fire room, in the fire room the cell sizes of 10 -20 cm were used, with the smallest in the fire region.

In total 10 minutes were simulated and the experimentally obtained HRR-curve was used as input to the simulation. Only the ground floor of the hospital building was modelled in the simulation. Spaces above the ground floor and also most of the patient rooms on the ground floor were treated as inactive blockages in the computer model. This was motivated by the fact that most of these locations were closed or did not interact with the fire development. However, some patient rooms on the ground floor, the rooms where victims were found, taken into account in the calculations. The doors to the rooms were closed in the CFD model but leakage of fire gases from the corridor to patient rooms was simulated by making ten cm high slots on floor level in the door walls. In the patient room at the end of the corridor (~40 m from the fire room) in which one person was killed and another severely injured by fire smoke, a ceiling vent (natural ventilation) was modelled.

In the simulation, fresh air was supplied to the house from the end of the corridor, opposite to the room with two victims mentioned above, through an opening 25 cm in width and with the same height as the corridor. Two metres from that end, a static pressure boundary was modelled, which allows for the flow of fresh air in and fire gases out of the calculation domain.

2.4.2.1 Fire source

The fuel in this scenario was a mattress, bedclothes, upholstered furniture, a TV-set, curtains, a desk and a PVC-carpet. The maximum heat release rate was about 2.4 MW and the burning time was substantially longer than in the single room case. The experimental HRR measured is shown in Figure 23.

3 Results

3.1 Small-scale experiments

One of the main advantages of using the Purser furnace is the possibility of creating a "quasi" steady-state combustion, i.e. since the fuel-feed and primary air supply into the reaction zone is constant, more or less static oxidation conditions are obtained. This makes it possible to study the reaction products under well-defined ventilation conditions.

Duplicate tests were run both at well-ventilated and under-ventilated conditions. The experimental settings used were selected according to what is described in ISO/CD 19700. Well-ventilated conditions were normally obtained with a high primary air-flow rate and with a furnace temperature of 650 °C. For under-ventilated conditions a lower primary air-flow rate was used with a furnace temperature of 825 °C.

During the experiments, the equivalence ratio was measured using the ϕ -meter. The measured value for well-ventilated conditions showed quite good agreement with the theoretical value. However, the vitiated value measured was too low compared to the theoretical ditto. A possible explanation for this is that there was a continued oxidation of the vitiated smoke in the mixing box before sampling of the gas was made to the ϕ -meter. The ϕ -value rarely became greater than 1.1-1.2, even when the combustion conditions clearly were such that the ϕ -value should be closer to 2.0. In Figure 10 is shown typical results from the measurements, even though the ratio is perhaps more stable here than in most cases, due to the very stable combustion conditions obtained for the wood material.

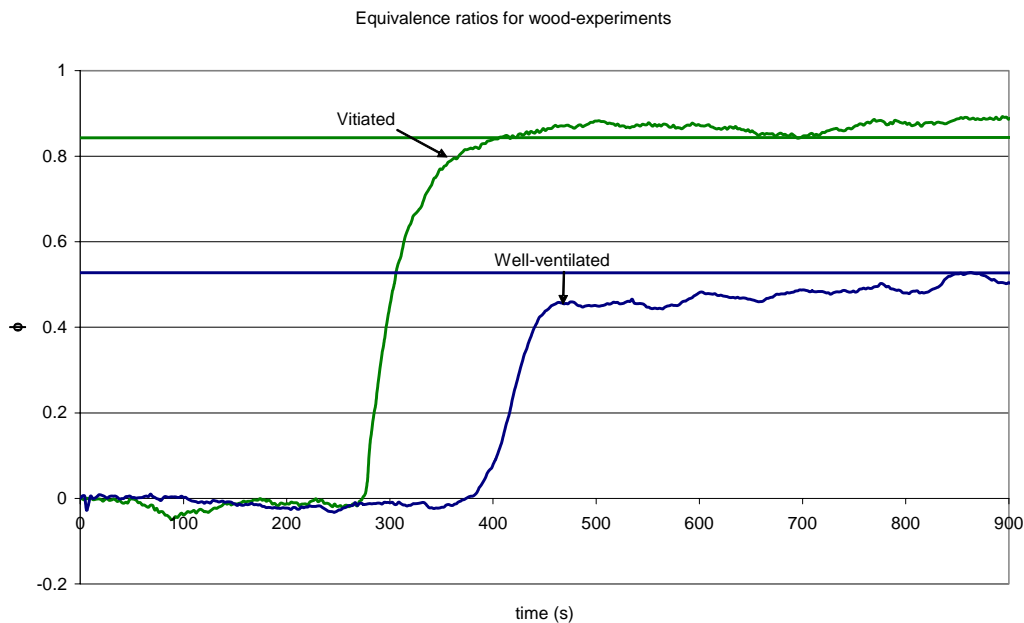


Figure 10 Estimated equivalence ratios for wood experiments.

3.1.1 Inorganic species

The results below are expressed as yields, often expressed as the quotient of mass of produced species and the mass of burnt fuel. Here, yield is calculated as the quotient of the production rate of species and the input rate of fuel (mass charge).

3.1.1.1 Wood

In Figure 11 is shown a comparison of CO and CO₂ production using well-ventilated or under-ventilated combustion conditions. It can be seen that at least the under-ventilated experiment might be considered as being performed under steady-state conditions. The figure also clearly demonstrates the shift in CO and CO₂ production when the ventilation condition is altered, which is in concordance with the common understanding of combustion chemistry.

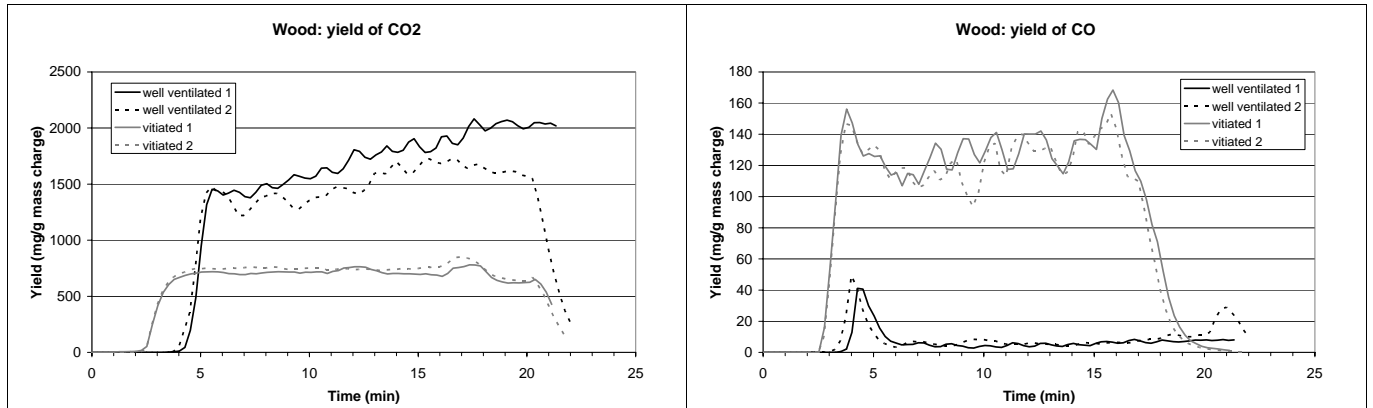


Figure 11 Results from wood combustion in the Purser furnace

3.1.1.2 PTFE-cable

The results from the Purser furnace experiments made with the PTFE-cable, is quite different from the wood experiments, which partly is explained by the fact that no flaming combustion took place. The production rate of the species measured are virtually unaffected by the different ventilation conditions and it is interesting to note that the quotient CO/CO₂ is similar to the quotient for under-ventilated wood combustion. It is also interesting to observe that the HCl mass production rate is of the same magnitude as the CO mass production rate. The HCl is developed from PVC-based material in the PTFE-cable and the production rate of HCl is in fact greater than the production rate of HF.

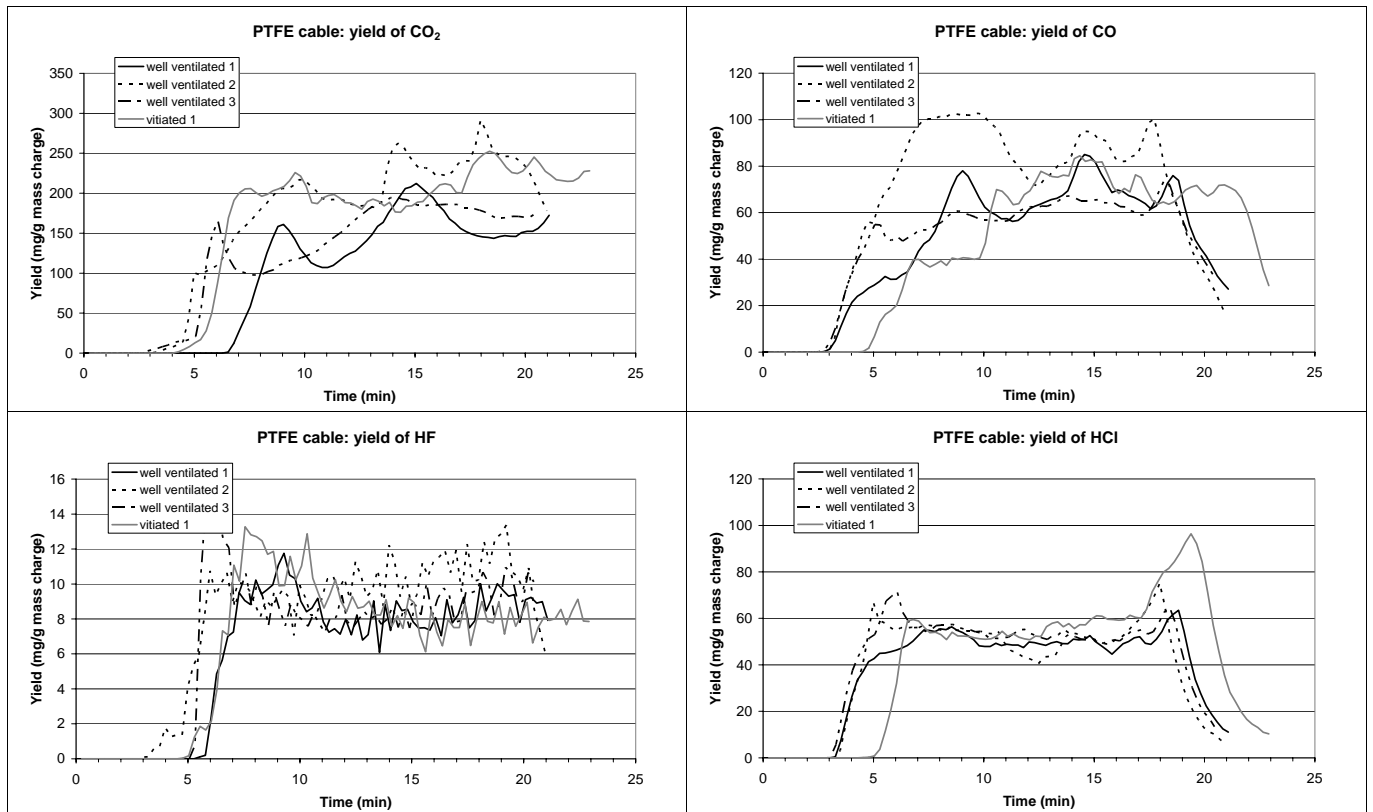


Figure 12 Results from PTFE-cable combustion in the Purser furnace

3.1.1.3 PVC-carpet

The PVC-carpet was of the same type as used in the full-scale Växjö hospital fire reconstruction and results from the small-scale experiments were used in the computer simulation of the fire. It can be seen that the CO-yield is only influenced slightly by the ventilation conditions and that in fact, the HCl-yield is higher than the CO-yield. The former fact can be explained by the flame-retardant effect of chlorides which makes total oxidation $\text{CO} \rightarrow \text{CO}_2$ difficult. The increased yield of HCl obtained for well-ventilated combustion compared to the vitiated case is explained by a more efficient combustion, i.e. a higher HCl production rate during well-ventilated conditions.

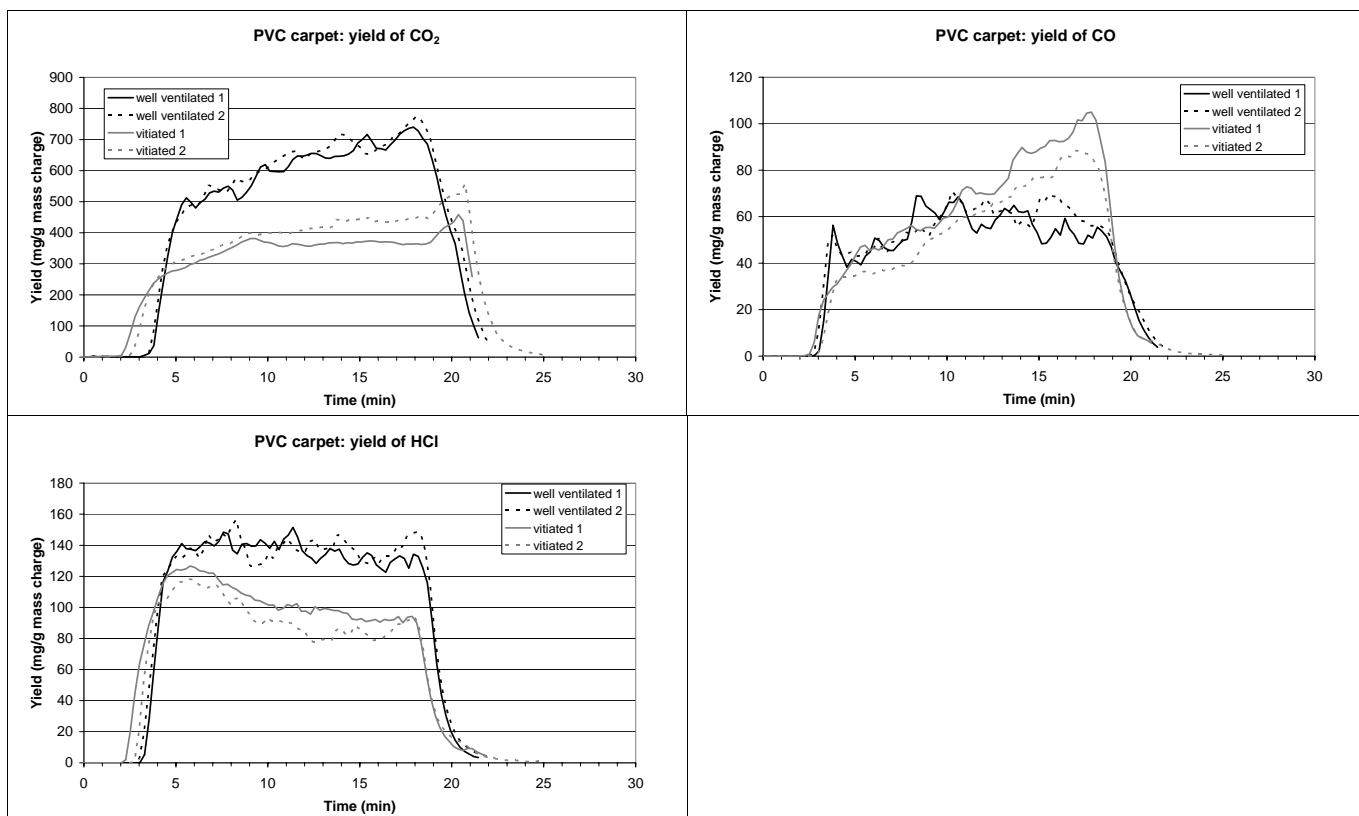


Figure 13 Results from PVC-carpet combustion in the Purser furnace

3.1.1.4 PVC-pellets

PVC-pellets were also tested in the Purser furnace and it might be interesting to compare this pure PVC-material to the carpet, which includes also other type of substances, such as softeners etc. A comparison between Figure 13 and Figure 14 reveals that the results are very similar. The difference between well-ventilated and vitiated HCl yield, however, seems to be less for the pellets than for the carpet.

