

# **Combination of CFD and evacuation models for determination of FED and FEC levels**

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Combination of CFD and evacuation models for determination of FED and FEC levels

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### Abstract

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*April 30<sup>th</sup>, 2014*

*Beom Jin Jeong*

## Abstract

Previously developed methods to evaluate FED and FEC level via combination of CFD and evacuation simulation have been verified by new features of FDS6 and extended to fire cases involving common building materials. The FED levels calculated by the conversion factor [1] based on carbon monoxide are compared with the direct calculation by way of mass fraction of carbon monoxide, hydrogen cyanide and carbon dioxide. FEC level is compared with FIC output of FDS6. Both values showed quite good agreement with each other when all the combustion products are exactly specified in the reaction formula. The difference between FDS5 and FDS6 is also investigated for the FED and FEC level of the cable fire case and the result shows approximately 10 percent difference on average, which may result from the new combustion model of FDS6, i.e. partially-stirred batch reactor model. As for fuel, a sofa and bookcases were selected to be representative common building items and assumed to be a mixture of different materials, composed of mainly polyurethane and wood respectively with small amounts of PVC. For each item, a single fuel formula and stoichiometry reaction were formulated and used for the FDS simulations. For all cases, FED and FEC levels remain below the tenability criteria. However, considering measurement uncertainties, sensitivity analysis reveals that the FIC level can exceed criteria in case of maximum HCl yield. Also when it comes to post-flashover condition, FED levels appear to be exponentially increasing far over the criteria due to the contribution of hydrogen cyanide. Lastly prediction of FED and FEC level for fires involving combination of both sofa and bookcase has been demonstrated.

## 요약 (KOREAN)

피난 시뮬레이션과 전산유체역학을 결부시켜 FED 와 FEC 수준을 평가하는 방법이 기존에 제안된 바 있으며, 이를 최근 발표된 FDS6 의 새로운 기능을 통해 검증하고 일반건물에 흔히 존재하는 가연물 화재에 확대 적용 하였다. 기존의 방식은 FED 계산시 일산화탄소 농도를 기반으로 하는 “환산율”에 의한 방법인데, 이것을 일산화탄소, 시안화수소, 이산화탄소 농도에 의한 직접 계산 방식으로 비교해 보았다. 환산율에 의해 계산된 FEC 는 FDS6 의 FIC 출력값으로 비교하였다. 그 결과 모든 연소 생성물들이 정확히 화학 반응식에 포함되었을 경우, FED 와 FEC 모두 비교값과 매우 일치하는 결과를 보였다. FED 와 FEC 를 계산함에 있어서 FDS5 와 FDS6 의 편차를 케이블 화재의 경우에 대하여 확인해 본 결과 평균 약 10%의 오차를 보였다. 이는 FDS6 에서 기존의 혼합비 모델 대신 새로이 채택한 연소모델인 partially-stirred batch reactor model 에서 기인한 것으로 보인다. 대표적인 건물 내 가연물로서 소파와 책장을 선정하였으며 각각 폴리우레탄과 나무를 주재료로 소량의 PVC 가 섞인 혼합물로 가정하였다. 각각의 물품에 대하여 분자식과 연소반응식을 구성하여 FDS 시뮬레이션에 적용하였으며 FED 와 FEC 모두 거주 한계조건인 0.3 보다 낮은 것으로 나타났다. 그러나, 측정오차 등 불확실성을 고려한 민감도 분석 결과 HCl 의 생성율이 가장 높을 경우 FIC 값이 기준치를 넘어서는 것으로 나타났다. 또한 소파 화재에 대하여 포스트 플래시오버 조건으로 시뮬레이션 했을 경우 오히려 FED 레벨이 시안화수소의 영향으로 기하급수적으로 증가하여 거주한계 기준치를 훨씬 넘어서는 것으로 해석되었다. 마지막으로 위의 결과들을 바탕으로 두 가지 가구류가 동시에 연소할 경우에 대하여 FED 와 FEC 레벨을 예측하였다.

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## List of abbreviations

$C_3H_4O$  : Acrolein

$CH_2O$  : Formaldehyde

CFD : Computational Fluid Dynamics

EC : EkonomiCentrum

EDC : Eddy Dissipation Concept

FDS : Fire Dynamics Simulator

FEC : Fractional Effective Concentration

FED : Fractional Effective Dose

$FED_{total}^*$  : FED value calculated by the HCN mass fraction OUTPUT from FDS

$FED_{total}$  : Sum of FED for CO and HCN

FIC : Fractional Irritant Concentration

HCl : Hydrogen Chloride

HCN : Hydrogen Cyanide

HF : Hydrogen Fluoride

HRR : Heat Release Rate

HV : Hyperventilation

LUNARC : Lund University Numeric Intensive Computation Application Research Center

MDF : Medium-Density Fiberboard

MPI : Message Passing Interface

OD : Optical Density

PUR : Polyurethane

PVC : Polyvinylchloride

RSET : Required Safe Egress Time

ASET : Available Safe Egress Time

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# 1. Introduction

## 1.1 Background

Tenability conditions can be examined by way of temperature, visibility, heat flux and so on but in addition to these criteria, it is also possible to investigate combustion products containing toxic species such as irritant gases and asphyxiant gases which are presented in terms of FED (Fractional Effective Dose) and FEC (Fractional Effective Concentration).

In 2010, Lund University performed research on the possibility of new methodology combining computational fluid dynamics and evacuation simulation in order to investigate how people are influenced by the content of smoke gases during evacuation [1].

In this case study, two kinds of cables were used as a fuel to calculate FED and FEC. The main difference between two cables was with respect to the type and composition of species produced during fire. Both cables belonged to the same Euroclass D (Euroclass: European Classification system for e.g. wall and ceiling linings, floor coverings and cables to be used for CE marking of products) but one cable was non-halogenated and the other one was halogenated. The non-halogenated cable produced carbon monoxide and carbon dioxide while the halogenated cable produced acrolein, formaldehyde and hydrogen chlorinate in addition to CO and CO<sub>2</sub>. FDS simulations were performed based on the fire scenario in the existing university building and based on the experimental data of cable burning.

On the other hand, several evacuation scenarios have been set up and simulated via the evacuation program, SIMULEX [25] to be combined with FDS results. Six scenarios have been simulated and the most representative scenario was chosen for further analysis [1]. Finally, FED and FEC calculations from the result of FDS, i.e. smoke products' concentration at the location of interest, have been done by means of MATLAB.

The results of this study showed that the halogenated cable creates critical condition due to the irritant smoke gases and lower visibility than non-halogenated cable which makes no problem in FED and FEC values. This case study also showed the feasibility of new numerical methods to determine FED and FEC but further study was still needed to uphold this methodology.

In the above mentioned case study, only cables were used as a fuel and no sensitivity analysis has been performed yet. The output of FDS can vary depending on a number of different input data, for example, cell size, material property and so on. Especially for visibility, mass extinction coefficient, soot yield, HRR and cell size are known as relatively more influential parameters to the output by the extensive uncertainty study [2]. Also due to the lack of experimental data

that measured various smoke gas species at the same time, such as soot, CO, HCN and HCl which are essential components of the FED and FEC calculation, there exists uncertainty as well in their yields [3],[4].

In case of building fires, various combustible materials can contribute to the fire load other than cables [5] and those combustibles are possibly composed of a mixture of materials or combination of multiple objects commonly used in public buildings. Toxicity and hazard of various smoke gases, which will be addressed in this thesis is briefly introduced in the following section.

## 1.2 Toxicity of combustion products

Common toxic combustion products can be categorized into two groups such as asphyxiant gases and irritant gases. CO, HCN, CO<sub>2</sub> and low oxygen belong to asphyxiant gases which are known to cause confusion and loss of consciousness followed by death from asphyxia when a sufficient dose is inhaled [24]. Incapacitation by CO is expected when a sufficiently high concentration of carboxyhemoglobin is reached in the blood. The main mechanism of poisoning by hydrogen cyanide (HCN) is prevention of oxygen metabolism in the mitochondrion by inhibition of cytochrome reaction with oxygen. Low oxygen hypoxia depends on inhaled CO<sub>2</sub> concentration and occurs at 10-12% of oxygen concentration [24]. In this thesis, low oxygen effect is not taken into account but the effects of CO, HCN and CO<sub>2</sub> will be mainly addressed.

Irritant gases include inorganic acid gases such as hydrogen chloride (HCl), hydrogen bromide (HBr), hydrogen fluoride (HF), sulphur dioxide (SO<sub>2</sub>) and nitrogen oxides (NO<sub>x</sub>). In addition, acrolein (C<sub>3</sub>H<sub>4</sub>O) and formaldehyde (CH<sub>2</sub>O) are called organic irritants [21]. These gases are known to cause painful stimulation of eyes, nose, mouth, throat and lungs along with some hypoxia due to breathing difficulties, which hinders evacuation and can be lethal depending on the concentration. Also it may cause lung inflammation and oedema which may be fatal usually a few hours after exposure depending on dose inhaled [24]. Among these gases, this thesis mostly focuses on HCl which is the essential species accounting for FEC level to evaluate irritancy of smoke. HBr is also quite often taken up but it is not addressed here since it was not detected in the experiment quoted in this thesis. In addition to HCl, acrolein, formaldehyde and NO<sub>2</sub> will be discussed as the effect of minor species.

In general, fire effluents are mixtures of irritants and asphyxiants. Toxicity models basically assume different asphyxiants are additive with each other, and different irritants are also basically proportionally additive with each other. The FED for CO and HCN are considered directly additive and all these will be increased according to volume fraction of CO<sub>2</sub> [24]. To normalize the fractional concentrations or doses of each individual toxicant, the combined effects can be summed for a tenability assessment. Evacuees are also possibly impeded by soot

particles, heat convection and radiation dose, so they are also briefly compared with effects of toxic gases but not in detail since it is not the main purpose of this thesis.

### 1.3 Objectives

The aim of this thesis is to extend previous study [1] to other materials which are very commonly present in public buildings, for instance, furniture such as chairs and sofas made of different type of foams, plastics, wood and so on. This means the fuel can be extended to mixture of materials or even combination of different mixtures. The objective is to see if people are influenced by the smoke gases via calculating FED and FEC with different design fires other than a cable fire.

For further verification, it is also an important part of this thesis to compare the previous study via FDS5 with the results via newly published FDS6. It became possible to verify the previously developed methodology by means of new outputs and function given by FDS6. Also, another objective is to check how uncertainty has an effect on the final result by sensitivity analysis over the variation of composition of different materials. Grid dependency will be investigated especially for the area where people are exposed to smoke gases longer time due to queuing.

### 1.4 Limitations

This thesis has several limitations listed below.

- Only temperature and visibility are compared with FED and FEC as a tenability condition since this thesis mainly focuses on the toxicity effect presented by FED and FEC.
- In consideration of FED, low oxygen effect is not taken into account.
- The latest version of FDS [11] is used for the CFD modelling and SIMULEX for the evacuation modelling respectively and these models have certain limitation in themselves with respect to fire behaviour, combustion model and human behaviour.
- As for the subject building, only one type of public building, which is the same as previous case study, has been chosen for the purpose of direct comparison between the results from this thesis and the previous work.
- A hypothetical design fire which is taken from limited experimental data sources may not be representative to this case study, thus fire growth can be different from real fire situations such as a large scale building fire by simplified assumptions about the heat release rate curve and so on.



## 2. Methodology

In the previous feasibility study [1], the following procedure was developed. The CFD simulation is performed for the specific fire scenario and then gas temperature, gas density, soot mass fraction and CO mass fraction are obtained as outputs. In order to investigate the effect of toxic gases on the people who evacuate, evacuation simulations need to be done for the same geometry. From the evacuation simulation, the position of evacuees over the time is retrieved as an output. At the last step, the information of people's location is combined to the toxic gas concentration by means of MATLAB software which is coded to convert soot and CO mass fraction into volume concentration ( $\text{kg}/\text{m}^3$ ) and then calculate FED and FEC level for each person per every time step according to the formula given in ISO TS 13571 [6]. The CO concentration is used to calculate other gas species' concentrations such as HCl, acrolein and formaldehyde by "conversion factor" which is the ratio of other gas' yield to CO yield. This methodology is called, "conversion method" onward in this thesis. More detailed procedure is addressed in the later part.