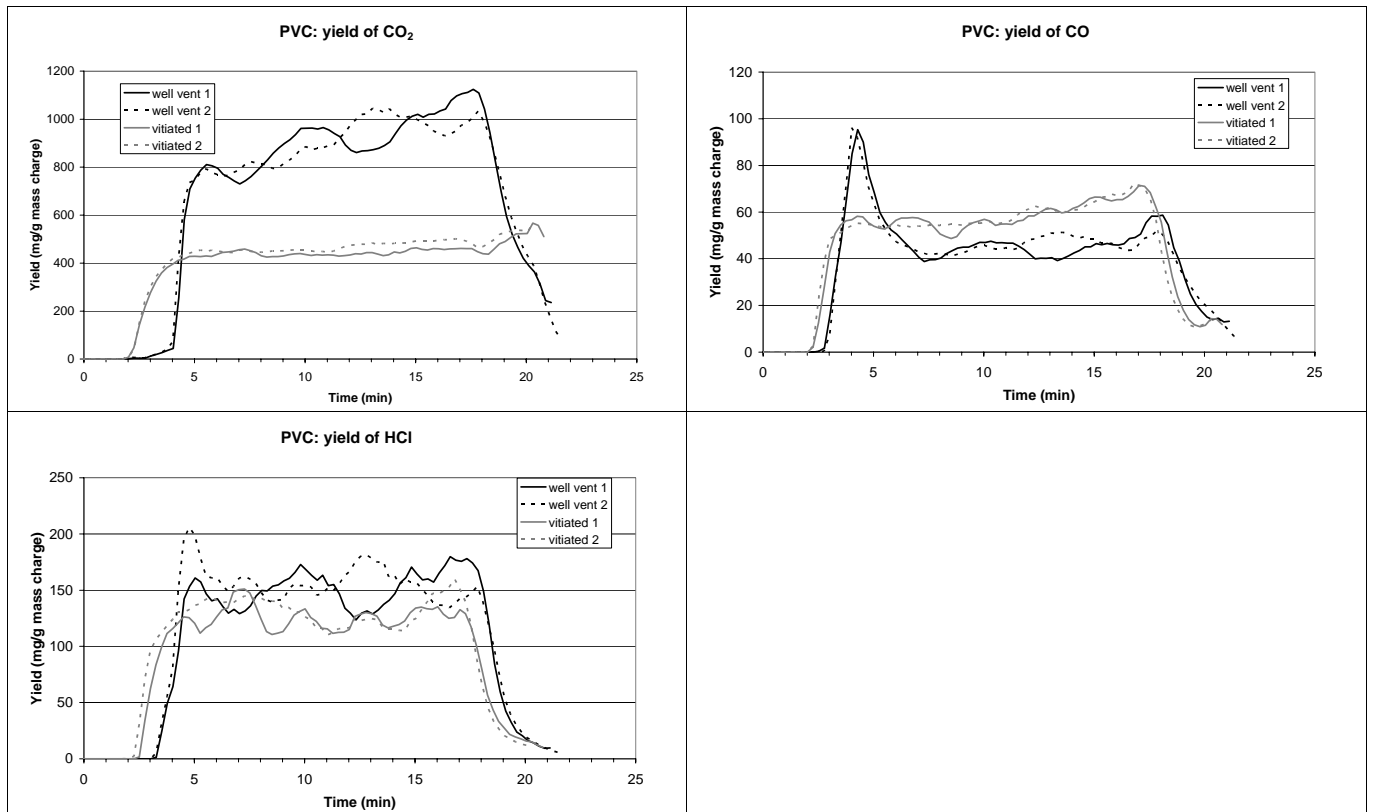


Figure 14 Results from PVC-pellet combustion in the Pursler furnace

3.1.1.5 Polyethylene-pellets

Another type of plastic pellets tested were polyethylene based and it can be seen that the results in Figure 15 are comparable to wood combustion (Figure 11).

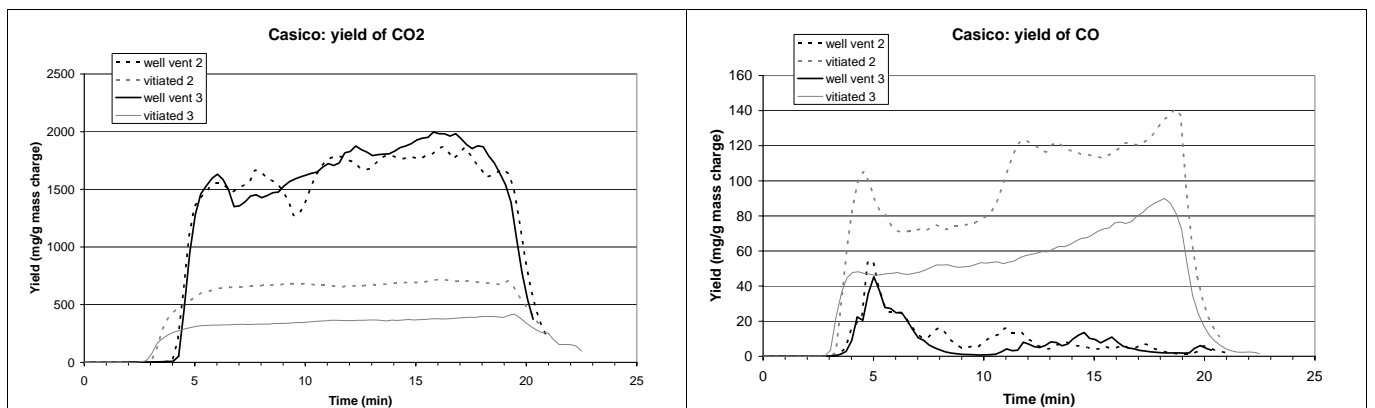


Figure 15 Results from polyethylene-pellet combustion in the Pursler furnace

3.1.1.6 Rigid PUR

The material tested were a flame retarded type which can be seen from the amount of HCl measured.

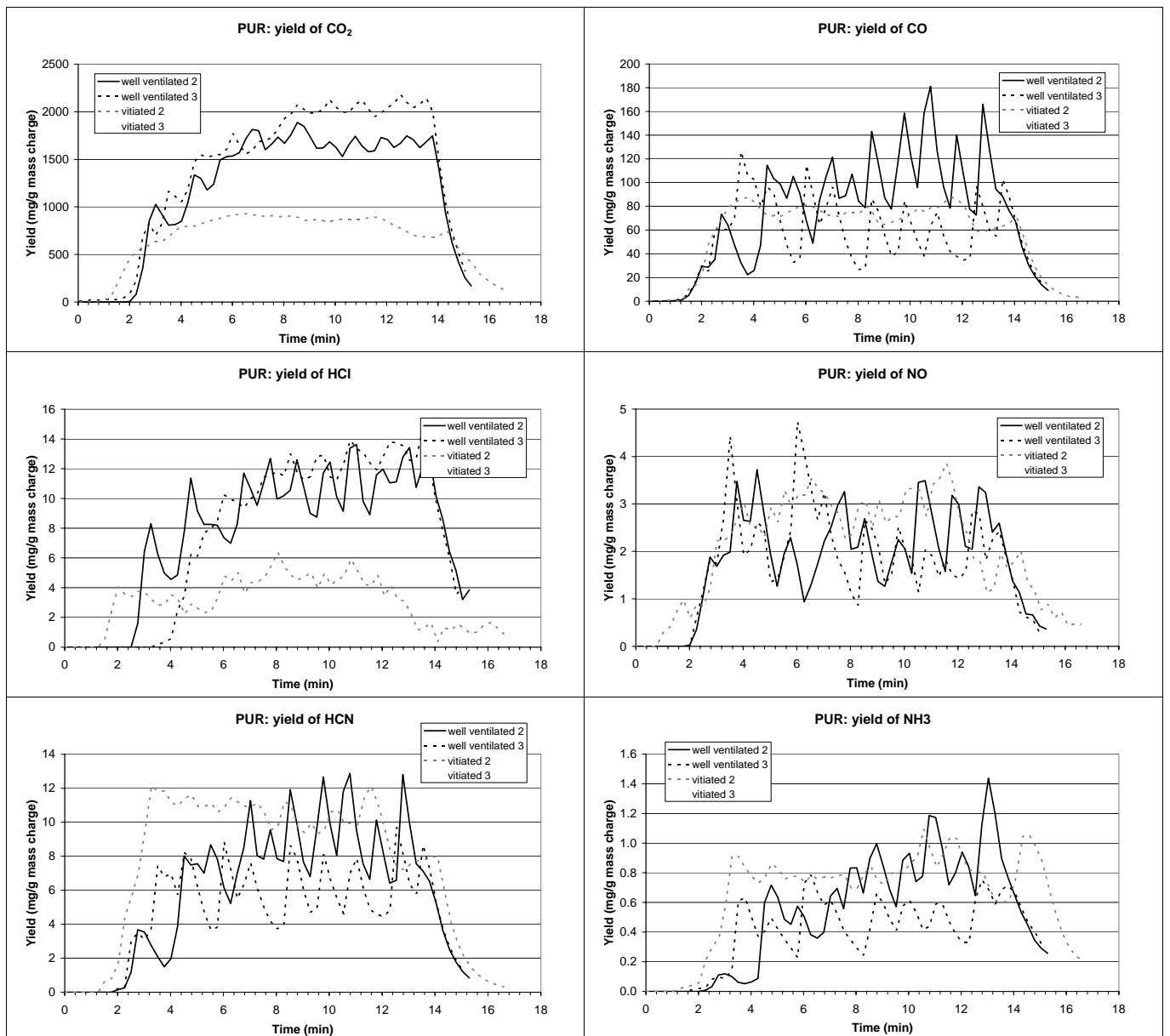


Figure 16 Results from rigid PUR combustion in the Purser furnace

3.1.1.7 Mattress

Mattress material from Växjö hospital of the same type that took part in the catastrophic fire incident were used in the full-scale reconstruction and also tested in the Purser furnace. The mattress consists mainly of PUR. The results in Figure 17 are also comparable to the findings in Figure 16 but it can be seen that the differences generally are smaller between vitiated and well-ventilated combustion in the rigid PUR-case compared to the mattress experiment, which is probably explained by the Cl-based flame retardant found in the rigid PUR.

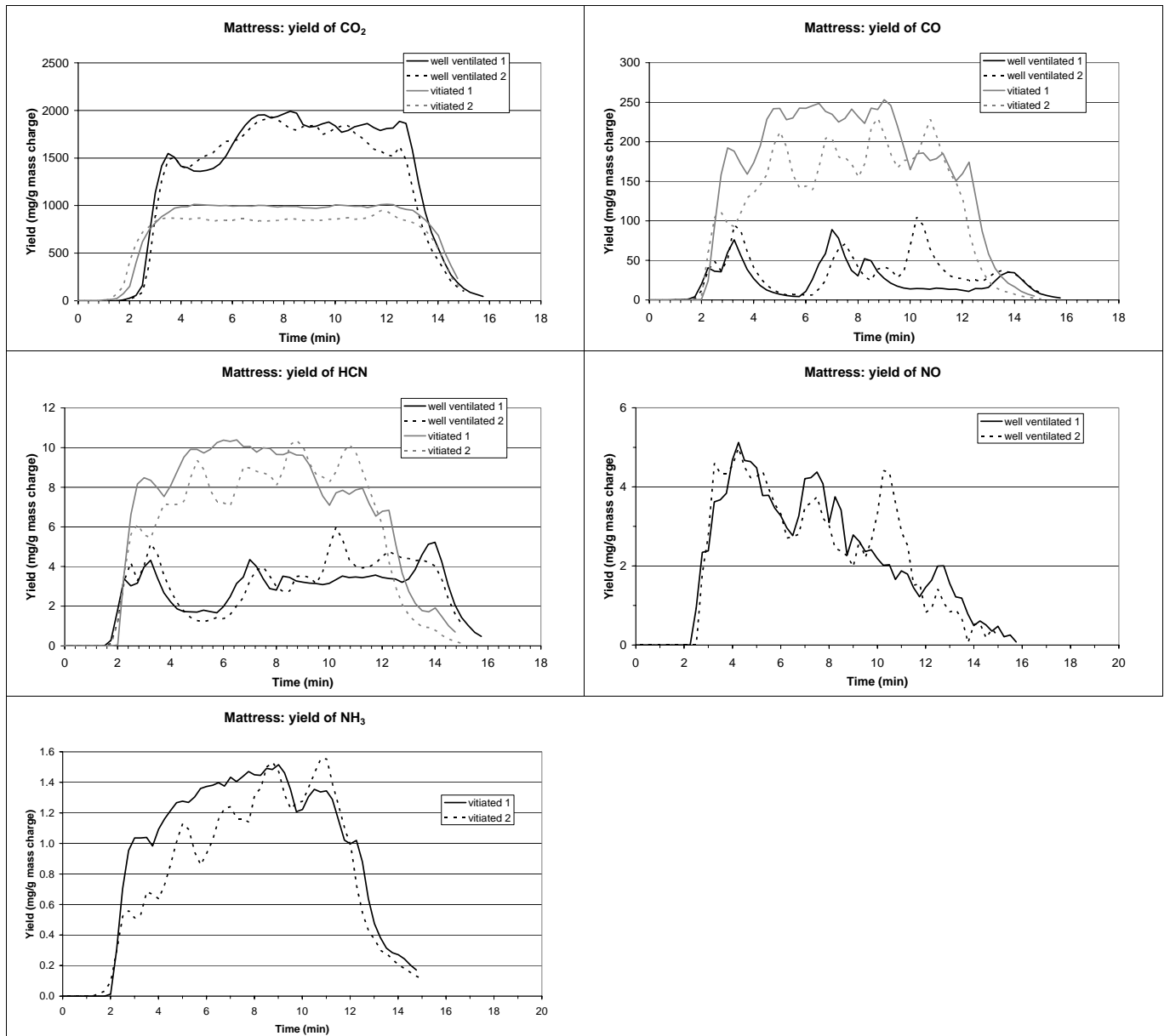


Figure 17 Results from mattress combustion in the Purser furnace

3.1.2 Particles

Particles in the smoke were measured as described previously in section 2.2.2.2. Only two materials were tested, the Våxjö hospital mattress and the PTFE-cable. The results are shown in Figure 18. It is interesting to note that the maximum in mass distribution in both cases increases for the under-ventilated experiment compared to the well-ventilated combustion. This is not illogical since the vitiated combustion will provide a denser smoke and, hence, greater possibilities for the creation of larger particle agglomerate.

The maximum values in mass distribution for the well-ventilated Purser furnace experiments are also approximately the same as those previously reported for well-ventilated combustion in the Cone calorimeter⁴.