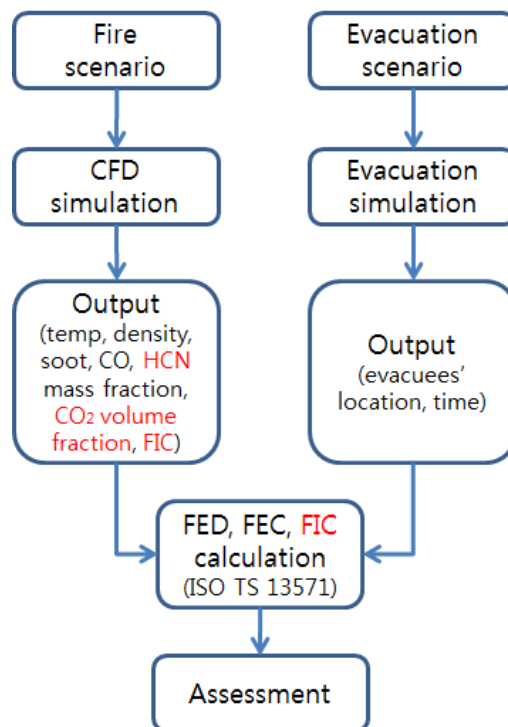


Figure 2.1 Schematic of calculation procedure

## 2.1 Selection of Building

Firstly, a public building is selected as a simulation subject. In this thesis, the same building used in the previous feasibility study [1] is adopted as well since evacuation experimental data is available and in order to compare the different smoke effects driven by different fire sources. This building is a three-story university building “EC3” which has a cafeteria, seminar rooms on the ground floor and auditorium, a data room and offices on the upper floors. It has also an atrium from the ground floor up to the first floor which has a balcony overlooking the ground floor to which is connected by two separate stairs at both ends of the balcony.

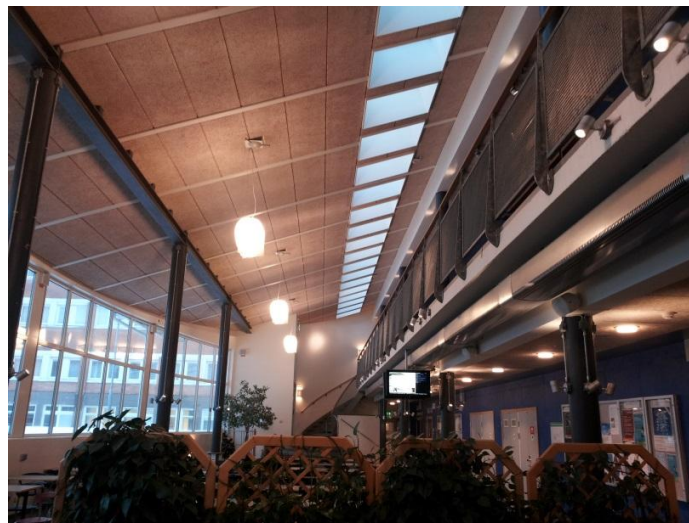


Figure 2.2 View from ground floor

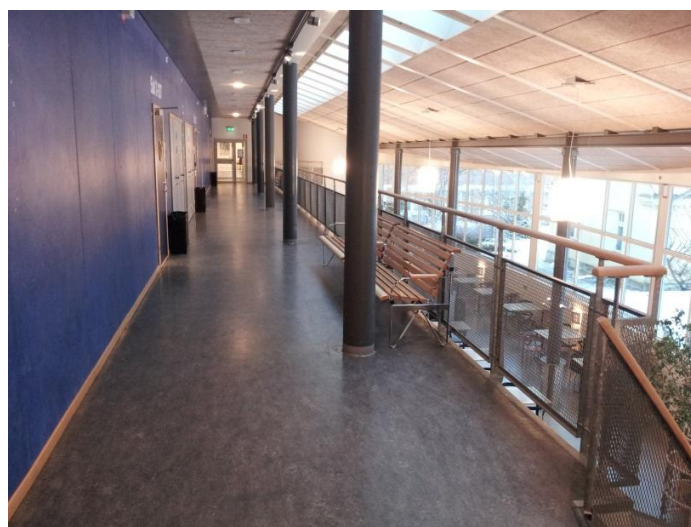


Figure 2.3 Balcony of the first floor



Figure 2.4 Cafeteria kitchen and serving area on the ground floor

## 2.2 CFD Simulation

Fire simulations are performed by FDS6, but FDS5 is also used in some cases for the purpose of comparison with the previous research. Due to the demanding computing time for the large scale building simulation, parallel computing has been performed in the LUNARC, which is a center for scientific and technical computing for research in southern Sweden. The Alarik cluster of LUNARC has performance of 3.0 GHz CPU, 2 to 4 GB memory per core and 16 cores on every node.

### 2.2.1 Selection of building material as a fuel

There are a variety of materials in public buildings and these can be a potential fuel in case of fire. Zalok and Eduful [5] did a research on the contribution of materials to the total fire load in office buildings and the result is reproduced in the table below. From this result, wood and paper account for 70% of total and the rest are plastic and textile.

Table 2.1 contribution of different materials to the fire load

material	Contribution (%)
paper	24
wood	46
Plastic	22
textile	8
Total fuel and fire load	100

Some of the major items related to the building subject to this simulation and their material composition are excerpted and summarized in the table below from literature [7]. This table shows that common items in buildings are mostly made of mixture of several different materials, which produce different combustion products as shown in Table 2.3.

Table 2.2 common combustible items and composition

Room	Item	Materials
All	cables	PVC, PE, Nitrile rubber
Living / Dining	Coffee table	Wood, MDF
	Bookcase	MDF, particle board
	Table and chairs	Timber, metal, PUR, fabric
	Sofa (or any other upholstered furniture)	PUR(upholstery), wood(frame), steel(frame), cotton, polyester
Kitchen	Cabinets	MDF, particle board, PVC
	Chairs	PVC, PP
	Appliances	ABS, PP, PC
Office	Desk	Timber, MDF
	Chair	PVC, PP, fabric, leather

Table 2.3 combustion products of materials

Material	Combustion products
Wood, PE, PP, PS, PVC, PUR	CO, CO <sub>2</sub>
Wool, nylon, PUR, ABS, nitrogen containing material	HCN, NO, NO <sub>2</sub>
PVC, Fluoropolymer, halogen containing material	HCl, HF
Rubber, wool, sulphur containing material	SO <sub>2</sub> , H <sub>2</sub> S

As this thesis mainly focuses on FED and FEC level resulting from common building items, CO and HCN should be included in the combustion products for the FED calculation and HCl for the FEC calculation. From all the above literature review, upholstered sofa and wooden furniture are concluded to be the most suitable and representative building material for the purpose of this thesis.

### 2.2.2 Design Fire

It is the best to adopt a full experimental data set containing the entire heat release rate curve and yields measurement of various species over the time including soot yield. But even though there are some large-scale fire tests that documented HCN and HCl yields for diverse materials [8] [9] [10], it is very rare and hard to find fire test data satisfying those all requirements.

Especially there is little documentation about the experimental data measuring soot yield, CO yield, HCN yield and HCl yield at the same time, which are essential species needed for the FED and FEC calculation.

According to the conclusion of the previous section, a very well-documented fire test data reported by NIST [4] regarding common building furniture, was finally selected and used for fire modelling in this thesis. This research is about room-scale tests including combustion products' yields for both pre and post-flashover of three items which were selected for diversity of physical form, combustion behaviour and yields of toxicants produced. The yields data are reproduced in the following table. The latter figures mean repeatability and measurement uncertainty, which will be subject to sensitivity analysis in the later section.

Table 2.4 Yields of combustion products (g/g)<sup>[4]</sup>

gas	Fire stage	sofa	bookcase
CO	Pre-F.O	$1.44 \times 10^{-2} \pm 35\%$	$2.4 \times 10^{-2} \pm 55\%$
	Post-F.O	$5.1 \times 10^{-2} \pm 25\%$	$4.6 \times 10^{-2} \pm 30\%$
HCN	Pre-F.O	$3.5 \times 10^{-3} \pm 50\%$	$4.6 \times 10^{-4} \pm 10\%$
	Post-F.O	$1.5 \times 10^{-2} \pm 25\%$	$2.5 \times 10^{-3} \pm 45\%$
HCl	Pre-F.O	$1.8 \times 10^{-2} \pm 30\%$	$2.2 \times 10^{-3} \pm 75\%$
	Post-F.O	$6.0 \times 10^{-3} \pm 35\%$	$2.2 \times 10^{-3} \pm 65\%$
NO <sub>2</sub>	Pre-F.O	$< 7 \times 10^{-2}$	$< 2 \times 10^{-2}$
	Post-F.O	$< 1 \times 10^{-3}$	$< 1 \times 10^{-3}$
Acrolein (C <sub>3</sub> H <sub>4</sub> O)	Pre-F.O	$< 8 \times 10^{-3}$	$< 2 \times 10^{-3}$
	Post-F.O	$< 1 \times 10^{-4}$	$< 1 \times 10^{-4}$
Formaldehyde (CH <sub>2</sub> O)	Pre-F.O	$< 2 \times 10^{-2}$	$< 2 \times 10^{-3}$
	Post-F.O	$< 8 \times 10^{-4}$	$< 4 \times 10^{-4}$

It should be noted that NO<sub>2</sub>, C<sub>3</sub>H<sub>4</sub>O and CH<sub>2</sub>O are not detected in their tests so that their yields are normalized relative to HCl concentration and calculated for the upper limit [4]. Nevertheless the above data is almost ideal for the purpose of this thesis since it is not the yield of pure material but mixture of different materials which this thesis is aiming to investigate. Each item in the table is compositionally complex and detailed description is quoted as follows from [4].

- Sofa : made of upholstered cushions supported by a steel frame. The fire retardant in the cushion padding contains chlorine atoms. Thus, this fuel would be a source of CO<sub>2</sub>, CO, HCN, HCl, NO<sub>x</sub>.

- Bookcase : particleboard with a laminated polyvinyl chloride (PVC) finish. This fuel would be a source of CO<sub>2</sub>, CO, HCN, HCl, NO<sub>x</sub>.

As the above reference does not include soot yield and heat of combustion for each item, they are adopted from other statistical source which provides design recommendations to conduct an FDS sensitivity analysis [3]. They established various model inputs for probabilistic modelling through extensive literature survey, from bench scale to full-scale fire tests, over a number of combustible material and items. Among a number of statistical data in this literature, recommended values for design purposes are taken as follows.

- Soot yield :  $0.018 \pm 0.0032$ <sup>[3]</sup> for furniture containing PUR foams.
- Heat of combustion :  $17,040\text{kJ/kg}$ <sup>[3]</sup> for furniture containing PUR foams.

In order to compare with the FED and FEC in case of the cable fire of the previous study, the peak heat release rate is decided to be the same, 1MW and fire growth rate is adopted from the experimental result of “fabric covered PUR foam single seater” given in Figure 5.2 of reference [3]. This is somehow moderate maximum value for a sofa fire but it was taken for the sake of this study. In this thesis, it is assumed that peak heat release rate is maintained for 3 minutes after 120 seconds of growth phase for simplicity. In fact, yield data in Table 2.4 were measured for approximately 4 or 6 minutes of room-scale fire tests.

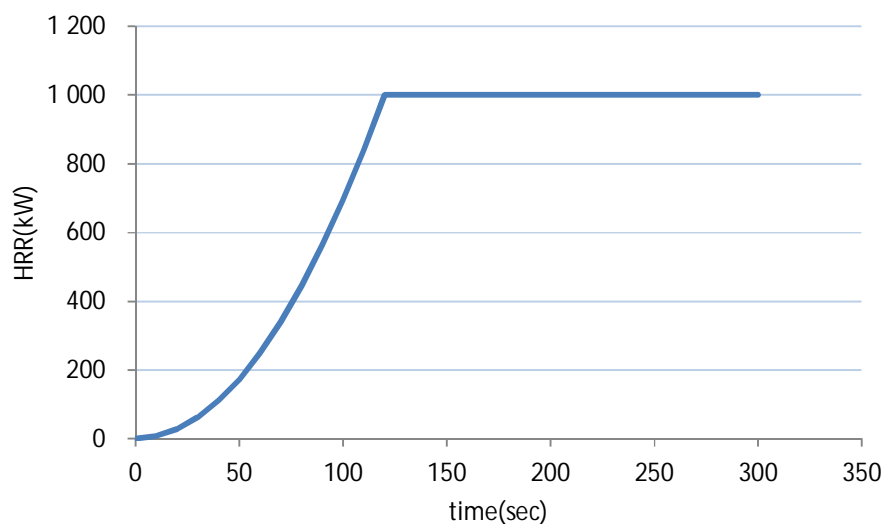


Figure 2.5 Heat Release Rate curve

### 2.2.3 Geometry and Mesh Set-up

The building space to be modelled is about 30m wide, 9m depth and 7m high, which includes a ground floor, a balcony of first floor and atrium. The cell size is decided according to the FDS user guide [11] and given in the table below.

Table 2.5 Mesh Resolution

Resolution	Coarse	Medium	Fine
$D^*/dx$	4	10	16
dx(mm)	241	96	60
Cell size(mm) used	200	100	50

Since it is practically challenging to model the whole building with a fine mesh, it is divided into 10 meshes depending on the importance of each area. The space near the fire source and the vertical plume area are modelled with a fine mesh, atrium and a balcony with a medium mesh and the rest area of little interest is modelled with a coarse mesh. Total number of cells counts up to about 3,330,000 which is the same mesh structure used in the preceding study [1].