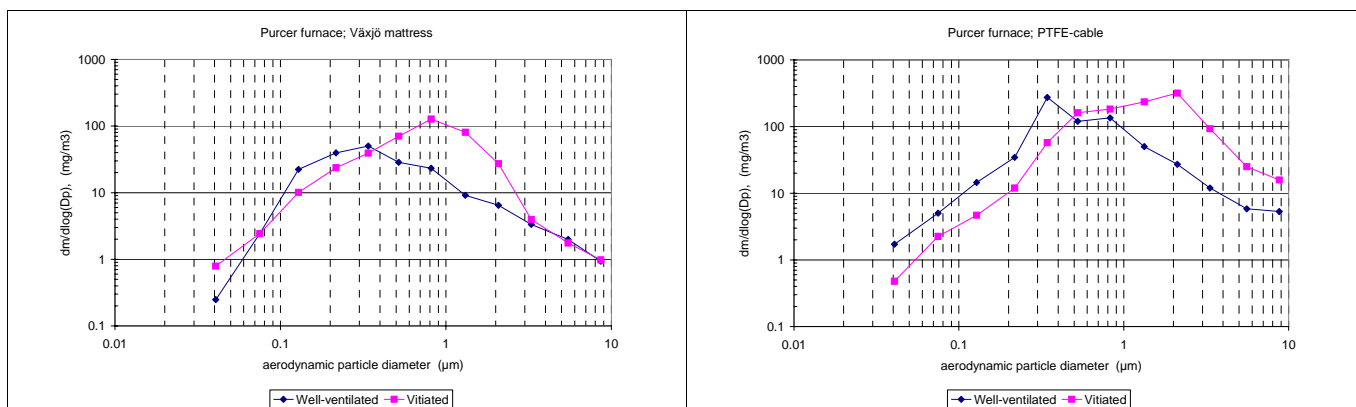


Figure 18 Particle mass size distributions from Purser furnace experiments.

3.1.3 Isocyanates

Analysis of isocyanates in the smoke gases was made in all tests except in the tests with PVC- and polyethylene pellets. Both the PUR and the mattress products are known to produce isocyanates when heated and this can also be seen in Figure 19. The index “v” in Figure 19 indicates “vitiated conditions” and it can be seen that there is small differences in mixing-box isocyanate levels between well-ventilated and vitiated combustion conditions.

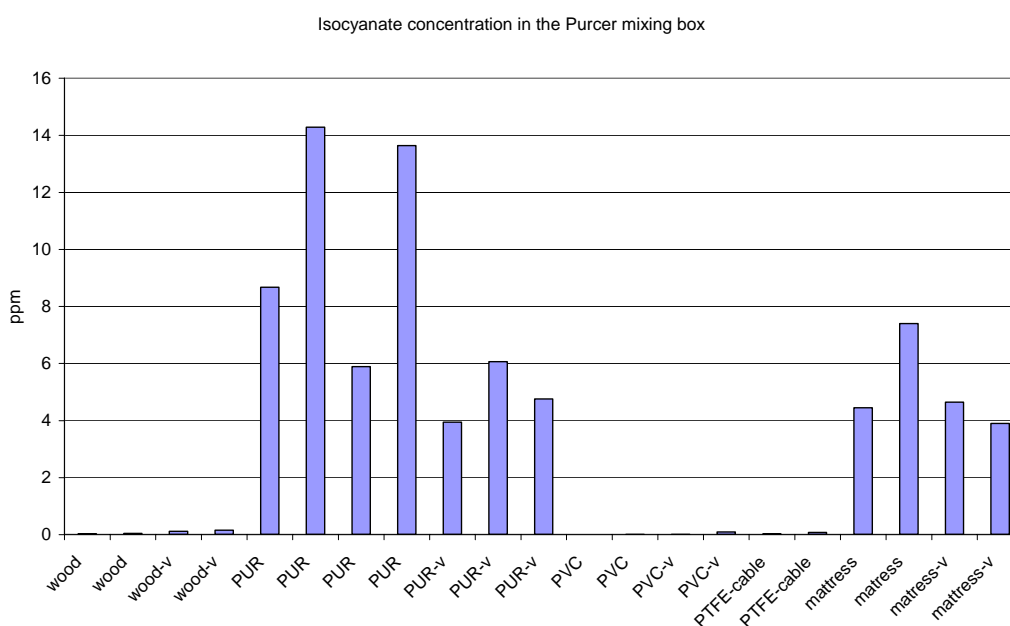


Figure 19 Total isocyanate concentration in the Purser furnace mixing box; “v” indicates vitiated combustion conditions

A tendency for isocyanate concentration decrease under vitiated conditions is however noted from the figure, which might be explained by the fact that other competing nitrogen reactions takes places during vitiated conditions, e.g. the HCN and NH_3 formation (see Figure 16 and Figure 17). It might, however, be difficult to compare directly due to variations in the test procedure (isocyanate sampling times, material feed-flow). A better comparison might be to look at the yield, based on the material feed into the furnace. Such comparison is shown in Figure 20 and it can be seen that the tendency for the PUR

product is the same as in Figure 19 but that the mattress isocyanate production rate is almost the same, whether well-ventilated or vitiated combustion conditions are applied.

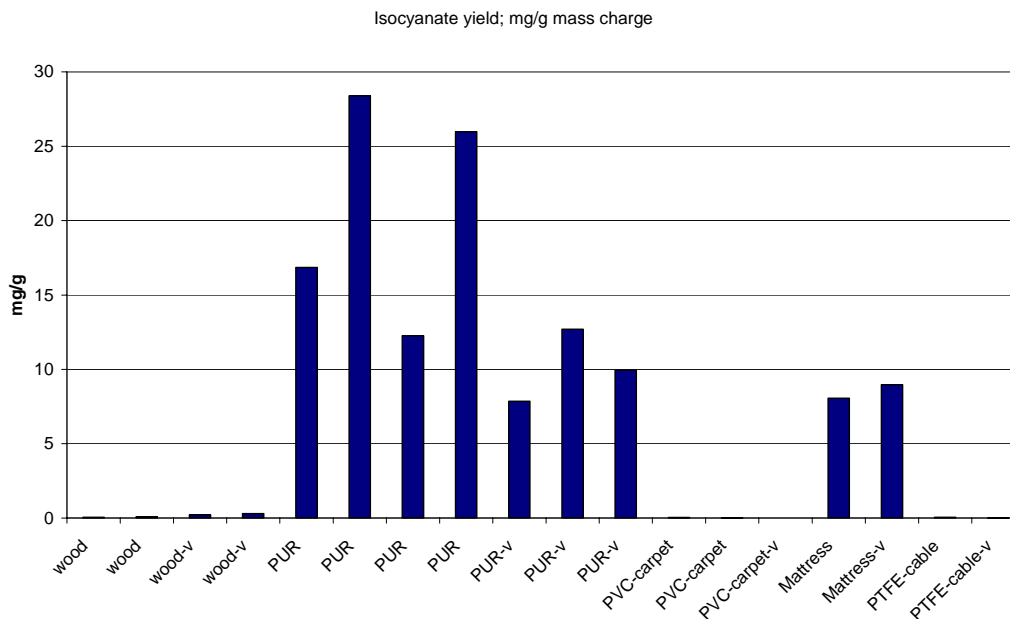


Figure 20 Isocyanate yield based on mean values of the total isocyanate production/minute of sampling divided by the sample feed/minute

3.1.4 Toxicity comparison

Comparing the toxicity between species having fundamentally different impact on humans is very difficult. Carbon monoxide, for a long time considered the sole explanation of smoke toxicity, and hydrogen cyanide are asphyxiates whereas hydrogen chloride and isocyanates are irritants. However, it is necessary to be able to use some kind of method for comparison if it shall be possible to compare fire hazards when using different kinds of materials.

One method for comparison is to use data from the American National Institute for Occupational Safety and Health, NIOSH, (www.cdc.gov/niosh). They define and lists concentration levels for different substances as being “Immediately Dangerous to Life and Health”, IDLH-values. The IDLH-values for the species found during the Purser furnace experiments are given in Table 1.

Table 1 IDLH-values (ppm)

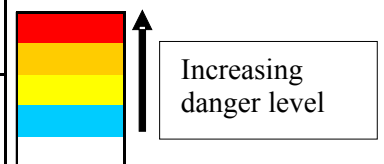
Substance	IDLH-value
Isocyanates	3
CO	1200
NO	100
HCN	50
HCl	50
NH ₃	300
HF	30

As can be seen from the table, there is a large variation in IDLH-values for the different species measured. The very low value for isocyanates should be noted. There are a large number of different isocyanates but only a few of them are listed in the NIOSH database, which is due to the fact that only a few have been thoroughly tested yet. However, the

acute toxicity of all isocyanates are usually considered to be comparable to the toxicity of toluene-diisocyanate, TDI, (IDLH=2.5 ppm) or methyl-isocyanate, MIC, (IDLH=3.0). If a comparison based on taking the quotient between the measured concentrations in the Purser furnace mixing box and the specie IDLH-value is made, the result given in Table 2 is obtained. Note that comparison only can be made between different species for an individual product. Comparison between different products is not possible in Table 2. The reason is that the figures presented in Table 2 are based on measured concentrations and that the input rate of material in some cases varied between materials.

**Table 2 Toxicity comparison based on mixing box concentrations and IDLH-values*
IDLH-quotient**

Substance	Isocyanates	CO	NO	HCN	HCl	NH3	HF
wood	0.01	0.62	0.00	0.00	0.00	0.00	0.00
wood	0.01	0.76	0.00	0.00	0.00	0.00	0.00
wood-v	0.04	2.44	0.65	0.00	0.00	0.00	0.00
wood-v	0.05	2.14	0.58	0.00	0.00	0.00	0.00
PUR	4.76	1.29	0.30	2.27	1.78	0.07	0.00
PUR	1.96	0.82	0.35	1.58	1.78	0.03	0.00
PUR	4.55	1.76	0.90	2.67	2.56	0.03	0.00
PUR-v	1.31	0.64	0.31	2.61	0.63	0.06	0.00
PUR-v	2.02	0.61	0.30	2.10	0.82	0.05	0.00
PUR-v	1.59	0.76	0.33	2.35	1.32	0.06	0.00
PVC	0.00	1.73	0.00	0.00	70.26	0.00	0.00
PVC	0.00	1.78	0.00	0.00	72.64	0.00	0.00
PVC-v	0.00	2.63	0.00	0.00	58.54	0.00	0.00
PVC-v	0.03	2.22	0.00	0.00	54.62	0.00	0.00
PTFE-cable	0.01	3.12	0.00	0.00	42.94	0.00	24.13
PTFE-cable	0.03	3.77	0.00	0.00	50.86	0.00	27.46
mattress	1.48	0.74	0.48	1.08	0.00	0.00	0.00
mattress	2.47	0.90	0.48	1.28	0.55	0.00	0.00
mattress-v	1.55	2.08	0.00	2.12	0.00	0.08	0.00
mattress-v	1.30	1.87	0.00	2.09	0.00	0.08	0.00
Polyethylene-pellets	0.00	1.19	0.00	0.00	0.00	0.00	0.00
Polyethylene-pellets	0.00	0.99	0.00	0.00	0.00	0.00	0.00
Polyethylene-pellets-	0.00	2.82	0.00	0.00	0.00	0.00	0.00
Polyethylene-pellets-	0.00	3.08	0.00	0.00	0.00	0.00	0.00
PVC-pellets	0.00	1.81	0.00	0.00	63.16	0.00	0.00
PVC-pellets	0.00	1.83	0.00	0.00	72.22	0.00	0.00
PVC-pellets-v	0.00	1.36	0.00	0.00	53.02	0.00	0.00
PVC-pellets-v	0.00	1.38	0.00	0.00	56.12	0.00	0.00



- Do not compare figures between different products.

It is interesting to note the difference in toxic content in the mixing box when changing from well-ventilated to vitiated combustion. The PUR and mattress experiments demonstrate a higher isocyanate than HCN-quotient during well-ventilated conditions but also a higher HCN than isocyanate quotient during vitiated combustion conditions. Also interesting to note is the very high HCl toxicity level obtained for the PVC-carpet and the PTFE-cable experiment as well as the high HF-level obtained for the PTFE-cable.

3.2 Full-scale experiments

The single mattress fire was mainly used for simulation comparison, using the flamelet model. This experiment did not develop a flash-over even though it was close; necessary HRR for a flashover in the Room-Corner enclosure is ~1 000 kW and the maximum

experimental value was somewhat more than 800 kW. The Växjö hospital fire reconstruction experiment did, however, reach well above the necessary effect for a flash-over. The HRR –curves obtained for the full-scale experiments are given in Figure 22 and Figure 23^{vii}.

In the reconstruction experiment, the fire developed quite slowly in the beginning but after some minutes, melting material from the mattress ignited the PVC-carpet and a kind of “local” flashover beneath the bed was attained, after which the fire developed quickly, involving all of the floor PVC-surface. The event is clearly seen in Figure 21.



Figure 21 Sequence of photos showing how the mattress and the PVC floor-carpet together provokes a “local” flashover that makes the fire spread over the entire floor, inducing at the same time a full flash-over situation with heavy smoke.

^{vii} The HRR-curve in Figure 22 shows the complete and undisturbed fire dynamics for a single mattress but the quick drop in maximum HRR seen in Figure 23 is due to water used for extinguishing the fire.

The PVC carpet material also provided a very dense smoke and a high smoke production rate, which gives an explanation for the smoke problem mentioned by rescue personal and smoke divers working to save patients in the Väjö hospital fire. Indeed, soot samples taken in the corridor and the patient room 40 m away from the fire where 2 victims where found were analysed with regards to its chloride content after the reconstruction was made and the analysis revealed that the soot contained 7-10 weight-% (!) of chlorides. This means that the smoke from the Väjö hospital fire contained a very high amount of HCl, which explains the dense fire smoke as chlorides have flame retardant qualities

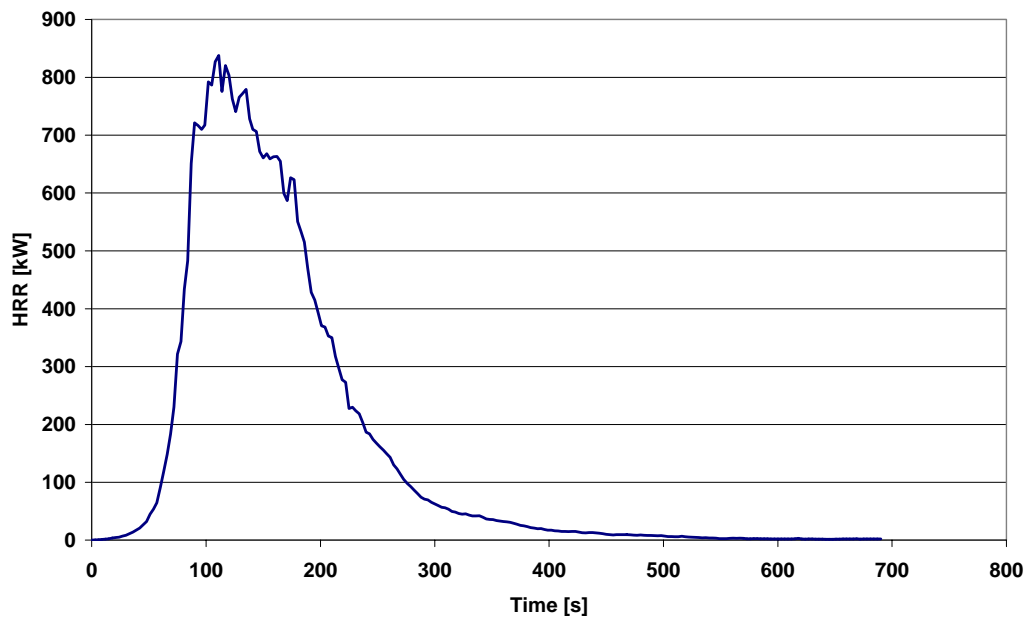


Figure 22 HRR-curve for the single mattress experiment

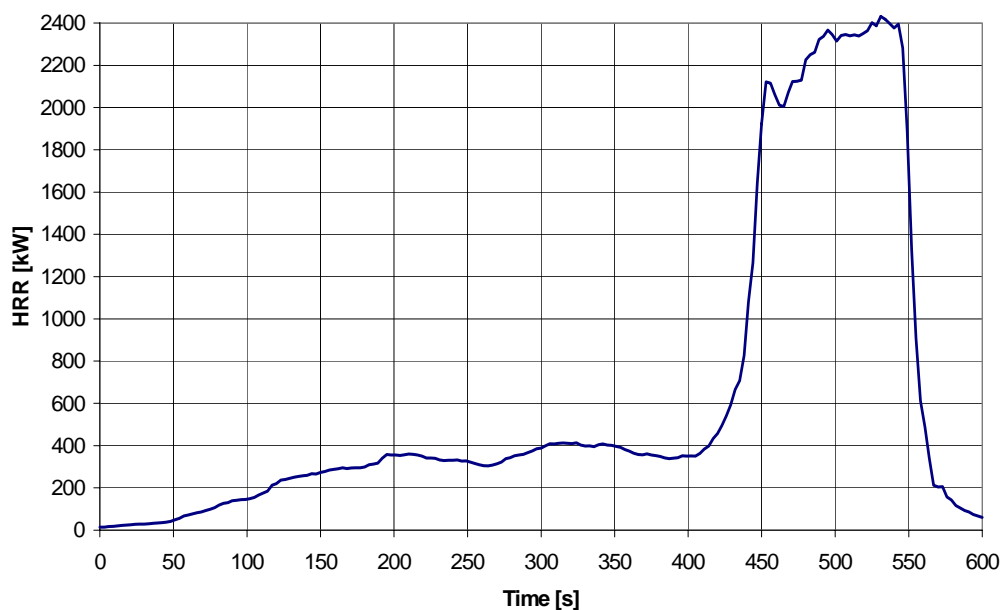


Figure 23 HRR-curve for the Väjö hospital fire reconstruction

The equivalence ratio for both experiments was measured using the ϕ -meter and the results of these measurements are shown in Figure 24 and Figure 25. The single mattress

fire did not provoke a flash-over situation and the equivalence ratio is during the entire experiment, firmly situated on a ϕ -value typical for a well-ventilated combustion.

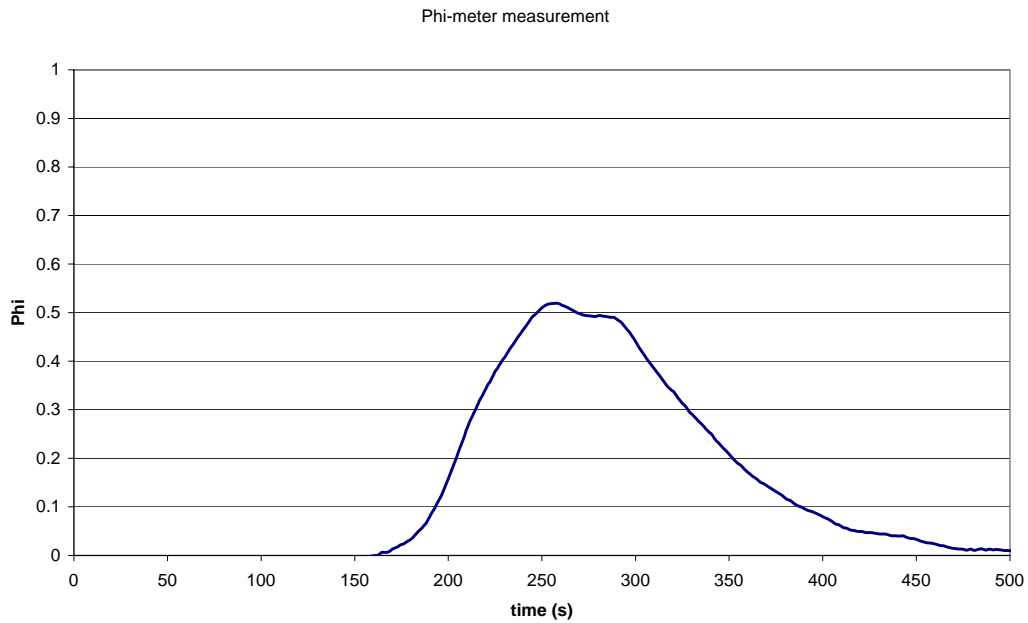


Figure 24 ϕ -meter measurements in the single mattress fire.

More surprisingly is the measured equivalence ratio for the reconstruction experiments since the ϕ -value does not pass the stoichiometric combustion figure (i.e. $\phi=1$) but in fact stays on the well-ventilated side. In this experiment, the flash-over should produce a much higher equivalence ratio. One explanation could be that the mixing in the door opening was such that fresh air from the outside was mixed with the smoke and therefore induced a higher oxygen concentration (i.e. a lower ϕ -value) than what was actually the typical combustion concentration in the room.

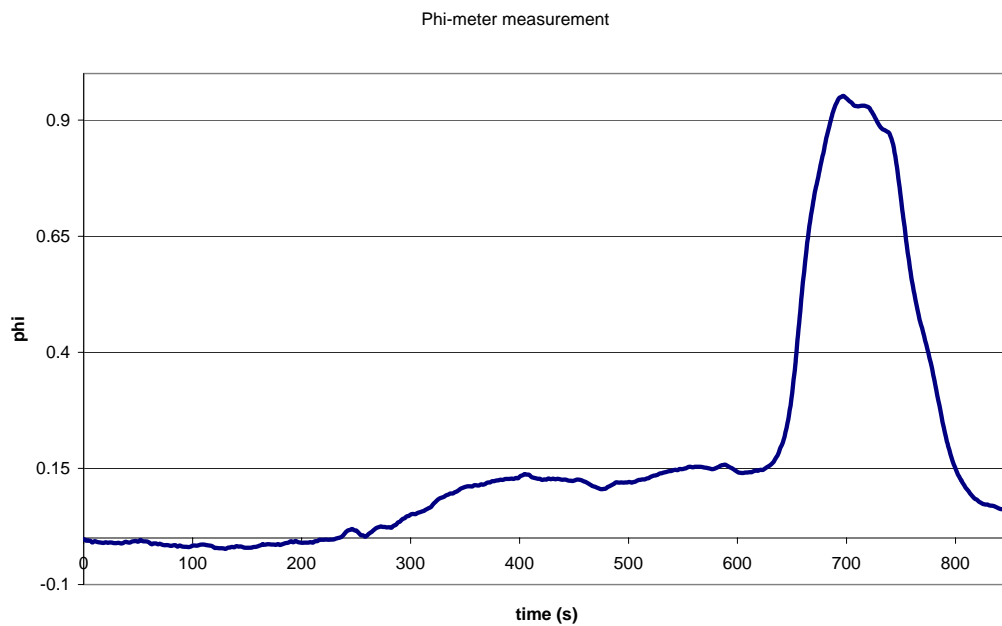


Figure 25 ϕ -meter measurements in the Växjö hospital fire reconstruction.

3.2.1 Inorganic species and isocyanates

3.2.1.1 Växjö fire reconstruction

Two patients died in the Växjö hospital fire and the medical explanation for this was intoxication by carbon monoxide. However, isocyanate metabolites (from toluene-diisocyanate) were also found in the lung tissues of both victims but it is not known in what way such substances might contribute to the survivability of fire victims. Findings from this project suggest that the impact of high concentrations of HCl on the fire victims also should have been more thoroughly investigated.

3.2.1.2 Toxicity comparison

In Figure 26 is given the concentrations of HCl and CO in the fire smoke from the Växjö fire reconstruction and it can be seen that they both are of the same magnitude. The literature provides different HCl-exposure limits as dangerous but using the NIOSH IDLH-values (see Table 1) it seems clear that Figure 26 points out HCl as being much more dangerous than CO.

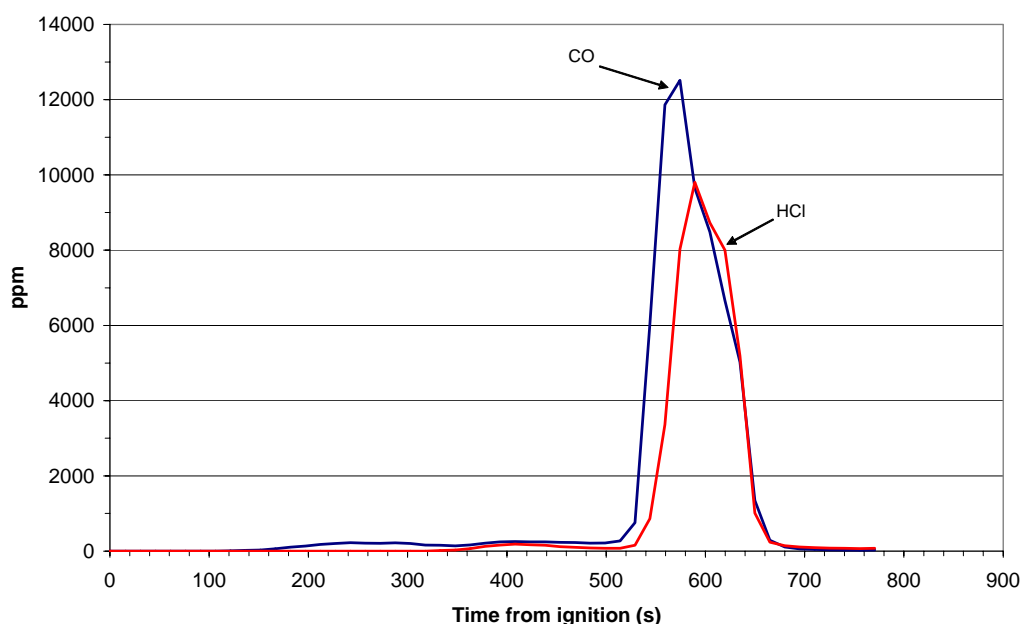


Figure 26 CO and HCl concentrations during the hospital fire reconstruction

The same IDLH-exercise performed for the couple HCN and isocyanates points at the isocyanates as being more dangerous than HCN see Figure 27. It is, however, also important to note that the isocyanates were measured over time intervals of 3+3+5 minutes, which means that the isocyanate concentrations given in Figure 27 are mean values over these periods of time. It seems highly probable that a true time resolved isocyanate measurement would have given a curve similar in shape as the inorganic species, i.e. that the maximum isocyanate concentration would have been much higher than shown in Figure 27.

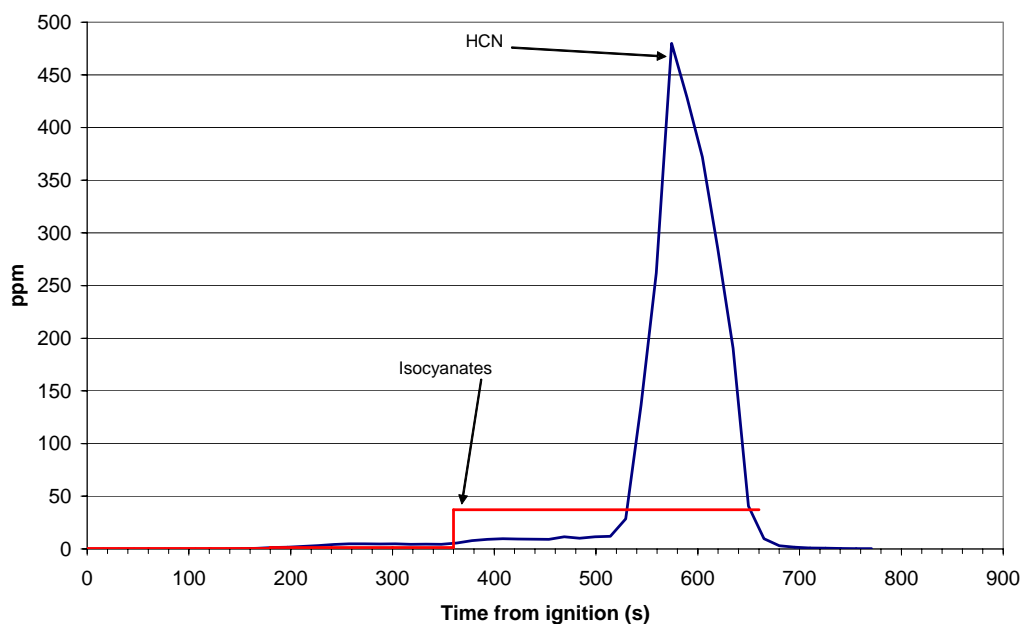


Figure 27 HCN and total isocyanate concentrations during the hospital fire reconstruction

If, for comparison of toxicity levels, the quotient between maximum substance concentration and IDLH-values (Table 1) for the different substances is taken (in the same way as in Table 2) the results given in Table 3 is obtained. Mean values taken over the last 5 minutes of the experiment are also given in order to be able to compare the inorganic specie concentration to the isocyanate measurement.

Table 3 Toxicity comparison based on smoke concentrations and IDLH-values

Substance	Max-value quotient	Mean value quotient
CO	10	2.6
HCl	196	44
HCN	9.6	2.2
Isocyanates	?	12.4

The results given in Table 3 shows that the most dangerous substance in the Växjö hospital fire reconstruction is HCl followed by isocyanates, with HCN and CO at approximately the same “level of toxicity”. It is remarkable that the two former substances are so much more dangerous (at least when we use the IDLH-values as a base for calculation) than the two latter as CO and HCN are the two species normally considered responsible for intoxication and death in relation to fires. A question one might ask is therefore if the medical investigation of fire victims too much focus on asphyxiates and not enough on irritants.

3.2.1.3 Mattress experiment

In the single mattress fire, no HCl was found in the smoke and the CO, HCN and isocyanate concentrations were significantly lower than in the reconstruction experiment. This was quite logical as the amount of combustible material was much lower and the experiment did not provoke a flash-over situation, i.e. the experiment was well-ventilated.

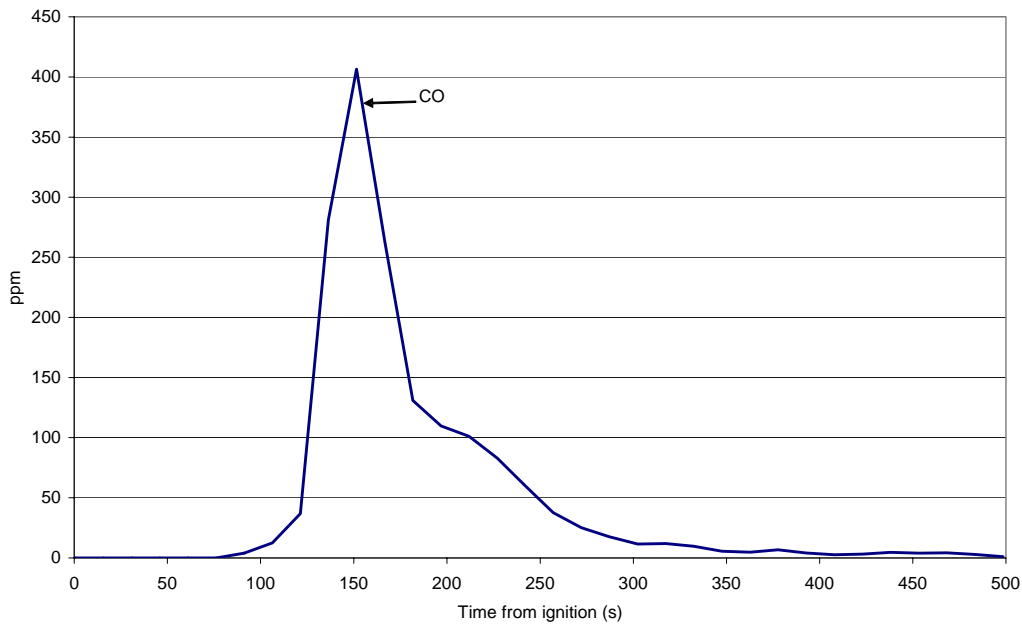


Figure 28 Concentration of CO in smoke from the single mattress fire.