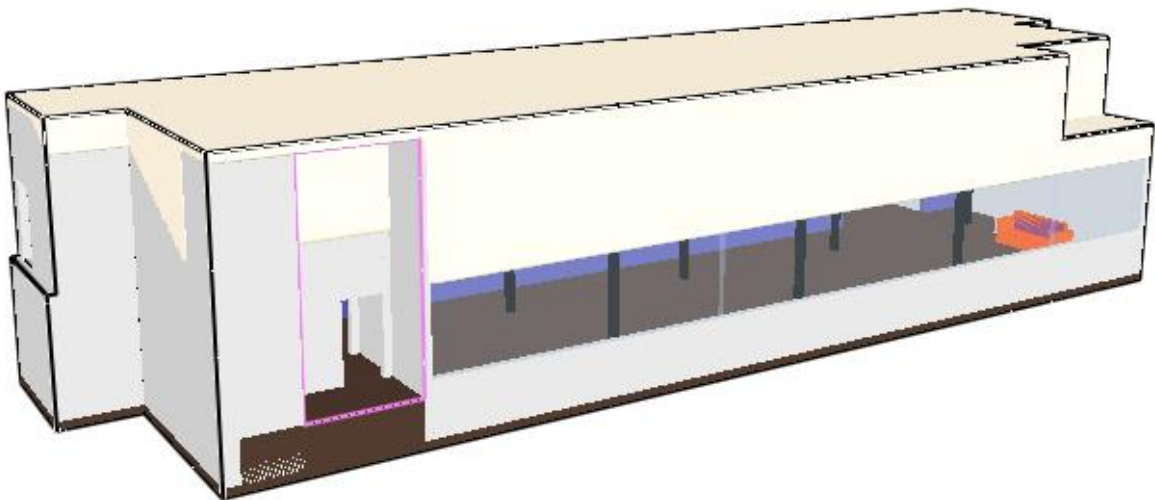


Figure 2.6 Geometry model of building "EC3"

As shown by the figure below, the fire source is assumed to be located just below the balcony of first floor.



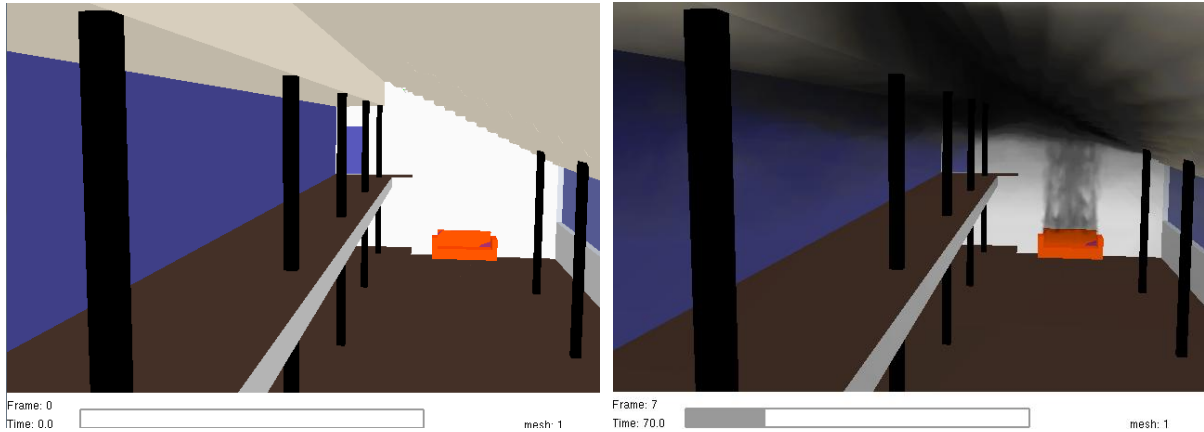


Figure 2.7 Modelling of inside building

## 2.2.4 Detection Time

The detection time is decided by the activation of the smoke detector specified in the FDS input. For all simulations in this thesis, the following setup is applied according to FDS guide [11].

```
&DEVC ID='SD_1', PROP_ID='Acme Smoke Detector', XYZ= 5.8, 9.0, 6.2 /
&PROP ID='Acme Smoke Detector', QUANTITY='CHAMBER OBSCURATION', LENGTH=1.8,
ACTIVATION_OBSCURATION=3.24 /
```

Figure 2.8 smoke detector set up

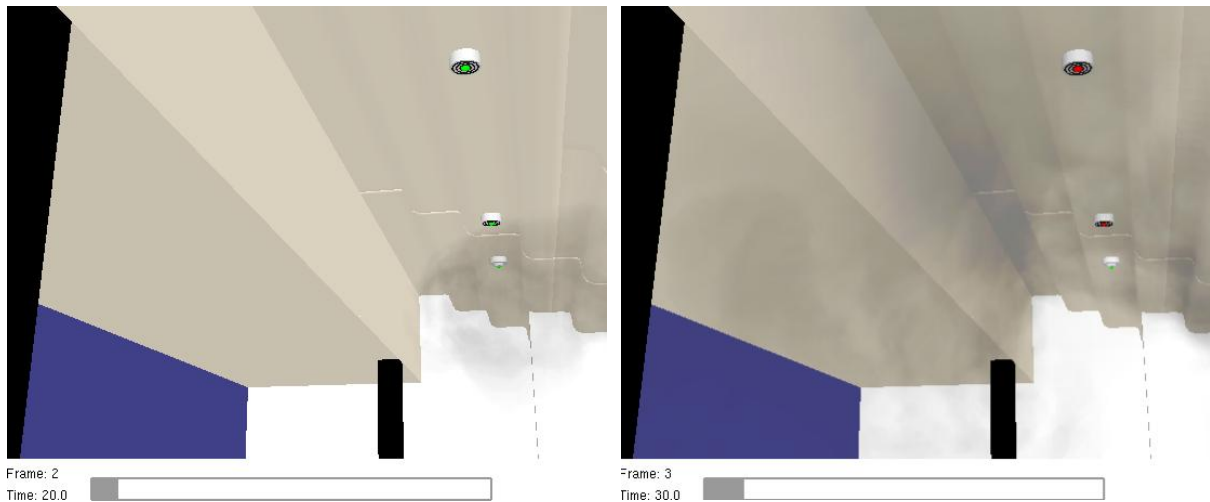


Figure 2.9 detector location and activation time

As shown by the picture (right) above, the smoke detector is activated after about 20 seconds. The exact activation time is 21s for the sofa fire and 19.8s for the bookcase fire in the preliminary simulation.



## 2.3 Evacuation Simulation

In fire safety engineering, generally the following equation is used for the escape design [23].

eq. (1)

$$t_{\text{detection}} + t_{\text{alarm}} + t_{\text{pre-movement}} + t_{\text{travel}} = t_{\text{escape}} = RSET < ASET$$

Where the detection time is defined as activation of automatic system and obtained from the CFD simulation, which was found to be about 20 seconds before. The second term, the alarm time, is assumed to be 10 seconds, which means the time from detection to a general alarm being given. Either evacuation experiment or evacuation simulation should determine pre-movement time and travel time. Finally, it will be checked whether the FED or FEC levels for each person exceeds the tenability criteria during the travel time. If so, the time at which it exceeds represents ASET (Available Safe Egress Time).

For the evacuation simulation, SIMULEX [25] is used. Specific location information of evacuees who are mostly exposed to smoke gases is retrieved from SIMULEX. This evacuation simulation is based on the unannounced real evacuation experiment at the building "EC3" performed on April 9<sup>th</sup>, 2008. The whole evacuation process was filmed and documented by observers, through which important input data for evacuation simulation such as pre-movement time and exit choice could be provided. In the presented thesis, the evacuation simulation was not performed. Instead, the simulation results from the preceding study [1] have been used in order to compare thesis' results with the cable fire in the same configuration. Thus, detailed procedure for the simulation is not given here, but only the principal part of the results is summarized in this section.

From the evacuation experiment, the pre-movement time was decided to be 10±10 seconds, which means the range of 0 to 20 seconds can be taken for each person to start movement in the evacuation simulation. In the SIMULEX simulation, 446 people in total were used for the different exit choice scenarios. Plane layout and evacuation route of each floor is illustrated in the figures below. In the chosen evacuation scenario, 25% of the people in room 2:1, 2:2 and 2:3 are assumed to use the exit to EC2 where is the next building connected by a corridor as shown by the table below, because they are not willing to wait long in the queue for the main stair. It should be noted from Figure 2.7 that the ceiling of this building has a slope along which smoke flows up and accumulates as a smoke layer above a balcony, hence deteriorating the tenability condition compared to the ground floor. In conclusion, people evacuating on the first floor are most likely to build a queue in front of a main stair and must stay at the balcony for relatively longer time, being exposed to worst tenability condition caused by toxic gases. Therefore, those who are on the balcony will be taken into account for the FED and FEC calculation in MATLAB.

Table 2.6 Evacuation scenario <sup>[1]</sup>

Floor	Room	No. of People	Exit choice
Ground	1:1	18	Main exit
Ground	1:2	18	Main exit
Ground	1:3	60	Main exit
Ground	1:4	60	Main exit
Ground	1:5	0	Main exit
First	2:1	35	Exit to EC2
First	2:2	75	Main exit
First	2:2	10	Exit to EC2
First	2:3	79	Main exit
First	2:3	6	Exit to EC2
First	2:4	85	Secondary exit
total		446	

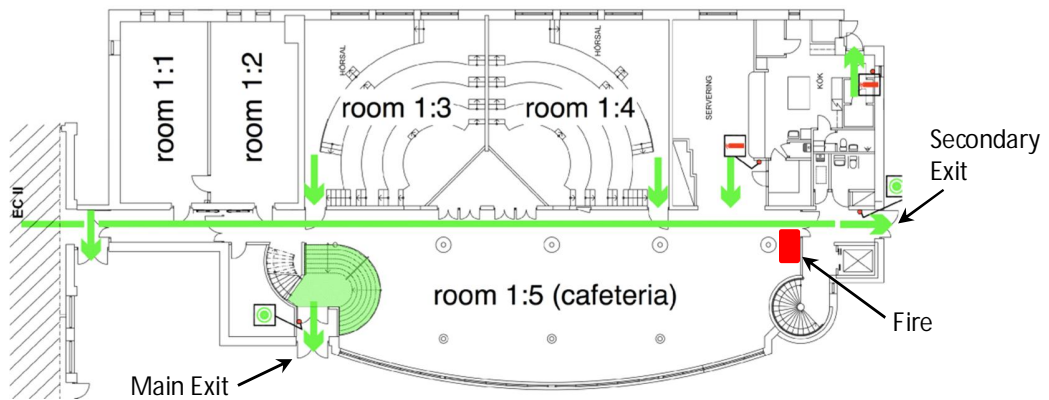


Figure 2.10 Evacuation route and exit choice on the ground floor <sup>[1]</sup>

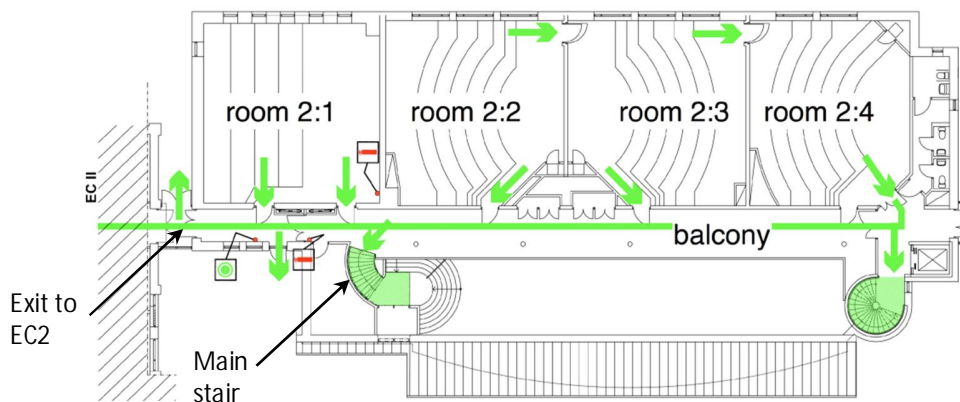


Figure 2.11 Evacuation route and exit choice on the first floor <sup>[1]</sup>

## 2.4 FED and FEC Calculation

In order to evaluate the FED and FEC level for each person, the location of a person at a certain time should be coupled with FDS output.

### 2.4.1 Formula

The FED and FEC are given by the following formula according to the ISO document [6]. Asphyxiant gas model for calculating fractional effective dose is;

eq. (2)

$$\mathbf{FED} = \sum_{t_1}^{t_2} \frac{\varphi_{CO}}{35000} \Delta t + \sum_{t_1}^{t_2} \frac{\exp\left(\frac{\varphi_{HCN}}{43}\right)}{220} \Delta t$$

**where,  $\varphi_{CO}$  is CO concentration in ppm**

$\varphi_{HCN}$  is HCN concentration in ppm

$\Delta t$  is time increment in minutes

In case where CO<sub>2</sub> concentration is over 2% by volume, each term of the above equation at each time increment shall be multiplied by a hyperventilation factor,  $\mathbf{v}_{CO_2}$ .

eq. (3)

$$\mathbf{v}_{CO_2} = \exp\left(\frac{\varphi_{CO_2}}{5}\right), \quad \varphi_{CO_2} \text{ is } CO_2 \text{ concentration in \%}$$

The irritant gas model for calculating fractional effective concentration is;

eq. (4)

$$\mathbf{FEC} = \frac{\varphi_{HCl}}{F_{HCl}} + \frac{\varphi_{HBr}}{F_{HBr}} + \frac{\varphi_{HF}}{F_{HF}} + \frac{\varphi_{SO_2}}{F_{SO_2}} + \frac{\varphi_{NO_2}}{F_{NO_2}} + \frac{\varphi_{acrolein}}{F_{acrolein}} + \frac{\varphi_{formaldehyde}}{F_{formaldehyde}} + \sum \frac{\varphi_{irritant}}{F_{Ci}}$$

**where,  $\varphi$  is concentration in ppm**

$F$  is the concentration of each irritant gas, expected to cause incapacitation in ppm

$F_{HCl}$  1000 ppm    $F_{NO_2}$  250 ppm    $F_{acrolein}$  30 ppm    $F_{formaldehyde}$  250 ppm

In addition to toxic gases, FED driven by radiant heat and convective heat can be also calculated. The tenability limit for exposure of skin to radiant heat is approximately 2.5kW/m<sup>2</sup> [6] which corresponds to a source of surface temperature maintaining approximately 200 °C.

Convective heat accumulated per minute is suggested as follows for fully clothed subjects,

eq. (5)

$$t_{conv} = (4.1 \times 10^8) T^{-3.61}$$

Where  $t_{conv}$  is the time in minutes and  $T$  is the temperature in Celsius ( $^{\circ}\text{C}$ ).

Then the total effective dose of heat acquired during exposure can be calculated by the following equation. The formula of radiative heat accumulated per minute is not given here.

eq. (6)

$$\mathbf{FED}_{Heat} = \sum_{t_1}^{t_2} \left( \frac{1}{t_{rad}} + \frac{1}{t_{conv}} \right) \Delta t$$

In areas where the radiant flux to skin is under  $2.5\text{kW/m}^2$ , the first term of above equation is set to be zero which is the case of this thesis simulation. It should be noted that FED is an accumulative value over the time but FEC is instantaneous value at a certain time.

#### 2.4.2 MATLAB Calculation

As mentioned before, since FED is time-integral value for each person moving continuously, it cannot be retrieved directly from FDS. Instead, MATLAB is used to extract OUTPUTs from ASCII files of FDS' SLCF and calculate FED and FEC according to the formulas given in the previous section.

From the result of the evacuation simulation, it was known that people on the balcony are mostly exposed to smoke gas in this fire scenario. MATLAB is coded to scan all the position of people at each time increment from the result file of SIMULEX and identify people on the balcony at that time so that FEC and FED are calculated for those people.

In order to calculate FED and FEC, it is necessary to get OUTPUTs from FDS such as gas temperature, gas density, soot mass fraction, CO mass fraction and  $\text{CO}_2$  volume fraction. Mass fraction (kg/kg) of each species is once converted into concentration ( $\text{kg/m}^3$ ) by multiplying gas density and then converted into ppm by ideal gas law.  $\text{CO}_2$  concentration is checked for each person at each time step to take hyperventilation factor into account. If it exceeds 2% by volume at that time, eq. (3) is multiplied to each term of FED formula eq. (2) [6].

In the preceding study [1], concentrations of all other species, for example HCl, other than CO were calculated based on the conversion factor, i.e. the ratio of the species yield to CO yield, but hyperventilation factor and HCN concentration were not included in FED calculation. For the purpose of this thesis, HCN concentration is taken into account in two ways. One way is to calculate it by the conversion factor as before, and the other way is to get it as a direct OUTPUT of HCN mass fraction from FDS, which becomes possible due to the new feature of FDS version

6, officially released in November 2013 [11]. These two methods are compared to check if both coincide with each other for the purpose of verification. MATLAB is coded to calculate FED for each person by both conversion factor and HCN mass fraction accordingly.

In addition, another new feature of FDS6 allows FEC value, which is calculated by the conversion factor, to be verified by the new OUTPUT of FDS, FIC. In the previous version of FDS5 [12], there was no built-in output about measurement of irritant concentration but FDS6 provides FIC (Fractional Irritant Concentration), which is FEC for irritants and basically the same as FEC of ISO TS 13571 [6] by definition, except the incapacitation concentration of each irritant gas that is expected to cause incapacitation in eq. (4). MATLAB is coded to calculate the FIC for each person and FEC by the conversion factor as well to compare the both values. Schematic of calculation procedure is given in the figure below and details can be found in the MATLAB script in Appendix 14.2.

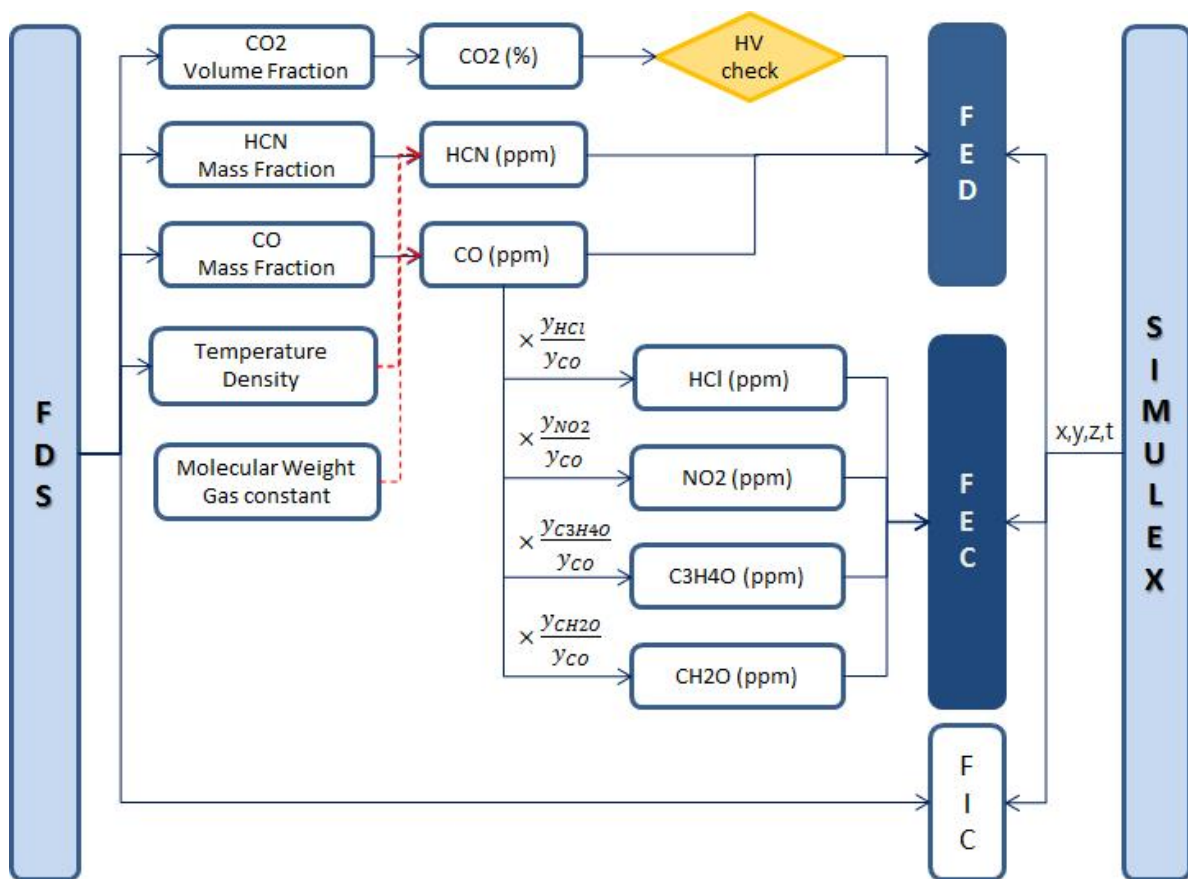


Figure 2.12 schematic of MATLAB calculation for toxic gases

## 2.5 Assessment

By definition, the FED and FEC value of 1.0 means incapacitation of people who have average susceptibility to escape for themselves. However, taking into account population group who are more sensitive and vulnerable to toxicity, threshold criteria of 0.3 could be used instead for the general group of people [6].

For the effect of smoke particles, a soot concentration of  $0.8 \text{ g/m}^3$  is used for criteria based on smoke obscuration model according to ISO Technical Specification [6]. In this concentration, occupants are supposed to be unable to see more than about 0.5m.

A visibility criterion is set to be the soot concentration, which corresponds to a visibility of 10m. Suggested tenability limit is 5m (OD; 0.2) for small enclosure, and 10m (OD; 0.08) for large enclosure in reference [14]. In this thesis, the equivalent soot concentration is given by the equation below that is the aerosol mass concentration at which threshold visibility occurs for light-reflecting signs [6].

eq. (7)

$$\mathbf{threshold\ concentration} = \frac{\mathbf{0.3}}{\mathbf{L}} [\mathbf{g \cdot m^{-3}}], \quad \mathbf{L = 5m \sim 15m}$$

### 3. Review of the Cable Fire in FDS6

It would be worthy to check how the FED and FEC levels are affected by different version of FDS. In this section, the result of halogenated cable fire [1] performed by FDS5 before is implemented again with new FDS version 6 and compared with each other.

#### 3.1 Comparison of FDS5 and FDS6

There is an important change in FDS6 which was officially released in November 2013, especially for the combustion modelling [13] as follows.

##### 3.1.1 Difference in combustion modelling

FDS5 models combustion by means of a Mixture Fraction Model as a default which tracks each species by two parameters, namely mass fraction of unburned fuel and mass fraction of burned fuel. These two parameters are only computed explicitly in FDS5. Hence, users should not explicitly list the reactants and products.

Instead, FDS6 models combustion by means of a Mixing-Controlled Model as a default which tracks three lumped species, namely air, fuel and products, of which the last two are explicitly computed. If the fuel is such a pre-tabulated one in FDS, for example hydrocarbons, the stoichiometric chemical reactions are still not needed to be specified. But, this is not the case for a PVC cable fire since it is not tabulated.

In this comparison, a cable containing chlorine is used, whose item number is C0506T1. Principal material properties and input data are as follows.

Table 3.1 input for combustion modelling

material	PVC
Formula	$C_2H_3Cl$
Soot yield (g/g)	0.1
CO yield (g/g)	0.1333
Heat of Combustion (kJ/kg)	16,533.33
Peak heat release rate (kW)	1,000
Time to reach peak HRR (s)	1,168

With the same input data above, PVC combustion is specified differently for each version of FDS.

### 3.1.2 FDS script of fuel

```

--- fuel ---
&REAC ID          = 'PVC'
  FYI             = 'Cable M - n(C_2 H_3 N_0 O_0 Cl_1),
  IDEAL          = .FALSE.
  HEAT_OF_COMBUSTION = 16533.33
  SOOT_YIELD     = 0.1
  CO_YIELD       = 0.133333333333
  N              = 0.
  C              = 2.
  H              = 3.
  O              = 0.
  OTHER          = 1.
  MW_OTHER       = 35.5 /

&SURF ID='BURNER', HRRPUA=832., TAU_Q=-1168, COLOR='RASPBERRY' /

```

Figure 3.1 PVC combustion modelling in FDS5

```

--- My fuel ---
&SPEC ID = 'C0506T1',          FORMULA = 'C2H3Cl' /
&SPEC ID = 'OXYGEN',           LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'NITROGEN',        LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'HYDROGEN CHLORIDE', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'WATER VAPOR',     LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'CARBON MONOXIDE',  LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'CARBON DIOXIDE',   LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'SOOT',            LUMPED_COMPONENT_ONLY = .TRUE. /

&SPEC ID = 'AIR', BACKGROUND=.TRUE.,
  SPEC_ID(1) = 'OXYGEN', VOLUME_FRACTION(1)= 1,
  SPEC_ID(2) = 'NITROGEN', VOLUME_FRACTION(2)= 3.76 /
&SPEC ID = 'PRODUCTS',
  SPEC_ID(1) = 'WATER VAPOR', VOLUME_FRACTION(1) =          1 ,
  SPEC_ID(2) = 'NITROGEN', VOLUME_FRACTION(2) =          6.882142857 ,
  SPEC_ID(3) = 'CARBON DIOXIDE', VOLUME_FRACTION(3) =          1.181547619 ,
  SPEC_ID(4) = 'CARBON MONOXIDE', VOLUME_FRACTION(4) =          0.297619048 ,
  SPEC_ID(5) = 'HYDROGEN CHLORIDE', VOLUME_FRACTION(5) =          1 ,
  SPEC_ID(6) = 'SOOT', VOLUME_FRACTION(6) =          0.520833333 /

&REAC FUEL = 'C0506T1',
  SPEC_ID_NU = 'C0506T1','AIR','PRODUCTS', NU=-1, -1.830357143, 1,
  HEAT_OF_COMBUSTION = 16533.33, CHECK_ATOM_BALANCE=.TRUE. /

&SURF ID='BURNER', HRRPUA=832., TAU_Q=-1168, COLOR='RASPBERRY' /

```

Figure 3.2 PVC combustion modelling in FDS6

While FDS5 needs only soot yield and CO yield, FDS6 needs to list up air, fuel and products with complete atomic balance, which is specified by soot yield and CO yield given.