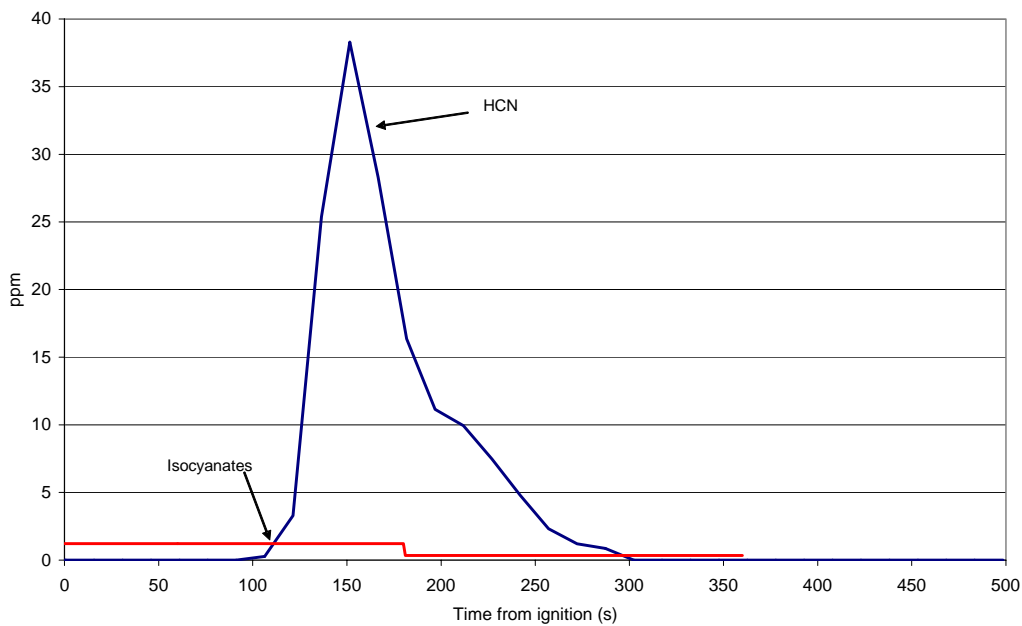


Figure 29 Concentration of HCN and isocyanates in smoke from the single mattress fire.

3.2.2 Particles

Particles were sampled in the full-scale experiments in the same way as in the small-scale experiments and the result of this investigation is seen in Figure 30. The reconstruction experiment gave as mentioned previously, a very high smoke density and some of the sampling plates in the measurement instrument (the Impactor) became overloaded, i.e. some of the plates obtained more particles than they could collect. This is shown in Figure 30 by using unfilled squares (the last 6 points). The mattress curve demonstrates a maximum around the same particle diameter, $0.3 \mu\text{m}$, as the small-scale experiments (see Figure 18).

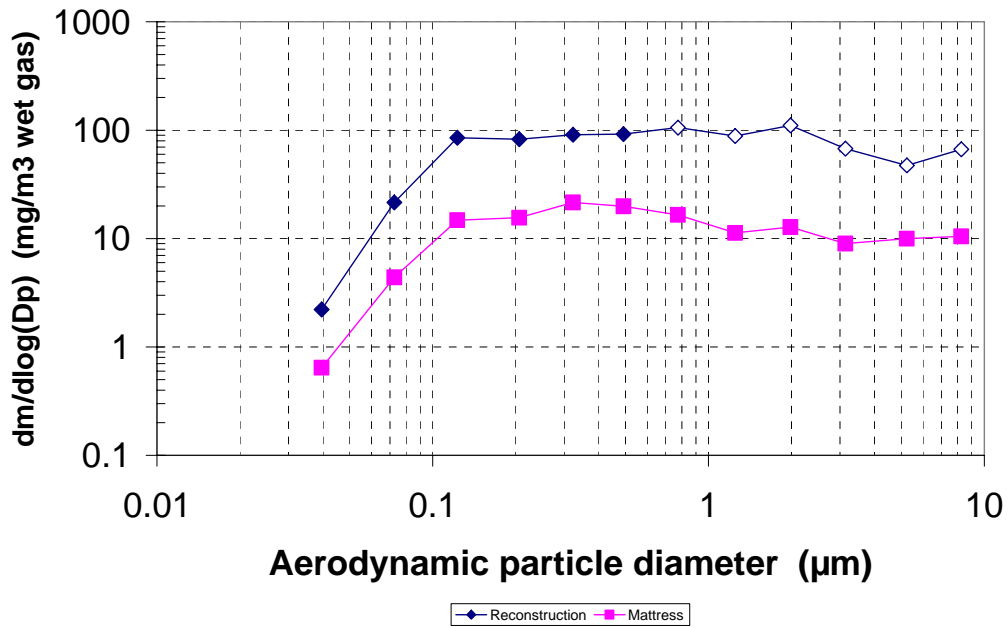


Figure 30 Mass size distributions for the 2 full-scale experiments

The particle concentration was also measured based on a light attenuation measurement, according to the ISO 9705 standard and the results can be seen in Figure 31 (reconstruction) and Figure 32 (mattress).

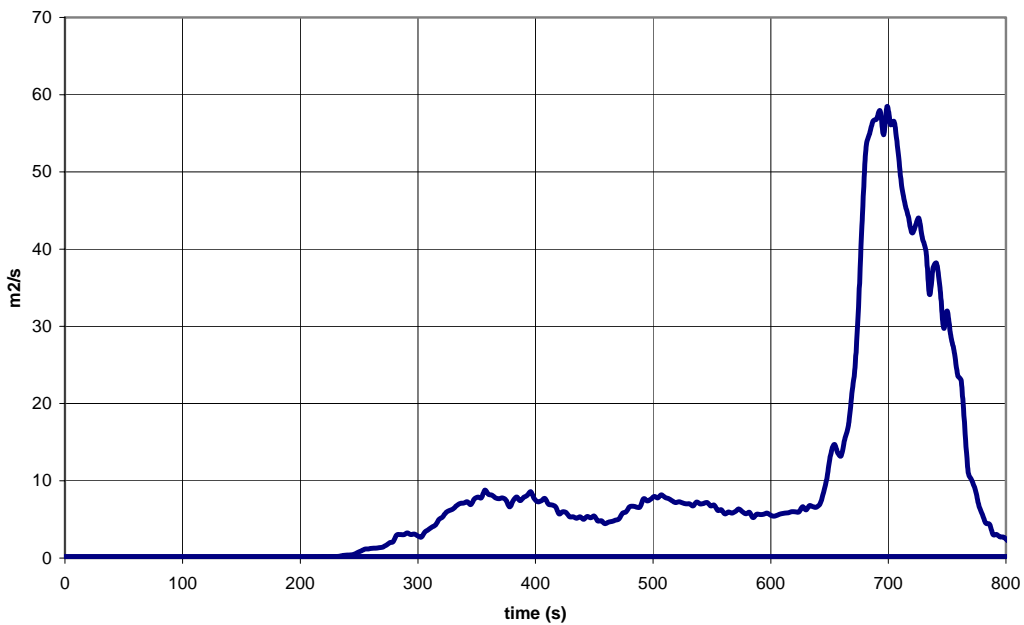


Figure 31 Smoke density in the exhaust duct of the Room-Corner scenario (Figure 3) during the Växjö hospital fire reconstruction.

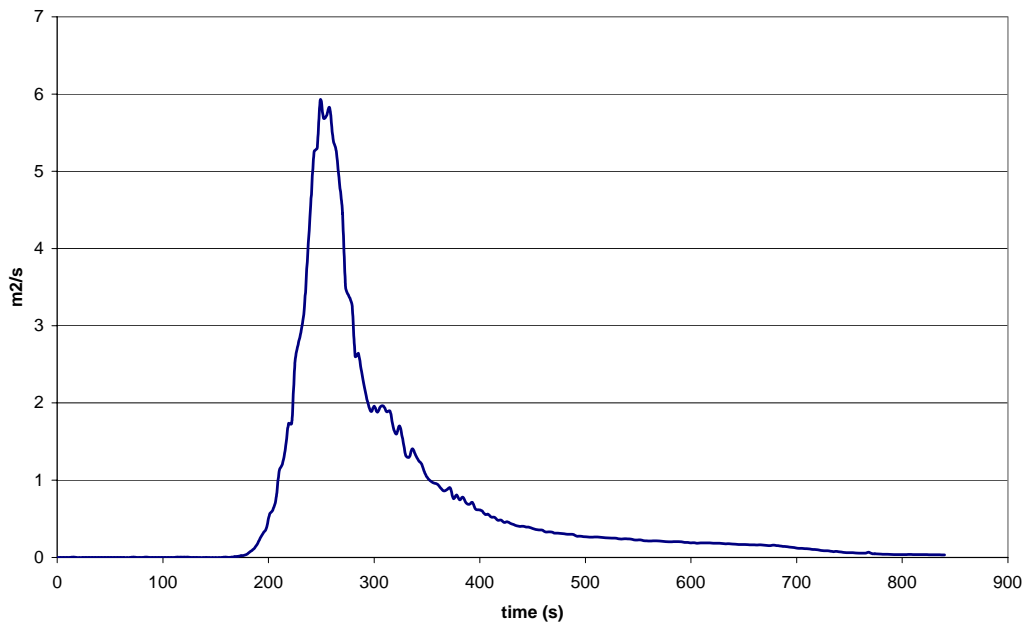


Figure 32 Smoke density in the exhaust duct of the Room-Corner scenario (Figure 3) during the single mattress fire.

3.3 Simulation

3.3.1 Single room scenario

The measurements of the toxic product were done in the door opening to the fire room. The CFD program calculates the product concentrations in the whole calculation domain. Calculated values are thus compared with the measured values at the door opening. Measurements were made over part of the door opening where the outflow of gases from the room was expected. To measure the representative value of concentrations the mean value in 6 points diagonally across the flow, according to Figure 8 was used. In the CFD simulations the mean value of these six points are represented in the comparisons.

The comparison of calculated concentrations of HCN using the flamelet model is shown in Figure 33. The maximum value of calculated HCN concentration is about 10 % lower than the measured maximum value. The curves have very similar shapes. The curve presenting the calculations, however, is not as wide as measured with respect to the time axis. The discrepancy in “wideness” can be attributed to uncertainty in the position and the thickness of the gas outflow region in the door opening. A similar comparison for CO is shown in Figure 34. Also in this case the curves are quite close and quite similar in shape; however the simulated concentration is somewhat higher than the measured one.

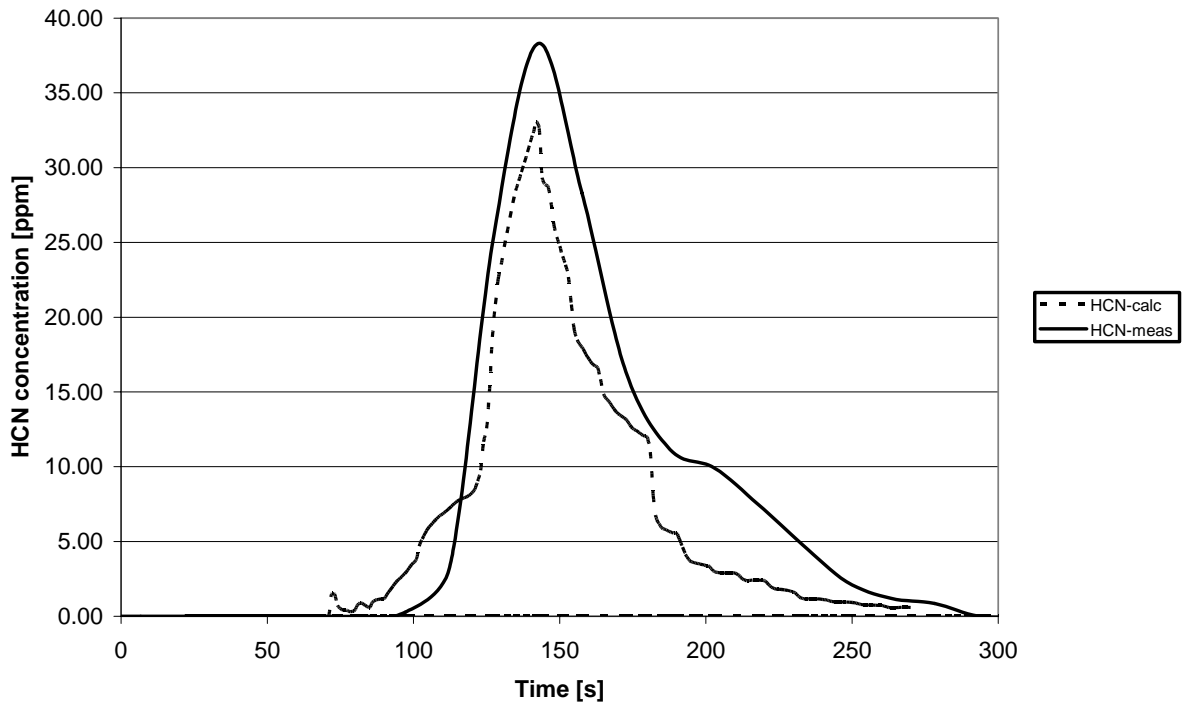


Figure 33 Comparison of the calculated HCN concentrations with measured results in the gas flow from the room. Solid line – measured, dotted line – calculated.

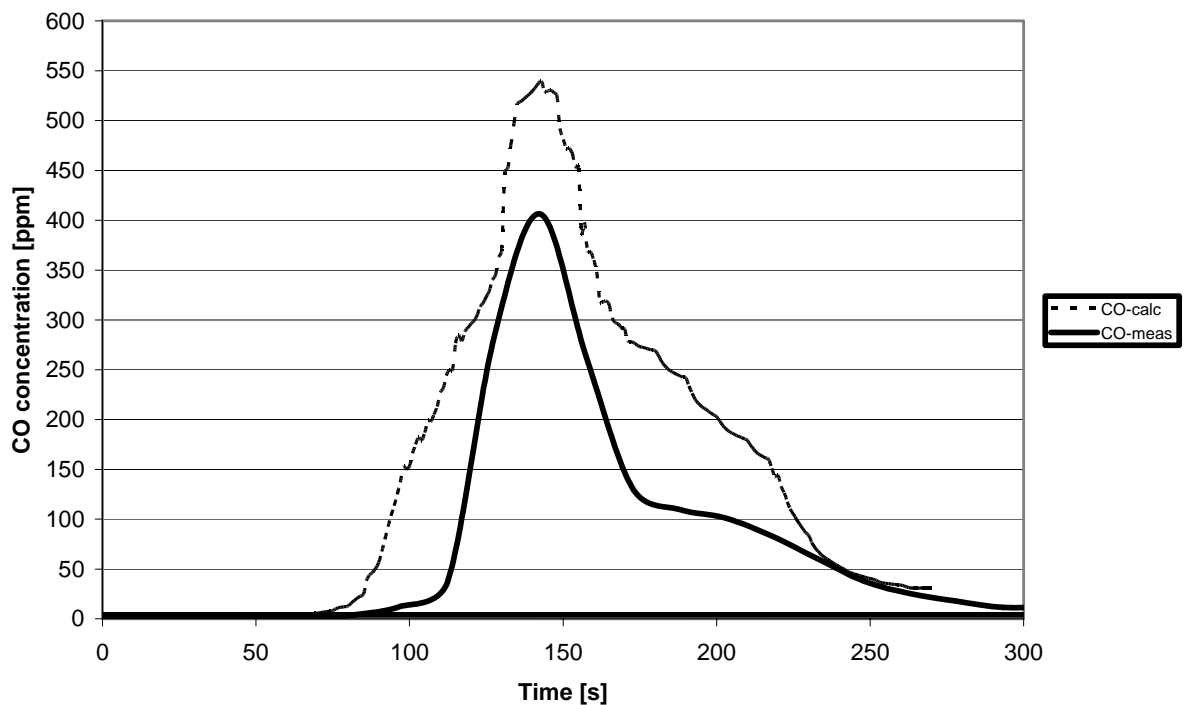


Figure 34 Comparison of the calculated CO concentrations with measured results in the gas flow from the room. Solid line – measured, dotted line – calculated.