### 3.2 Results and Analysis

In this simple comparison, FED is calculated only by CO and FEC only by HCl due to the lack of data for other species such as HCN, acrolein and formaldehyde. Based on experimental data, the conversion factor for HCl is set to be 2.7625 in MATLAB calculation. Detection time plus alarm time was determined to be 90 seconds by the FDS simulation. Thus, evacuation starts between 90 seconds and 110 seconds after ignition depending on the pre-movement time given in the section 2.3 for each person.

Table 3.2 Cable fire result summary

OUTPUT		FDS5	FDS6	deviation
FED <sub>CO</sub>	Avg.	2.54x10 <sup>-4</sup>	2.29x10 <sup>-4</sup>	9.8%
	Max.	0.00313	0.00295	5.8%
FEC <sub>HCl</sub>	Avg.	0.00472	0.00424	10.2%
	Max.	0.37497	0.32224	14.1%
Soot concentration (g/m <sup>3</sup> )	Avg.	0.00193	0.00173	10.4%
	Max.	0.15112	0.12988	14.1%
FED <sub>heat</sub>	Avg.	5 x10 <sup>-5</sup>	5 x10 <sup>-5</sup>	-
	Max.	0.00032	0.00034	6.3%

These results show more or less 10% deviation in overall average between two versions. Differences in peak value of FEC and soot concentration are somewhat bigger than those of FEDs in this case. As a result, the number of people who are exposed to more than threshold value of 0.3 is less in FDS6 than in FDS5. The possible reason will be discussed later.

Table 3.3 People exposed to threshold FEC (≥ 0.3)

Version	Number of people affected
FDS5	8 of 446
FDS6	3 of 446

Except for FEC, other measurements such as FED and soot concentration are quite lower than threshold value, e.g. smoke density 0.8g/m<sup>3</sup>. Also, the effect of heat dose is very little because the temperature increase is not so much due to very slow fire growth rate, i.e. 20min to peak HRR. FED level and FEC level for each person are plotted in the figures below. The plots of the FED level for heat dose and smoke concentration are not given here as their values are very low.

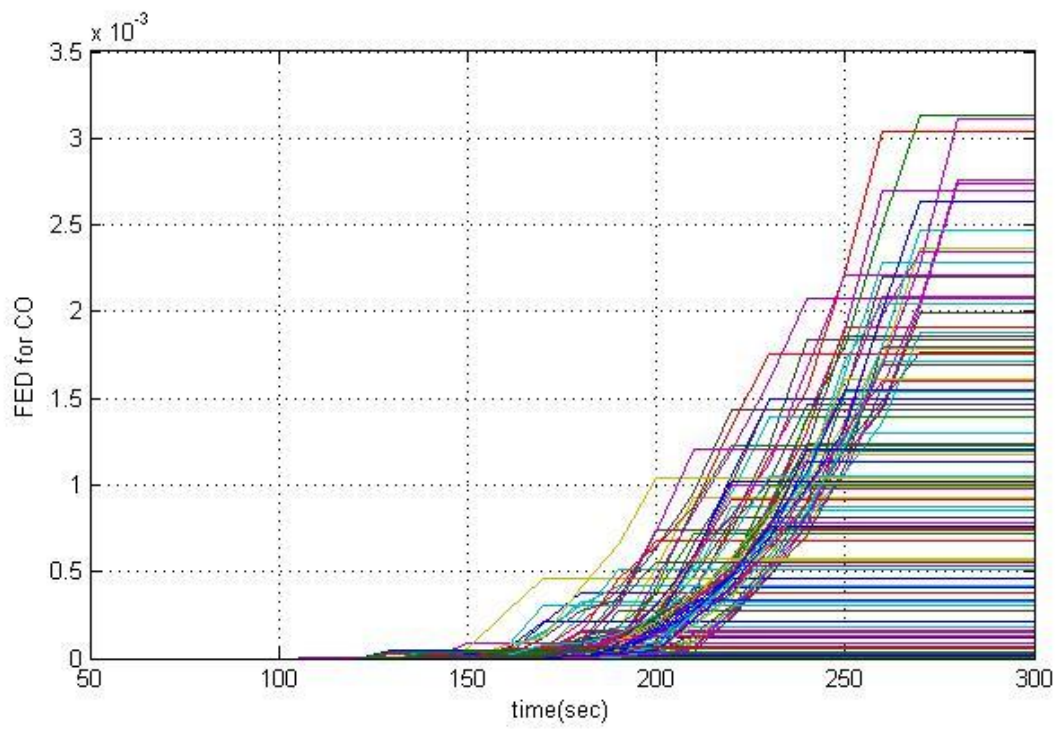


Figure 3.3 Cable Fire: FED by FDS5

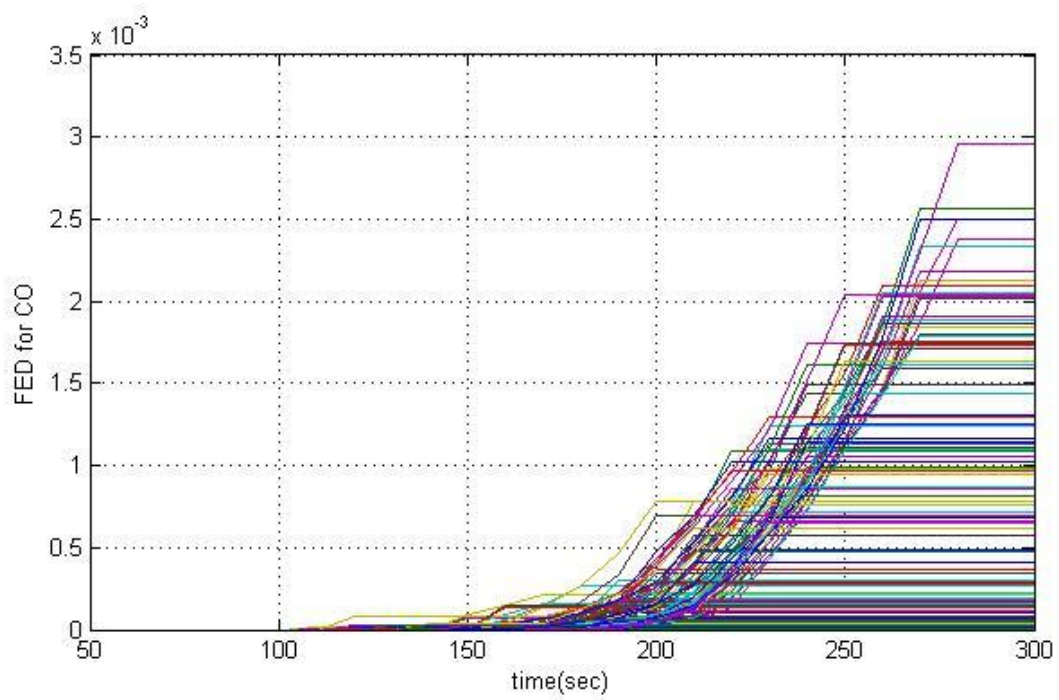


Figure 3.4 Cable Fire: FED by FDS6

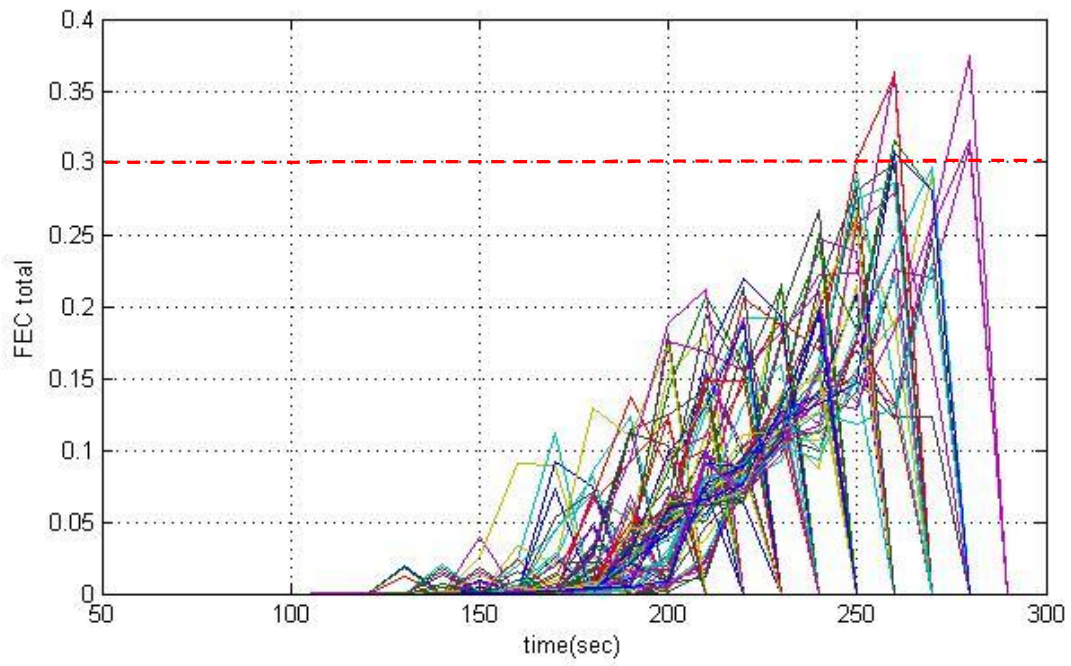


Figure 3.5 Cable Fire: FEC by FDS5

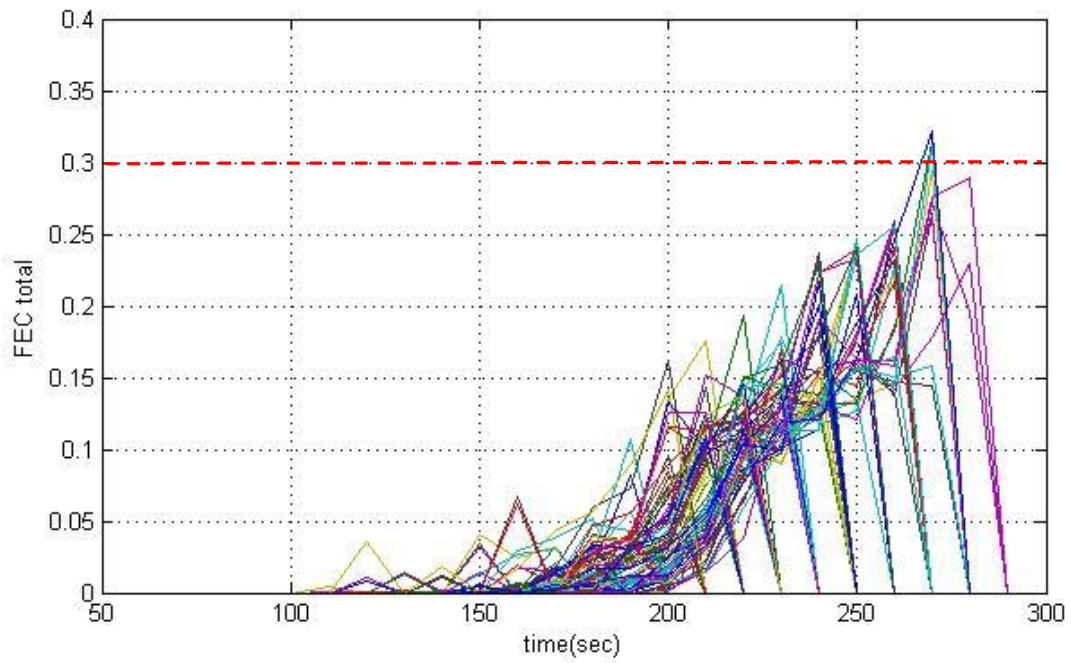


Figure 3.6 Cable Fire: FEC by FDS6

### 3.3 Discussion

The results from the new version of FDS showed about 10% lower FEC and FED level on average value and this is deemed to result from following aspects.