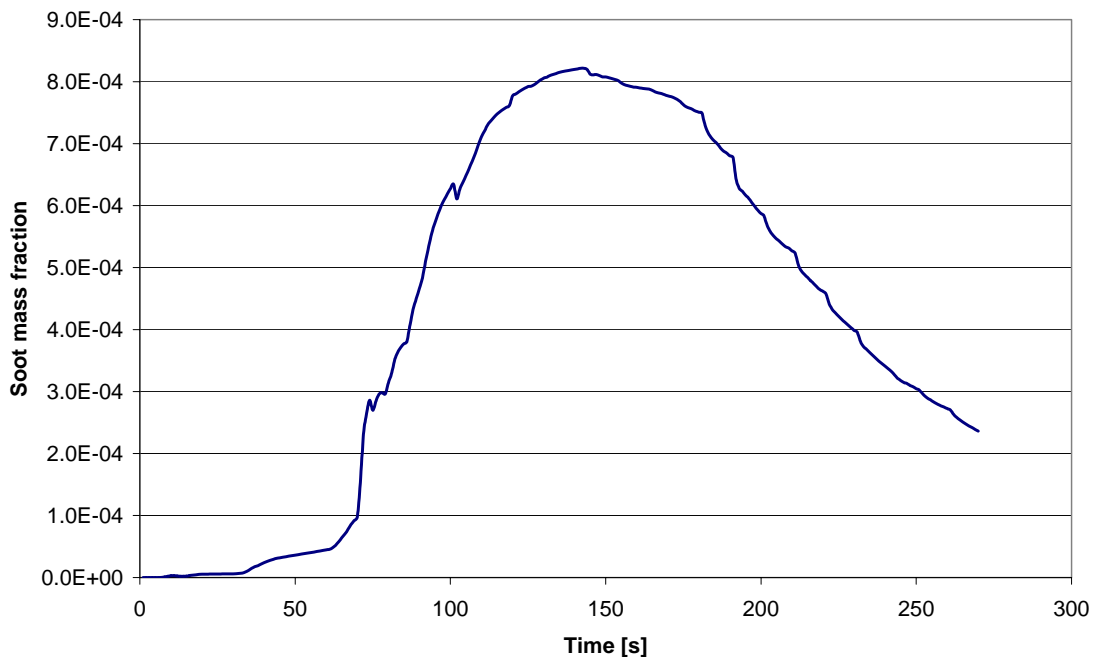


Figure 35 Calculated soot mass fraction in the gas flow from the room.

3.3.2 Ground floor scenario

3.3.2.1 The spreading of toxic products along the corridor

All the doors to open air were closed during the real fire incident, which made the situation worse. The ground floor was rapidly filled by toxic smoke from the fire. In the simulation, the door in the fire room was assumed open and all doors to other patient room were kept closed. Small leakage openings were simulated in those patient rooms where the dead or injured persons were found. The leakages were located in the door walls at floor level. In one patient room at the end of the corridor (room 137) soot in the ceiling around a ventilation opening indicated that this had been open during at least a part of the fire. This was modelled in the simulation as a “natural ventilation” (no fan).

A comparison between measured and simulated HCN-levels (passive scalar simulation) for the smoke in the door opening of the fire room is shown in Figure 36. The simulation input for HCN is based on small-scale Purser furnace experiments and it can be seen that the agreement between the two curves is quite good.

The results from the simulation, given as graphs of toxic gas concentrations, indicate that the most dangerous situation (part from the fire room itself) for the patients will develop at the longest distance from the fire. The hot smoke layer is cooled down when moving from the fire along the corridor. The gas gets heavier and mixes with fresh air below the layer. Figure 37-Figure 40 shows the concentrations of HCN, HCl, CO and O₂ respectively at the corridor centreline at heights 10, 100 and 170 cm, nine minutes after the ignition.

As seen in Figure 37, the maximum concentrations of HCN reach a value between 30 and 35 ppm at the closed end of the corridor, even near the floor. When toxic gas concentrations at lower levels increase, the danger for persons in the building increases. If the leakage of fire gases from the corridor to patient rooms occurs through the letter slit underneath the door, as it is assumed, the most dangerous conditions will first arise at the end of the corridor. Actually, one person was found dead and another severely intoxicated in the room situated at the longest possible distance from the fire, about 40 meters.

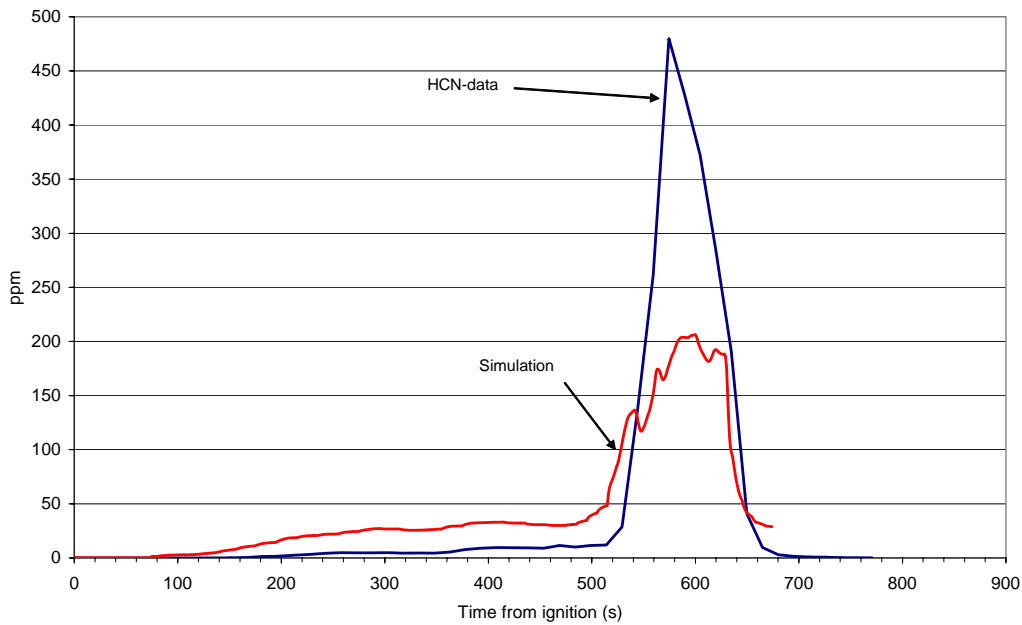


Figure 36 HCN concentrations in the smoke leaving through the door opening of the Room-corner scenario; measured and simulated values.

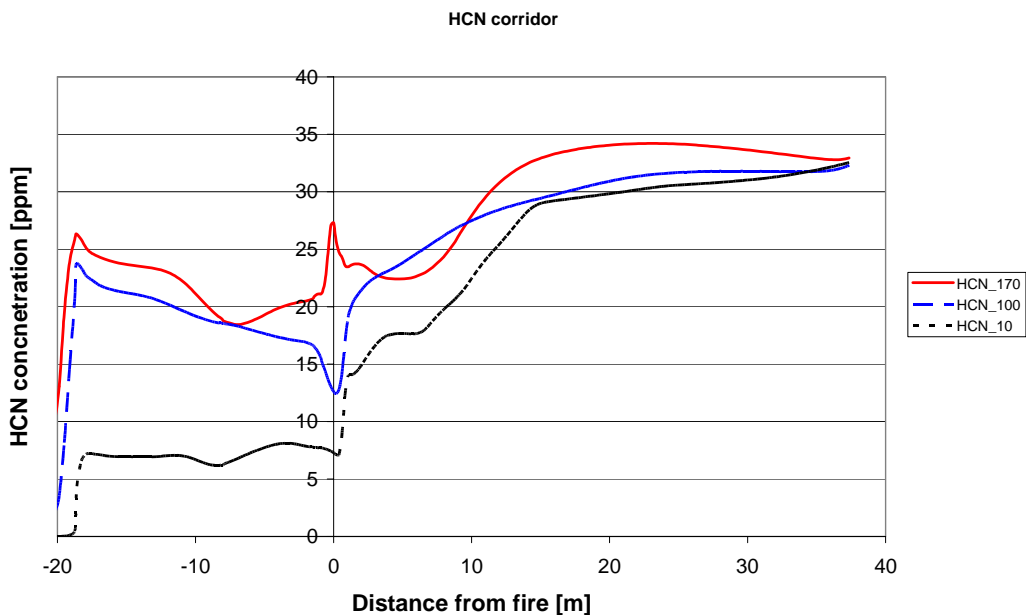


Figure 37 Calculated HCN concentrations in the corridor 9 minutes after ignition at heights 10, 100 and 170 cm.

At high temperatures, HCN might oxidise to H_2O , CO/CO_2 and NO_x if the oxygen content in the gases is sufficiently high. In this case, however, the fire became under-ventilated shortly after the PVC-carpeted were involved in the fire. Since the amount of oxygen that co-existed with HCN in the fire gases was low, the calculated concentrations of HCN outside of the fire room might very well be correct, i.e. HCN was not oxidised.

The calculated HCl-concentration reach very high levels in the corridor, about 2000 ppm, as shown in Figure 38. At the end of the corridor even at floor level values of ~ 2000 ppm were found. The simulated HCl came in this case was from a PVC carpet, while the HCN source was a polyurethane-based mattress.

Also the calculated levels of carbon monoxide are very high, about 3.5 % by volume (35 000 ppm) at the end of the corridor at floor level. This is also a high value compared to the IDLH value which for CO is 1200 ppm. At a level of 170 cm the simulated maximum value of CO is close to 4 % by volume, see Figure 39.

Oxygen concentration is shown in Figure 40. At the end of the corridor the simulated O_2 concentration is ~15 %. In addition to toxic product the shortage of oxygen decreases the human survival. People get easier disoriented and also loose consciousness due to toxic gases faster if the oxygen concentration is lowered (20.9-14.4% - only slight loss of exercise tolerance).

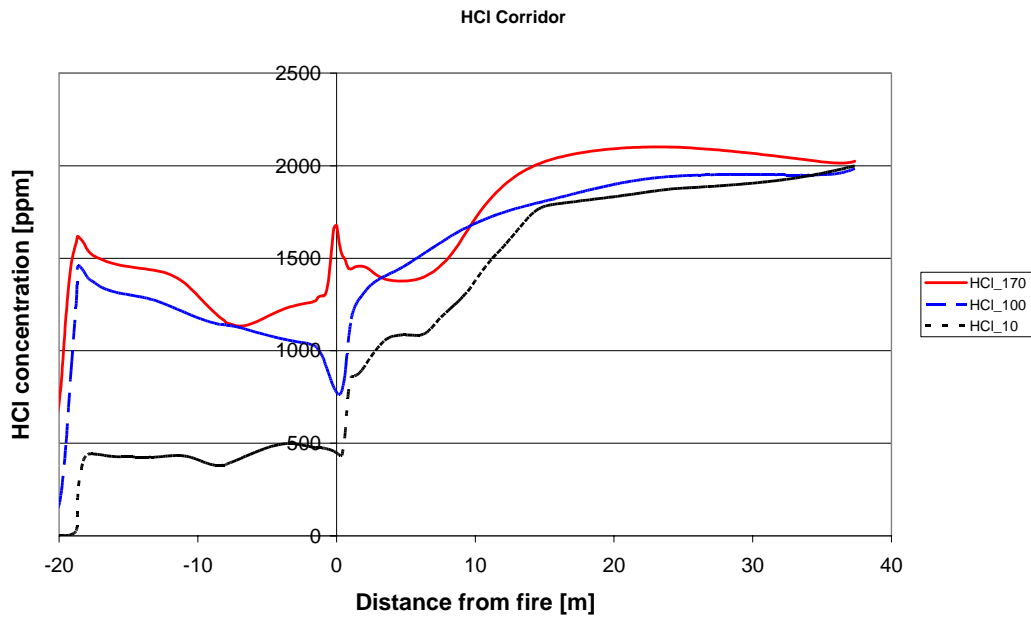


Figure 38 Calculated HCl concentrations in the corridor 9 minutes after ignition at heights 10, 100 and 170 cm.

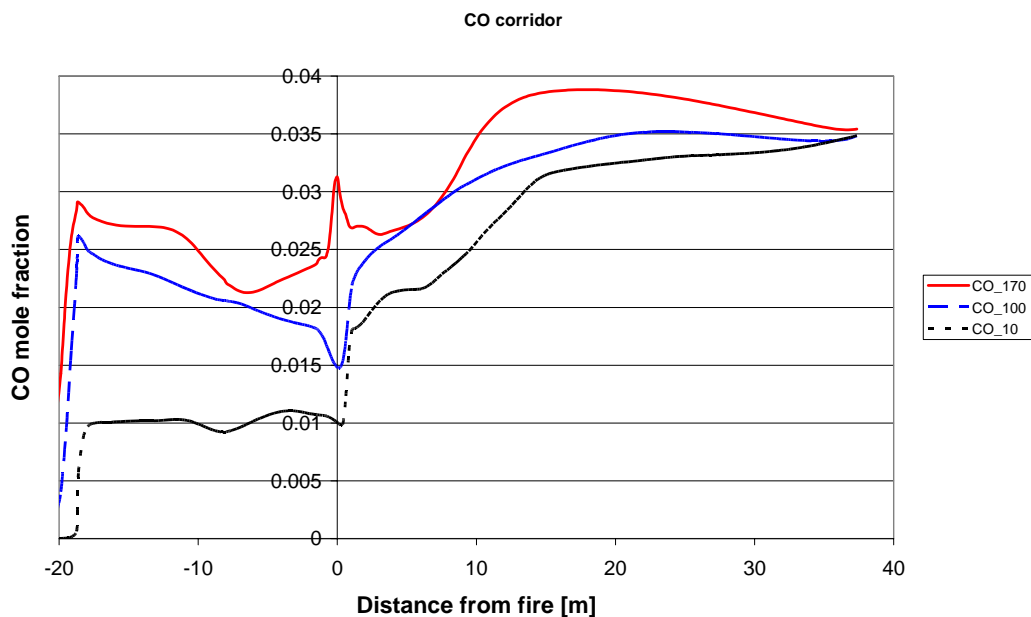


Figure 39 Calculated CO concentrations in the corridor 9 minutes after ignition at heights 10, 100 and 170 cm.