First of all, the new combustion model of FDS6 is “lumped species method” which is different from “mixture fraction model” of FDS5. For most applications of FDS, the assumption that the chemical reaction is considerably faster than mixing is valid and mean chemical source term for the fuel is modelled by Eddy Dissipation Concept (EDC) [16] in FDS6. But, when it comes to complex reactions such as CO and soot formation, mixing time scale and reaction time scale can be overlapped. FDS6 copes with this by the newly developed Partially-Stirred Batch Reactor model in which the degree of mixing based on mass fraction of species evolves in time at a simple subgrid environment called “mixed reactor zone” and the degree of mixing is generally dominated by turbulence [13]. As FDS6 also features improvement in the turbulence model, which provides higher resolution for a coarse mesh, mixing rate would be more correct than before when the same grid is used, which is the case of this simulation.

The FED and FEC calculation methodology in this thesis are based on the CO mass fraction. Since local mass fraction is not only 0 or 1 at the subgrid level but also can be mixed-mean value varying over time, it can be more precise than the mixture fraction model which is a simple linear combination of mass fraction of fuel and carbon-carrying combustion products, i.e. CO, CO<sub>2</sub> and soot [15]. Without implication of degree of mixing in a subgrid level, mixture fraction model may over-predict or under-predict CO and soot formation. As discussed above, taking into account that FDS6 is more enhanced in both combustion and turbulence model, FDS5 is deemed to over-predict local mass fraction of CO and soot approximately by 10% or more so that the FED and FEC level are also higher than those of FDS6 in this case study.

## 4. Furniture Fire : Mixture of different materials

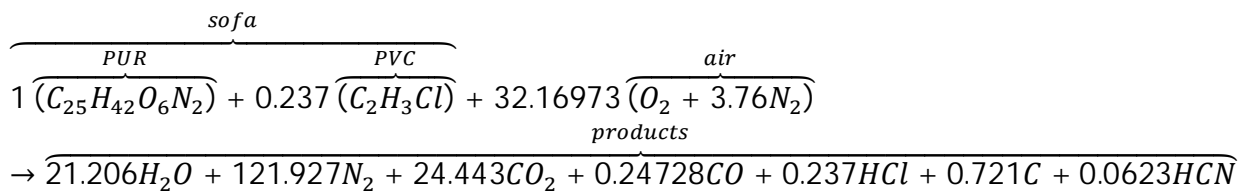
In general, the fire source or fuel in real building fire cases is not a pure material, but mostly a mixture of different materials as shown by Table 2.2. As the most common combustible items in building fire, upholstered sofa and wooden furniture were suggested in section 2.2. The FED and FEC level for those materials' fire is investigated in this section.

### 4.1 Fuel formulas

HCN is one of the secondary species in the FED formula but if once it is present in the smoke, it has an influence exponentially by the second term of the formula shown in eq. (2). Two nitrogen containing fuels as follow are addressed here to calculate FED implying HCN effect.

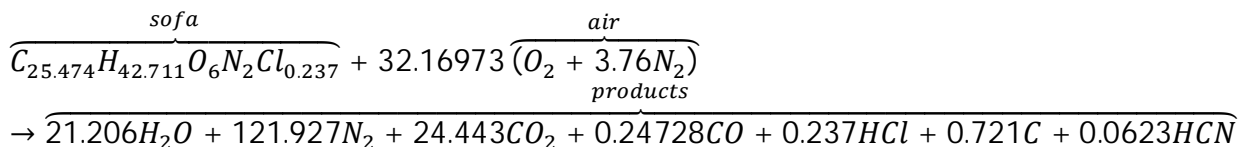
#### 4.1.1 Sofa

Due to the lumped species method of FDS6, formulating customized fuel has become possible. In reality, the combustion process of solid material mixture is quite complex and may have multiple reaction steps. But in this thesis, it is assumed for simplicity that one step reaction, well-ventilated combustion and no other species than HCl, HCN, CO, CO<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>O and soot are produced. From the description of section 2.2.2, the sofa is assumed to consist of only two materials that is PUR and PVC for simplicity. PVC is used for cushion cover and fire retardant [17] and the frame of sofa, which is steel, is not taken into account. Complete reaction stoichiometry for the sofa is specified as follows. The whole atomic balance is made by yield (pre-flashover) of each species for sofa fire given in experimental data, Table 2.4. Soot yield, fire growth rate and heat of combustion are also given in the section 2.2.2.



Based on lumped fuel composition, a single formula for the sofa can be constructed.

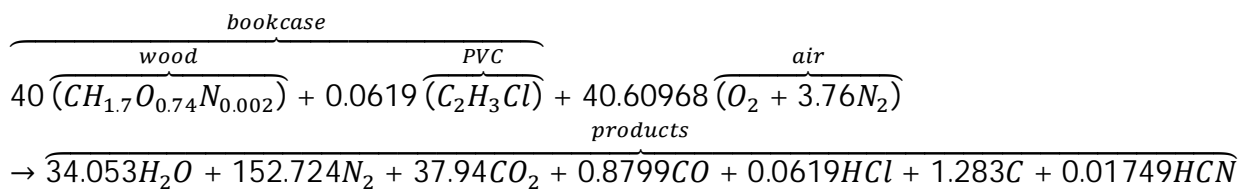
eq. (8)



As a result, the sofa, consisting of mainly polyurethane and small amount of PVC, is formulated as a single fuel that is specified in &SPEC line of FDS input file.

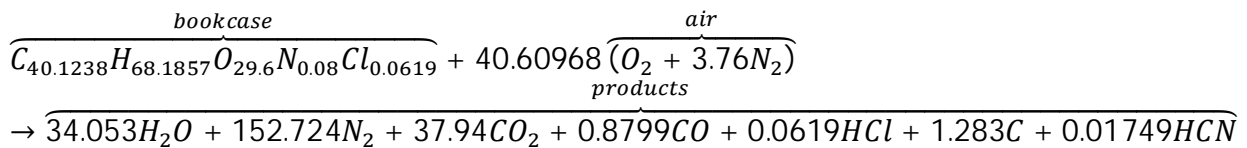
#### 4.1.2 Bookcase

The same assumption used in sofa combustion is still applied for bookcase combustion. From the description of section 2.2.2, the bookcase is assumed to consist of only two materials such as wood and PVC. Very little amount of PVC is used for finishing material over the wood, so this item is made of mainly wood. Complete reaction stoichiometry for the bookcase is specified as follows. The whole atomic balance is made by yield (pre-flashover) of each species for bookcase fire given in experimental data, Table 2.4. Soot yield is taken to be 0.015 from the other reference [19].



Based on lumped fuel composition, a single step reaction of a single formula for bookcase can be constructed.

eq. (9)



As a result, the bookcase, mainly consisting of wood, is formulated as a single fuel that is specified in &SPEC line of FDS input file. The detailed script is provided in Appendix 14.1.

The heat of combustion of wood can be various range depending on the reference, however it is known to be around 17,000kJ/kg [18] which is almost the same as that of furniture data in section 2.2.2. Therefore, for the purpose of comparison, the same heat of combustion is applied for both sofa and bookcase.

For the single formula of each fuel, the final material composition of them is determined as follows by molecular weight.

Table 4.1 Material composition of each furniture (wt.%)

Item	PUR	Wood	PVC
Sofa	97%	-	3%
Bookcase	-	99.6%	0.4%

## 4.2 FED and Verification

Even if FDS5 provides FED output, it is incomplete since it does not include the HCN term of eq. (2) and only uses CO concentration [12]. After introduction of FDS6, HCN is included in the calculation and FED value is provided for BNDF and DEVC output. Thus, it is possible to calculate FED including HCN by retrieving its mass fraction directly from FDS, which is called “direct calculation” and denoted as  $FED^*$  onward in this thesis. It is also possible by the “conversion method” based on CO yield as stated in methodology section. MATLAB is coded to do both methods in order to compare the result with each other.

### 4.2.1 Summary of Results

The results of both items are summarized as below. It can be noted that the  $FED_{total}$  level given by both methods are almost identical.

Table 4.2 FED for each furniture

OUTPUT		Sofa	Bookcase	Remark
$FED_{CO}$	Avg.	0.00153	0.00327	Max. at 270s
	Max.	0.01169	0.02557	
$FED_{HCN}$	Avg.	0.00490	0.00297	
	Max.	0.03173	0.01493	
$FED_{total}$	Avg.	0.00660	0.00631	Conversion method
	Max.	0.05089	0.04412	
$FED_{total}^*$	Avg.	0.00660	0.00631	Direct calculation
	Max.	0.05091	0.04412	

\* This means total FED value calculated by direct calculation with HCN mass fraction from FDS to be distinguished from the value calculated by conversion method.

The FED level for each person is plotted in the figures below, in which every single coloured solid line indicates FED level over the time per person. It should be noted that the detection time plus alarm time is 30 seconds in a preliminary simulation as stated in the section 2.3. Therefore, evacuation starts between at 30s and 50s depending on the pre-movement time of each person. The results show that the total FED levels of both items are far below the tenability criteria, 0.3.



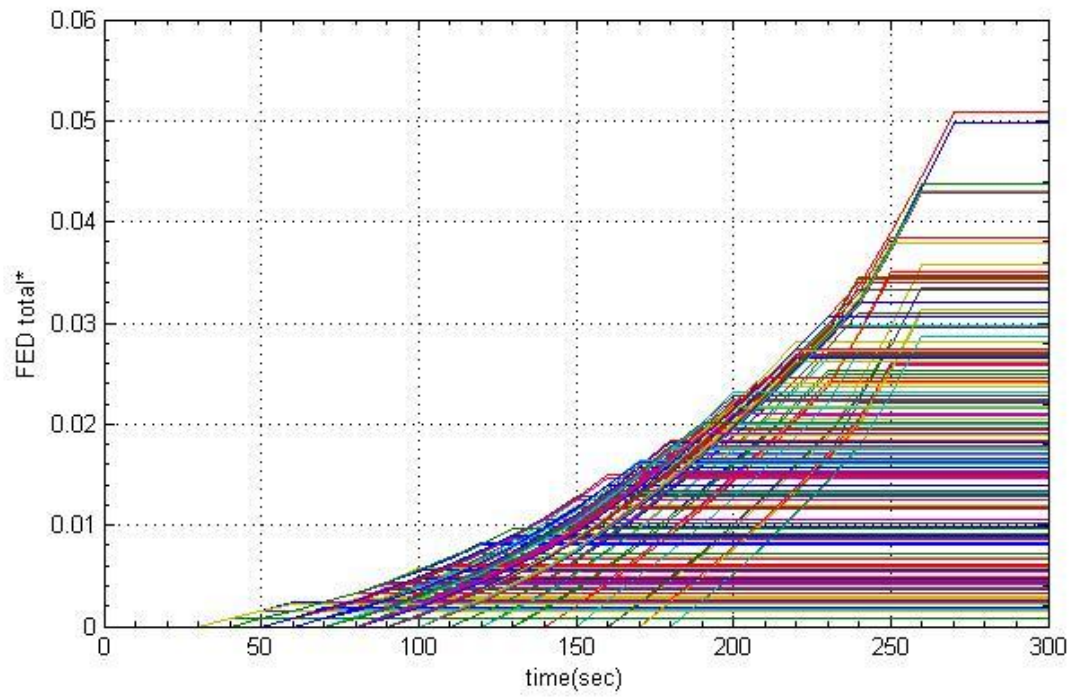


Figure 4.1 FED level for the Sofa fire

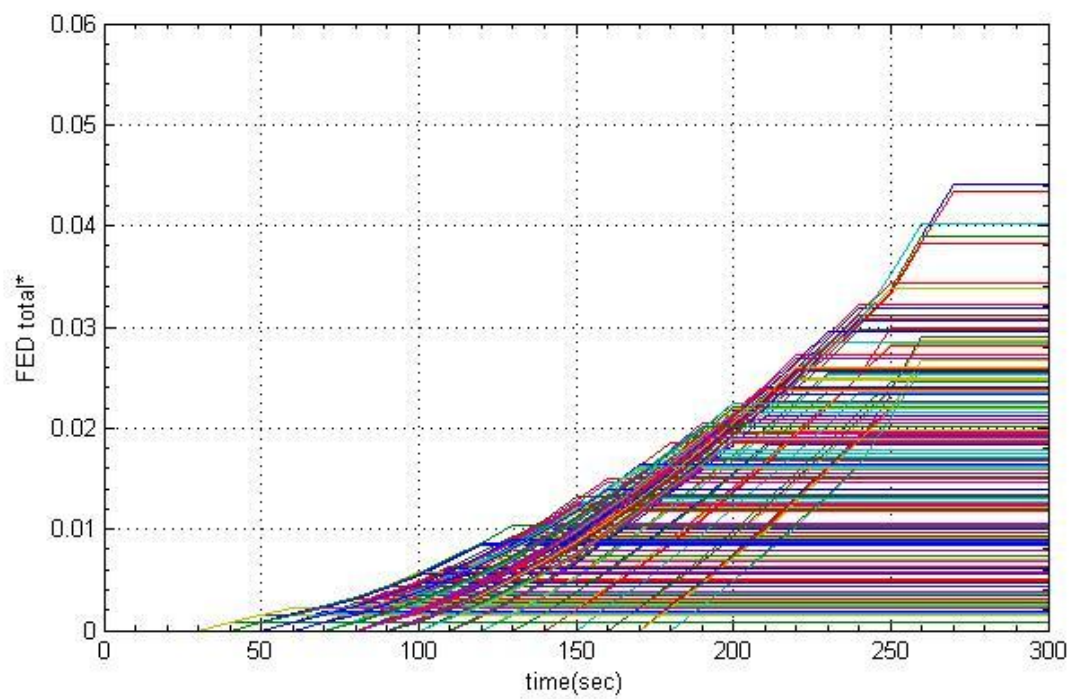


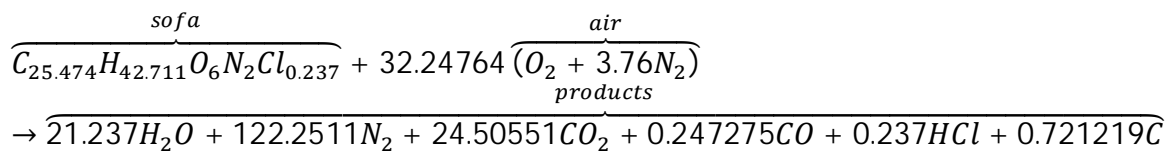
Figure 4.2 FED level for the Bookcase fire