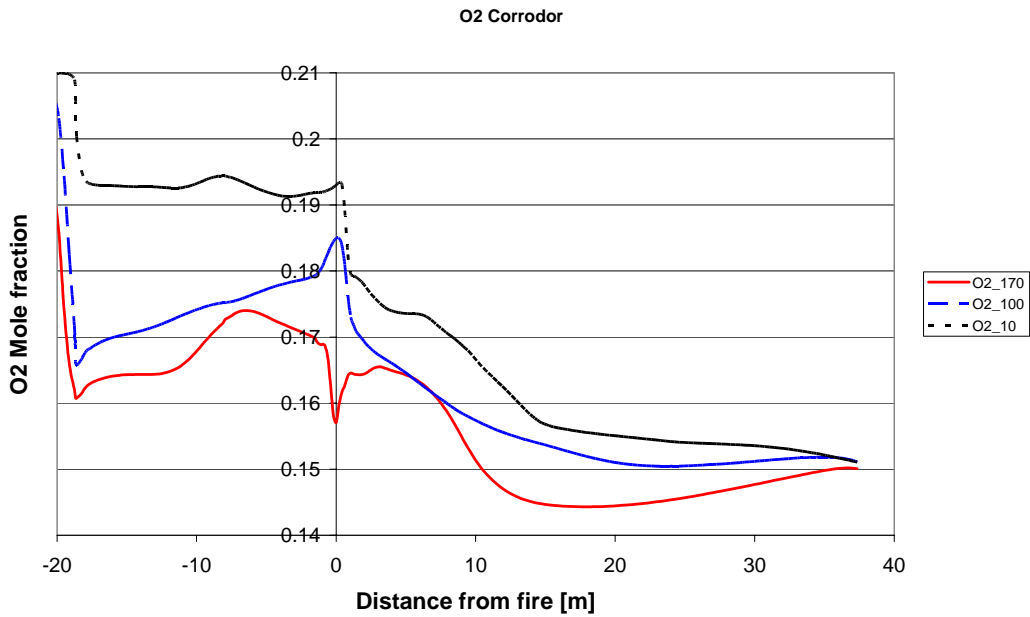


Figure 40 Calculated O₂ concentrations in the corridor 9 minutes after ignition at heights 10, 100 and 170 cm.

The polyurethane mattress and the PVC carpet in this fire were large sources of soot. The soot (smoke) in the fire gases reduces the visibility, and hence is one of the most decisive factors in evacuation. Figure 41 shows the simulated soot mass fraction in the corridor. In the real case there were quite much traces of soot in the corridor and also at the floor and lower parts of the walls in the patient room at the end of the corridor.

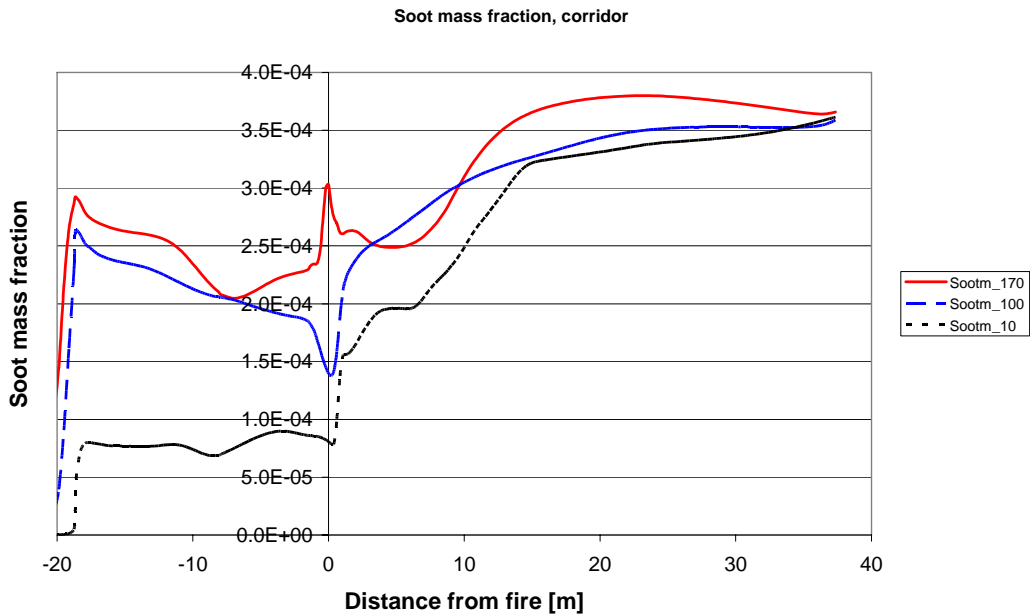


Figure 41 Calculated soot mass fractions in the corridor 9 minutes after ignition at heights 10, 100 and 170 cm

Figure 42 shows simulated temperature profiles in the corridor. The fire gases at a height of 170 cm are just over 300 °C at the centre of the corridor. The temperature at that height decreases almost linearly to 125 °C when moving towards the end of the corridor. At the floor level, the temperature is constant in the whole length of the corridor, about 100 °C.

The fact that the temperature sinks in the gas layer is the reason why there are most toxic products at lower levels at the end of the corridor. The smoke layer is getting colder, i.e. heavier, and thereby goes down at the end of the corridor.

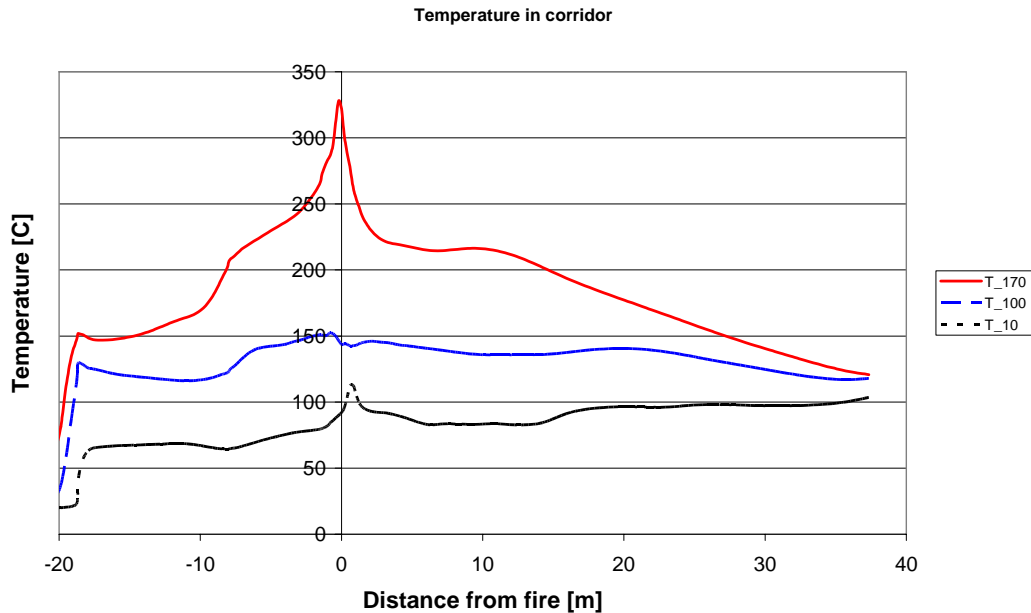


Figure 42 Calculated temperatures in the corridor 9 minutes after ignition at heights 10, 100 and 170 cm.

3.3.2.2 Toxic products in patient room located 40 m from the fire

One patient was found dead and another severely injured by fire gases in the patient room number 137, which was located about 40 m away from the fire. As discussed in the previous section the simulations have shown that the longer the distance was from the fire, the more dangerous was the situation for patients still in their rooms, since fire gases then went down to floor level. The concentrations of HCN, HCl, CO and O₂ as a function of time in patient room 137 are shown in Figure 43-Figure 46. Figure 47 shows the soot mass fraction in the room and Figure 48 the simulated temperature.

According to the simulations, toxic smoke starts to flow into the room about 7.5 minutes after the fire starts. It occurs shortly after the fire effect start to increase rapidly. Due to the rapid pressure increase and that the smoke layer has sunk down to floor level, the inflow of smoke into the patient room also increases rapidly. One minute later, the simulated levels of toxic gases concentrations have raised to ~90 % of their maximum levels, which occurs after one more minute, i.e. a little more than 9 minutes after the start of the fire.

The maximum values of HCl are just below 500 ppm at height 1.7 m a half metre from the back wall (i.e. the opposite wall to the door wall) in the room. CO concentration reaches 8500 ppm at the same location. The maximum level of HCN is about 8 ppm at that point. Also at lower height, 1.0 m above the floor, the maximum concentration values are high; about 90 % of those simulated at 1.7 m. However, in the middle of the room at a height 1.0, the maximum values of all toxic substances are somewhat lower, about 70 % of the maximum values at height 1.7 m. The reason to this locally lower value is probably that the roof vent in the simulations was located at that point which changed the flow pattern. Also the soot concentration follows the same pattern as toxic substances, see Figure 47.

The oxygen concentration is reduced to a minimum value of 19.6 % from the atmospheric value 21 %. As expected, the minimum of oxygen concentrations in the room occurs at the same points and time as the toxic substances reach their maximum concentrations.

The temperature in the room increases only to 35 °C at height 1.7 m. At height 1.0 m the maximum temperature is a couple of degrees lower, see Figure 48.

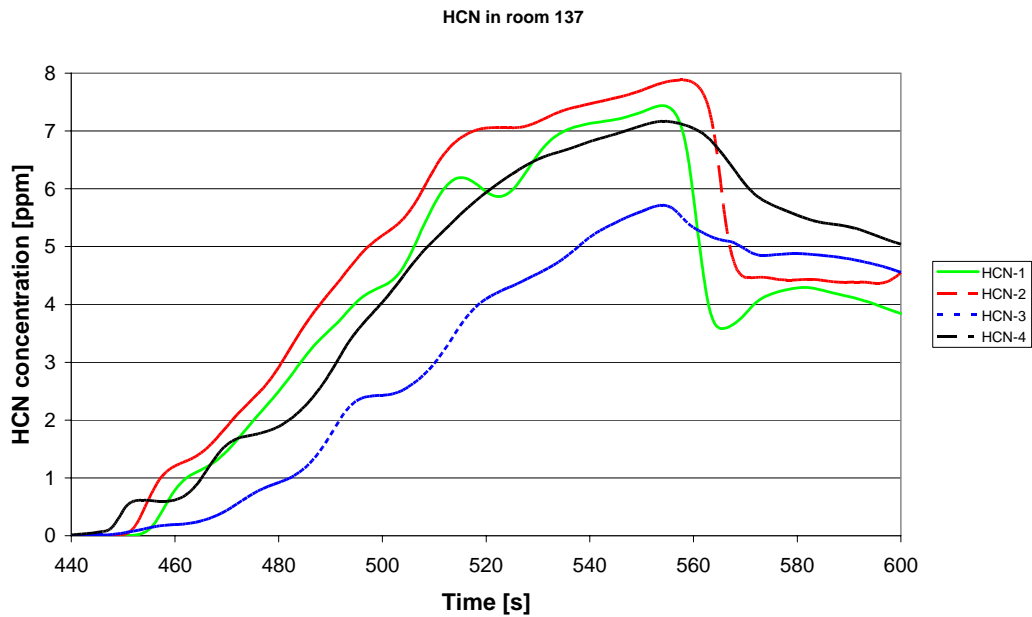


Figure 43 Calculated hydrogen cyanide concentration in the patient room 137 located 40 m from the fire. The numbers in legend denote the location; 1) 0.5 m from back wall in the room at height 1.0 m, 2) 0.5 m from back wall at height 1.7 m, 3) at middle of the room at height 1.0 m and 4) at middle of the room at height 1.7 m.

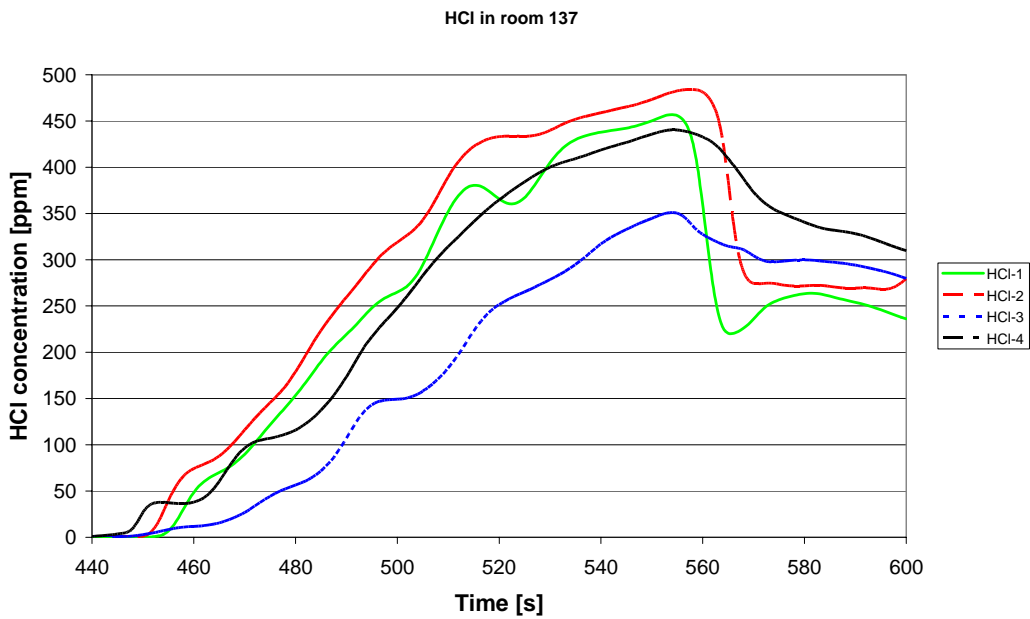


Figure 44 Calculated HCl concentrations in the patient room 137 located 40 m from the fire. The numbers in legend denote the location; 1) 0.5 m from back wall in the room at height 1.0 m, 2) 0.5 m from back wall at height 1.7 m, 3) at middle of the room at height 1.0 m and 4) at middle of the room at height 1.7 m

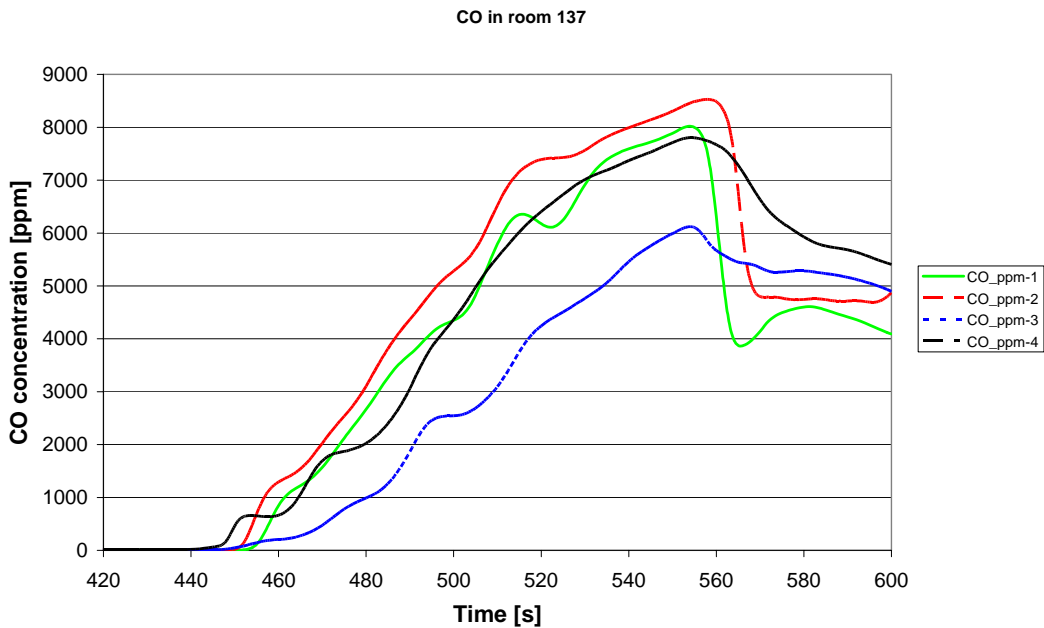


Figure 45 Calculated carbon monoxide concentration in the patient room 137 located 40 m from the fire. The numbers in legend denote the location; 1) 0.5 m from back wall in the room at height 1.0 m, 2) 0.5 m from back wall at height 1.7 m, 3) at middle of the room at height 1.0 m and 4) at middle of the room at height 1.7 m