#### 4.2.2 Influence of HCN in fire modelling

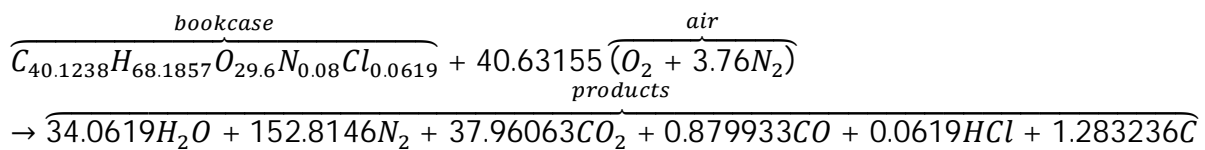
The previous results are given from the simulation based on eq. (8) and eq. (9) which includes HCN in combustion products. But it would be worthy to check how much HCN species affects the final result of FED and FEC level, because if it were not for FDS6, HCN yield could not be specified in &REAC line in FDS5. For this purpose, a reaction model without HCN is constructed with only soot and CO yield in lumped combustion products. Thus, eq. (8) for the sofa fire can be rewritten accordingly as below.

eq. (10)



In the same way, eq. (9) for the bookcase fire can be rewritten accordingly as below.

eq. (11)



In this case, only the conversion method is comparable and the results are summarized as follows. It can be noted that the effect of HCN in the reaction formula is not so much in the cases where HCN yields are relatively much lower than carbon monoxide's yield. The deviation for sofa fire is larger than bookcase fire as its HCN yield is larger by almost an order of magnitude than that of bookcase.

Table 4.3 Effect of HCN species

Item	OUTPUT		With HCN	Without HCN	Deviation
Sofa	FED <sub>total</sub>	Avg.	0.00660	0.00671	1.7%
		Max	0.05089	0.05226	2.7%
Bookcase	FED <sub>total</sub>	Avg.	0.00631	0.00630	0.2%
		Max	0.04412	0.04350	1.4%

### 4.3 FEC and FIC

The output of FEC was not provided by FDS5 before, so there was no choice but to calculate it by post-processing as described in 2.4.2. However, FDS6 provides a new built-in output; FIC which is comparable with FEC. FIC is provided as a fixed measurement in FDS, so it should be combined with people's positional information by MATLAB code. Both results are summarized and compared in the table below. It shows that all values of tenability are lower than 0.3.

Table 4.4 FEC and FIC for each furniture

OUTPUT		Sofa	Bookcase
FEC	Avg.	0.01099	0.00173
	Max.	0.22283	0.03569
FIC	Avg.	0.01221	0.00192
	Max.	0.24760	0.03969
Difference	Avg.	10%	9.9%
	Max.	10%	10%

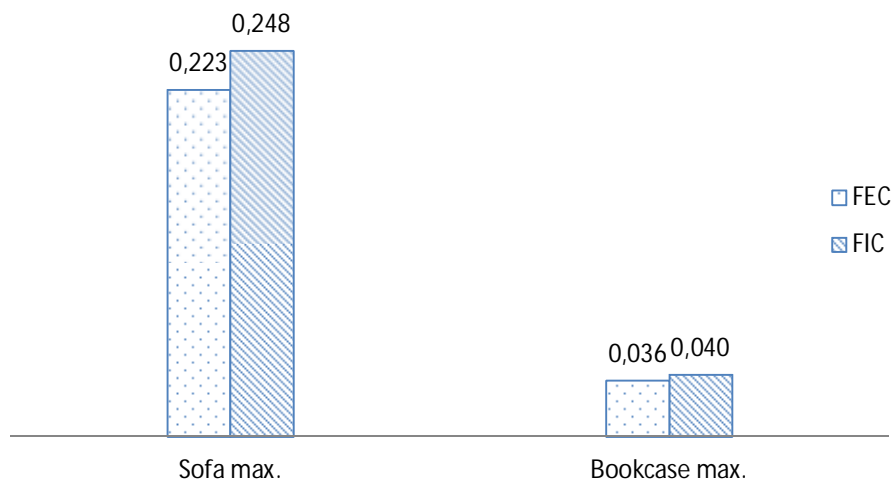


Figure 4.3 maximum FEC and FIC of each item

The FEC level for each person is provided in the following figures. The FEC of bookcase fire shows much lower level than that of sofa fire case.

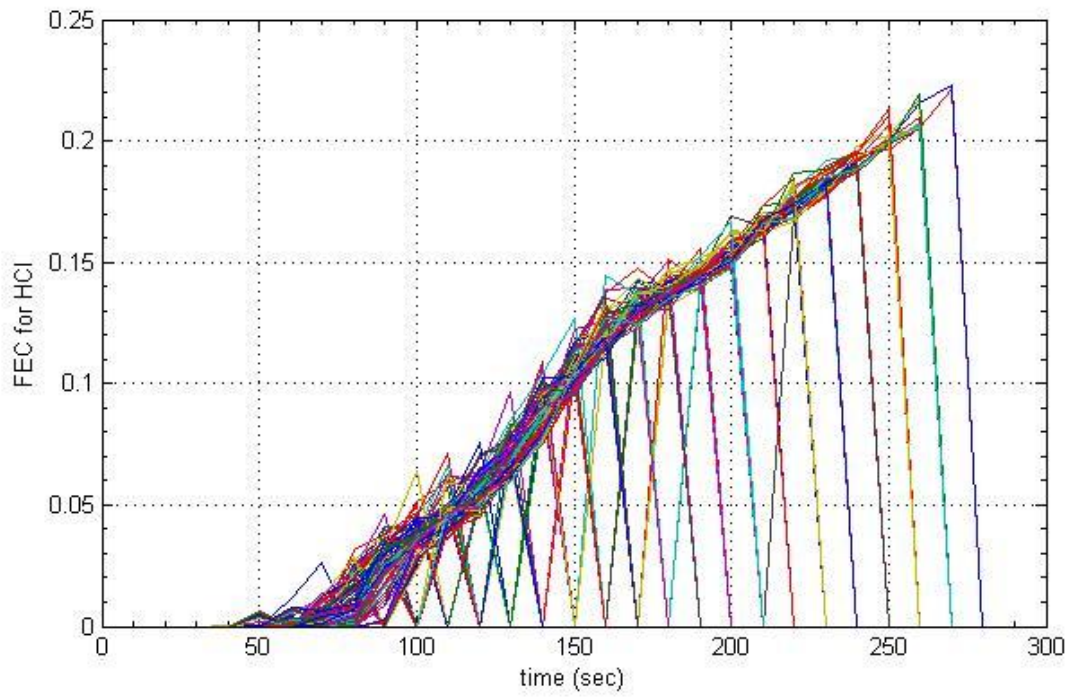


Figure 4.4 FEC level for the Sofa fire

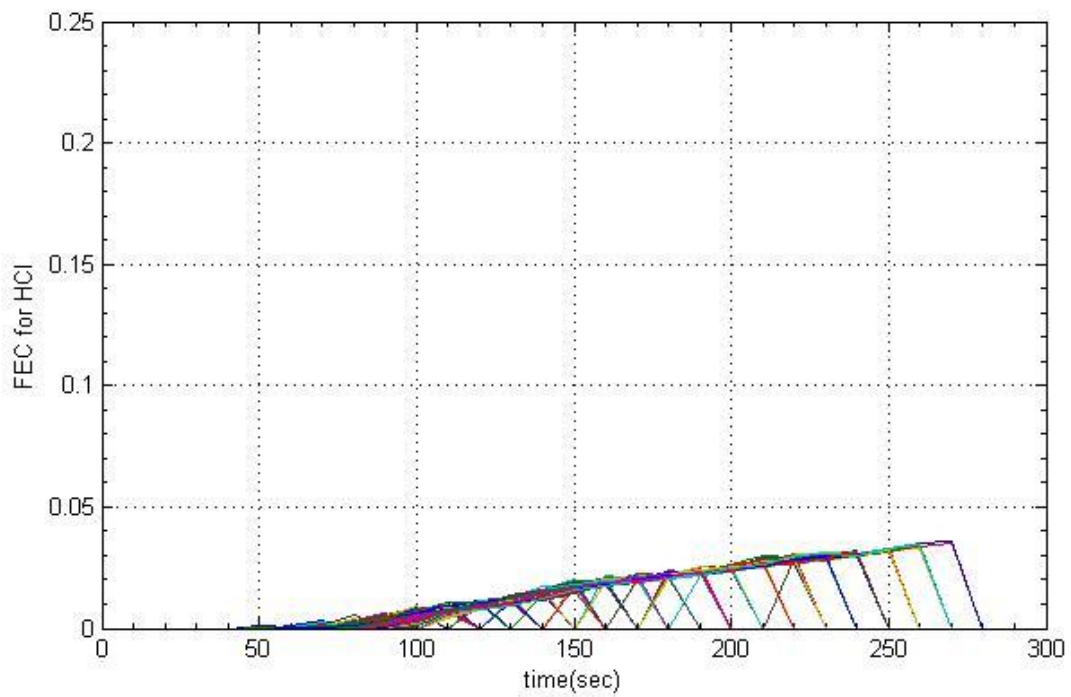


Figure 4.5 FEC level for the Bookcase fire

The FIC slice output from SMOKEVIEW of FDS is given in the following figures for each item. The height of slice is the same position, 1.6m where FEC is calculated by MATLAB, which was taken assuming mouth and nose height of people standing there.



Figure 4.6 FIC level at 1.6m high from the balcony for the Sofa fire (at 270s)



Figure 4.7 FIC level at 1.6m high from the balcony for the Bookcase fire (at 270s)

#### 4.4 Other Results

Fractional heat dose and soot concentration is summarized as follows. Both results are quite lower than the assessment criteria given in section 2.5. The fractional heat dose,  $FED_{heat}$  is found to be far below the criteria due to low temperature increase at the balcony during evacuation time.

Table 4.5 Fractional heat dose and Soot concentration

OUTPUT		Sofa	Bookcase
FED <sub>heat</sub>	Avg.	0.00559	0.00780
	Max.	0.05073	0.07153
Soot concentration (g/m <sup>3</sup> )	Avg.	0.014	0.015
	Max.	0.266	0.283

As for the visibility, according to the section 2.5, the threshold level for visibility of 10m is presented by a dashed line in the following figures. In case of sofa fire, 161 of 446 people undergo visibility problem less than 10m, and 160 people for the bookcase fire.