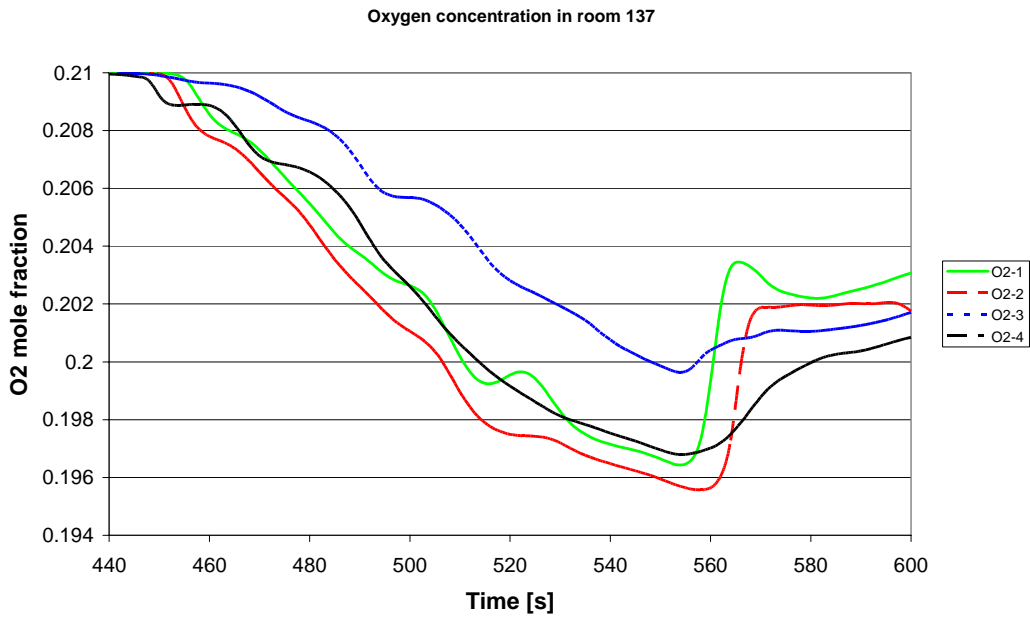


Figure 46 Calculated oxygen concentration in the patient room 137 located 40 m from the fire. The numbers in legend denote the location; 1) 0.5 m from back wall in the room at height 1.0 m, 2) 0.5 m from back wall at height 1.7 m, 3) at middle of the room at height 1.0 m and 4) at middle of the room at height 1.7 m.

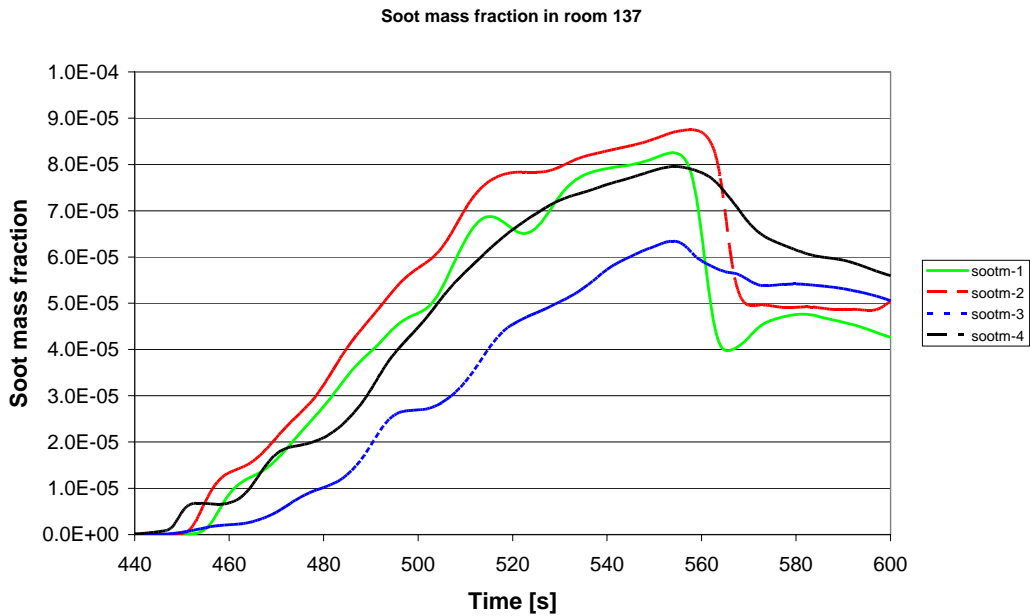


Figure 47 Calculated soot mass fraction in the patient room 137 located 40 m from the fire. The numbers in legend denote the location; 1) 0.5 m from back wall in the room at height 1.0 m, 2) 0.5 m from back wall at height 1.7 m, 3) at middle of the room at height 1.0 m and 4) at middle of the room at height 1.7 m.

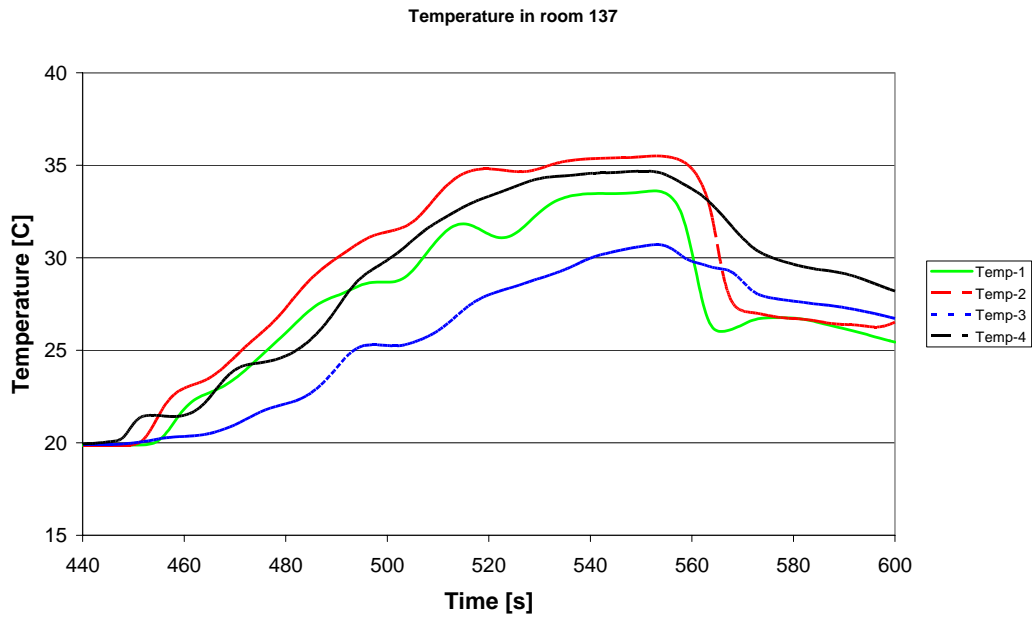


Figure 48 Calculated temperatures in the patient room 137 located 40 m from the fire. The numbers in legend denote the location; 1) 0.5 m from back wall in the room at height 1.0 m, 2) 0.5 m from back wall at height 1.7 m, 3) at middle of the room at height 1.0 m and 4) at middle of the room at height 1.7 m.

4 Conclusions-discussions

4.1 Small-scale experiments

Small-scale experiments in the Purser furnace was performed in accordance with ISO/CD 197005. A basic idea for this equipment is that a continuous, steady in-flow of combustible material and air to the reaction zone will generate a steady-state combustion, which permits investigating smoke content under well-defined oxidation conditions. The equipment is also well fit for making adjustments of the fuel/oxygen ratio in such a way that well-ventilated or under-ventilated (vitiated) combustion conditions are provided. This project has shown that steady-state conditions are attained reasonable well and that the test method is a good candidate for a small-scale toxicity test of smoke from burning materials.

Some weaknesses of the proposed test method have also been found. One of the basic premises of the test method defined by ISO/CD 19700 is that flaming combustion is taking place at well-ventilated or under-ventilated conditions. However, some materials such as the PTFE-cable investigated in this project do not burn but they do produce large amounts of toxic substances due to pyrolysis. The test method document suggests conditions also for pyrolysis but only at a significantly lower temperature than is used for the well-ventilated or vitiated combustion scenario. It is important that a test method for toxicity is able to show in what way products such as the PTFE-cable contribute to the overall toxicity when the material is exposed to fires.

Another material that was difficult to test was mineral wool (the results from these tests are, however, not included in this report). Such materials contain small amounts of combustible material in the form of a binder, but not enough to sustain a flaming combustion. However, this binder will produce relatively high amounts of isocyanates when heated³, which most likely will contribute to the overall toxicity in the fire smoke. Such materials too need to be testable.

Yet another obstacle might be that a tested material burns too well, i.e. that the flame-spread is faster than the fuel feed suggested by the method, which means that the burning surface increases and that a steady-state condition never is reached.

In spite of the difficulties mentioned, the suggested test method and equipment seems to be a very interesting candidate for a small-scale toxicity test and it should be possible to develop further the test protocol so that “difficult materials” such as the ones mentioned above, could be tested as well.

4.2 Full-scale experiments

Two full-scale experiments were performed in the project; one of these (a single mattress combustion in a room scenario) were mainly for simulation comparison. The other experiment, the reconstruction of the 2003 Växjö hospital fire, also aimed at understanding dynamics of the fire incident and in particular, the dense smoke produced.

The reconstruction clearly demonstrated that the floor PVC-carpet had a major impact on both the intensity of the fire and also the smoke produced. In the reconstruction, however, the mattress (which was taken from the actual hospital) was found to be the “engine” for the quick fire evolution. After a while, melting and burning mattress material started a pool fire on the PVC-carpet and a sort of “local” flashover was seen to occur under the bed. This was a significant event in the fire development and a full flash-over subsequently occurred where all of the PVC-carpet was burning.

The importance of the floor material in the fire development is often highly underestimated. It was found in the SP-reconstruction of the terrible discothèque fire, 1997 in Gothenburg, Sweden, where 63 young people were killed, that the floor involvement in the fire had a decisive influence on the final outcome.

The Växjö hospital fire clearly demonstrated the important impact of the PVC carpet on the fire development. It is true that a PVC carpet is not easily ignited but it was seen in this case that when the intensity of surrounding radiation is “big enough”, the material ignites and burns intensely. The flame retardant quality of chlorides explains the dense smoke as they will block a total oxidation, which means that soot is produced.

Due to the burning PVC-carpet, the HCl concentration was almost equal in magnitude to the CO concentration at the flash-over. In the room, upholstered furniture together with the mattress also produced high concentration of isocyanates in the fire smoke. In fact, based on an IDLH-value comparison (see 3.1.4), HCl was found to be (by large) the most dangerous substance in the fire smoke, followed by isocyanates, and CO and HCN almost at identical “magnitude of toxicity”.

After the reconstruction, analysis was made on soot-samples taken from the hospital a few days after the fire. A total chloride content of 7 -10% (by weight) were found. These samples were taken in the corridor (7%) a few meters away from the fire room and in the patient room (10%) 40 meters away from the fire where two of the victims were found. Samples taken from the fire room showed only small amounts of chlorides. This proves that the smoke did contain high amounts of chlorides, probably almost entirely from HCl.

Two patients died in the fire accident from smoke inhalation. Both victims were said to have been killed by CO-intoxication. However, the standard procedure when doing autopsy on fire victims, at least in Sweden, is to look for evidence of CO and HCN intoxication. These two substances are asphyxiates but other substances such as HCl or isocyanates are irritants that causes oedema and lung collapse and traces of such injuries are normally not looked for. In the light of the findings in this project one might suggest that fire victims should be investigated also with regards to irritants. It seems fully possible, or even probable, that high concentrations of irritants in the fire smoke will contribute to the overall cause of death.

Samples of lung tissue were taken from both fire victims and tested with regards to isocyanates. Traces of TDI (toluene-diisocyanate) metabolites were found in both victims but it is not known what this means, as no biological treasure values exists (i.e. a metabolite level “x” indicating a poisoning effect “y”). Further, most of the isocyanates in fire smoke is normally ICA (isocyanate acid), which do not produce any metabolites in the body.

4.3 Simulations

In the single mattress fire scenario the flamelet model was used in order to simulate the HCN concentration in the smoke leaving through the door opening in the Room-corner scenario. Chemical composition data from a mattress together with HRR-data and geometry from a single mattress combustion scenario were used as input to the CFD code. The calculated values were in excellent agreement with measured data. The flamelet model requires, however, a fine grid resolution to give adequate results. The time required for simulating the room/corridor scenario using the flamelet model would have been too long with the available computer capacity. It was therefore decided to use the alternative more simple model for this purpose.

In the simulation of the ground floor scenario, the formation chemistry of the toxic gases HCN and HCl were not calculated in the CFD code. Instead, small-scale experimental data from the Purser furnace were used as input to the CFD program. The program then calculated the spread of gases under the assumption that they did not react further. Comparing data from the Växjö hospital fire reconstruction with data simulated in this way showed good agreement, although not as good as for the flamelet model.

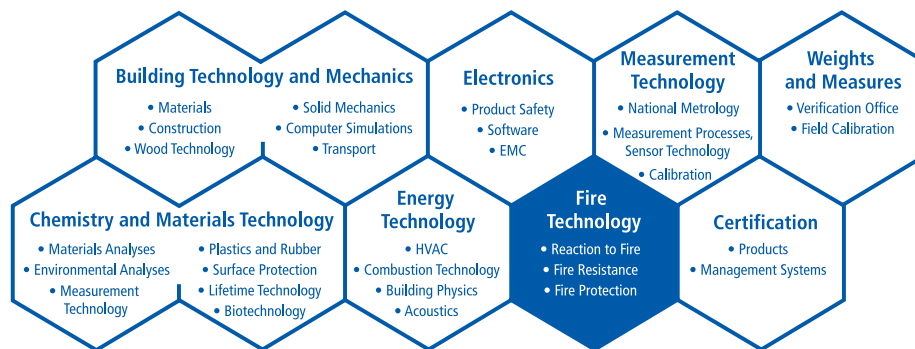
The simulations show that a local fire involving only one room in a room-corridor scenario might be very dangerous to persons situated at a long distance from the fire. In fact, the simulations indicate that under certain circumstances, it might be even more dangerous to be stuck at a longer distance since the smoke layer here earlier will reach the floor level.

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SP Fire Technology
 SP REPORT 2005:29
 ISBN 91-85303-60-7
 ISSN 0284-5172



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