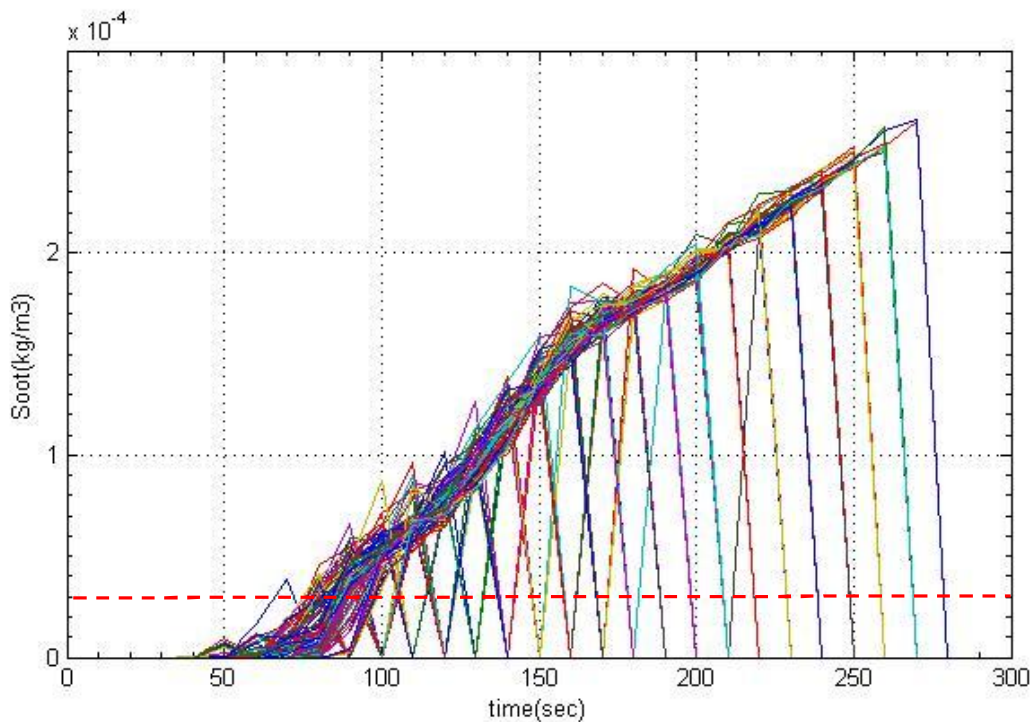


Figure 4.8 Soot concentration for the Sofa fire

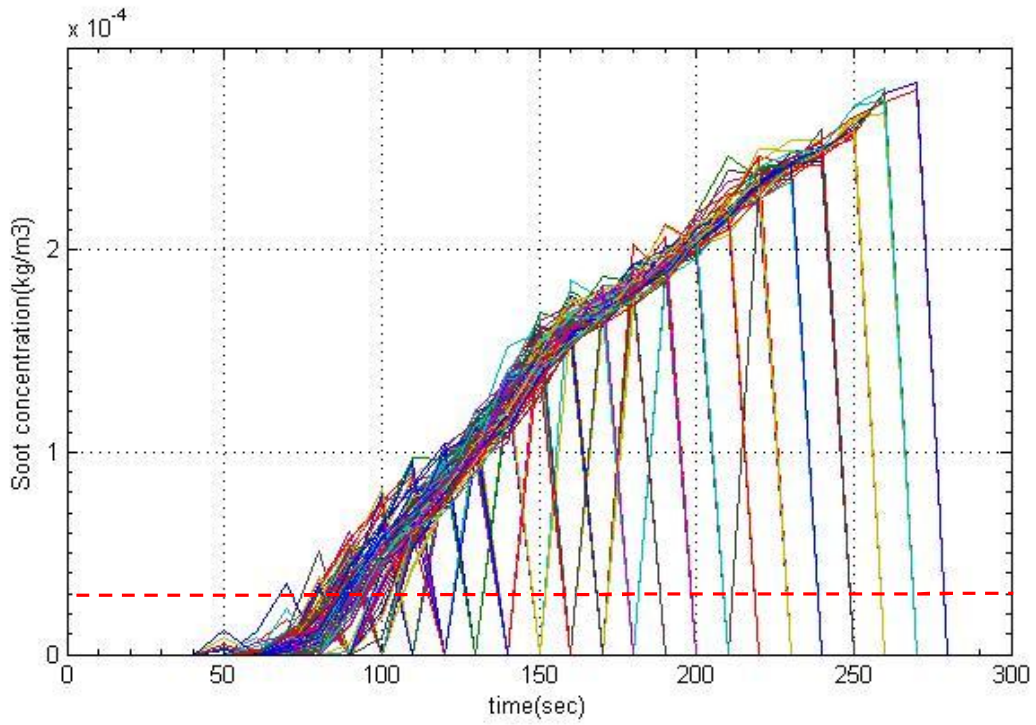


Figure 4.9 Soot concentration for the Bookcase fire

## 4.5 Discussion

The total FED level calculated by the conversion method was verified by direct calculation with HCN concentration from the FDS output and the result shows quite good agreement. In addition, it can be also compared with the FDS output of FED, which is a fixed measurement at the landing of the main stair on the first floor balcony (see Figure 2.11). Even if the figure below is information regardless of people's location, it shows very good match as well with maximum total FED level of Table 4.2, which is the value at 270s.

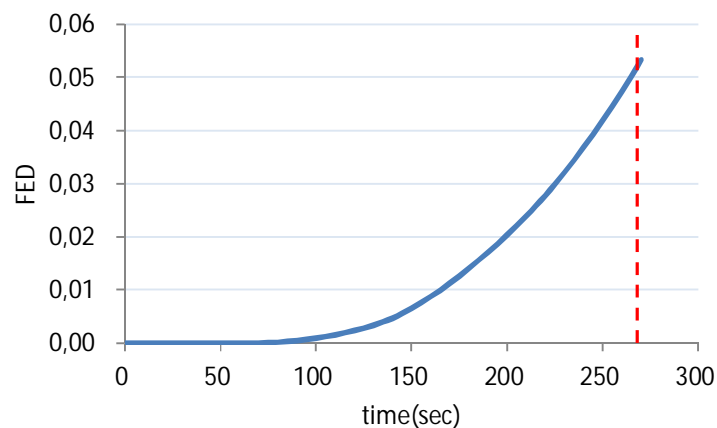


Figure 4.10 FDS output of FED: Sofa fire

The FEC level calculated by the conversion method is also verified by FDS output of FIC. Table 4.4 shows 10% difference between them, but which means quite good agreement in fact. While FEC uses 1000ppm for  $F_{HCl}$  in eq. (4), FIC uses 900ppm in its formula [11]; therefore there should be 10% difference between the two.

These good agreements are deemed to be because specifying combustion reaction of fuel in FDS6 is also based on the yields of combustion products like the conversion method which is based on the ratio of each species yield to CO yield. However, it should be noted that this coincidence is possible only if the exact stoichiometry reaction is specified including all combustion products. If some of the species are missing, for example HCN, it will make some deviation as investigated in section 4.2.2. And the higher yield of missing species is, the larger the deviation will be.

As for the sofa fire result, although HCN is secondary species having lower yield than CO by an order of magnitude, its contribution to FED is much higher than CO as shown in the figure



below. This is due to its exponential effect by definition of FED formula. But this is not the case in the bookcase fire because its HCN yield is much lower than CO by two orders of magnitude.

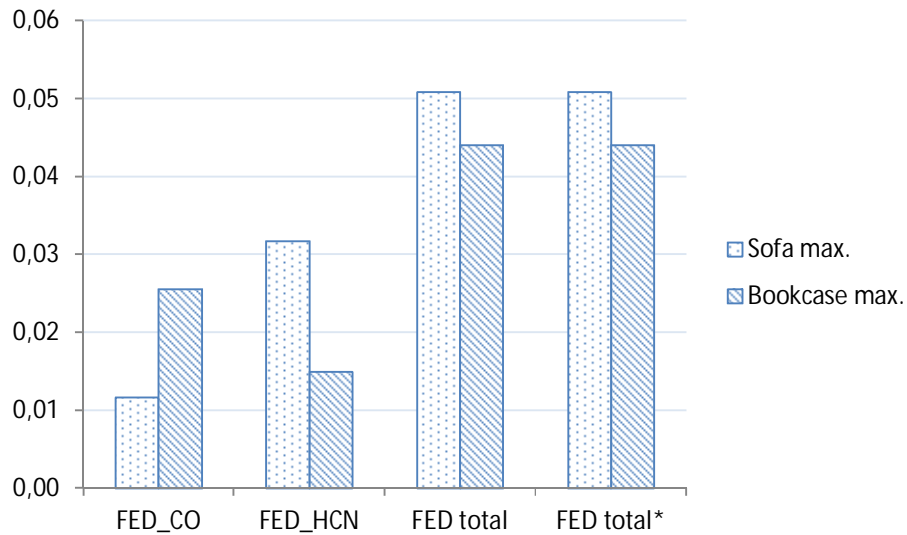


Figure 4.11 maximum FED comparison for each item

Also as HCl yield of bookcase is so lower than sofa by an order of magnitude, its FEC level is quite lower than that of sofa. In any case, the overall FED and FEC results of both sofa and bookcase are below the threshold criteria 0.3. Nonetheless, apart from the FED and FEC levels, it should be noted that the visibility problem occurs after approximately 70 seconds for both cases and one third of people suffer from the poor visibility that is less than 10m.



## 5. Sensitivity Analysis

This thesis is based on the experimental data of Table 2.4 but it also has measurement uncertainty, which is given in the table explicitly and indicates uncertainty in FED and FEC as well. For the sofa fire, one way sensitivity analysis has been performed for each yield to check how much those are influential to the FED and FEC level.

### 5.1 Result for $FED_{total}^*$

Obviously, the HCN yield is the most influential and then CO yield is secondary factor.

Table 5.1 Sensitivity result for  $FED^*$  : Sofa fire

Species	Uncertainty	Lower limit	Upper limit	Total variation
HCN	±50%	0.03722 (-27%)	0.07494 (+47%)	0.03772 (74%)
CO	±35%	0.04741 (-6.9%)	0.05472 (+7.5%)	0.00731 (14%)
HCl	±30%	0.05219 (+2.5%)	0.05173 (+1.6%)	0.05219 (2.5%)
Soot	±18%	0.04997 (-1.8%)	0.05022 (-1.4%)	0.04997 (1.8%)

Baseline value for  $FED^*$  is 0.05091

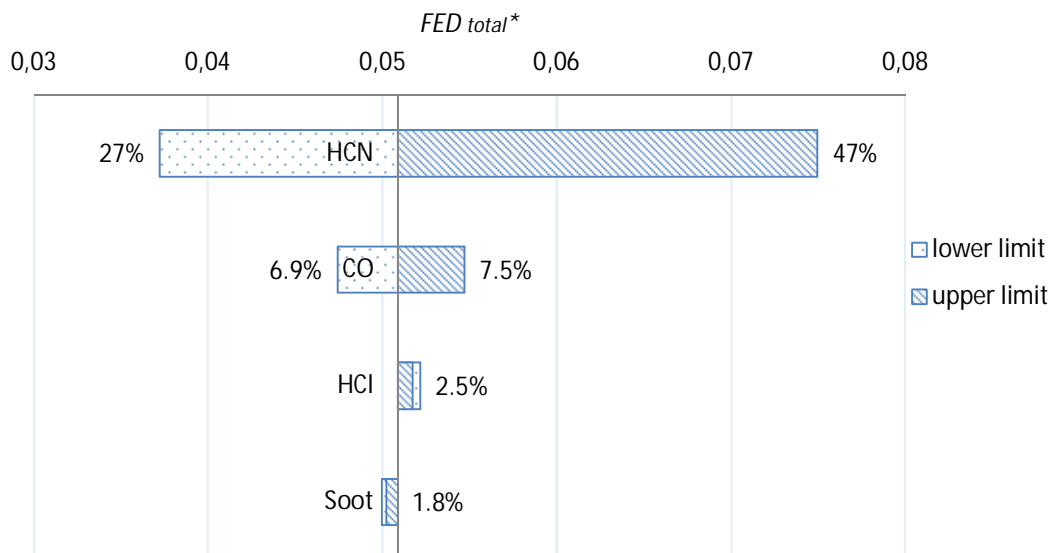


Figure 5.1 Sensitivity of  $FED^*$  to each yield : Sofa fire

It is remarkable that the effect of HCN yield is not equally proportional to both positive and negative direction. Given that the same amount of variation is applied, the effect for positive direction is much larger than negative direction. The reason will be discussed later.

## 5.2 Result for FEC

As expected, this value is most sensitive to the HCl yield's variation. Also, it can be observed that the effect of HCl yield's variation is almost equally proportional to both positive and negative direction not like the result of the *FED\**.

Table 5.2 Sensitivity result for FEC : Sofa fire

Species	Uncertainty	Lower limit	Upper limit	Total variation
HCl	±30%	0.15675 (-30%)	0.28116 (+26%)	0.12441 (56%)
HCN	±50%	0.22003 (-1.3%)	0.22785 (+2.3%)	0.00782 (3.5%)
Soot	±18%	0.22310 (+0.1%)	0.22904 (+2.8%)	0.22904 (+2.8%)
CO	±35%	0.22539 (+1.1%)	0.22491 (+0.9%)	0.22539 (+1.1%)

Baseline value for FEC is 0.22283

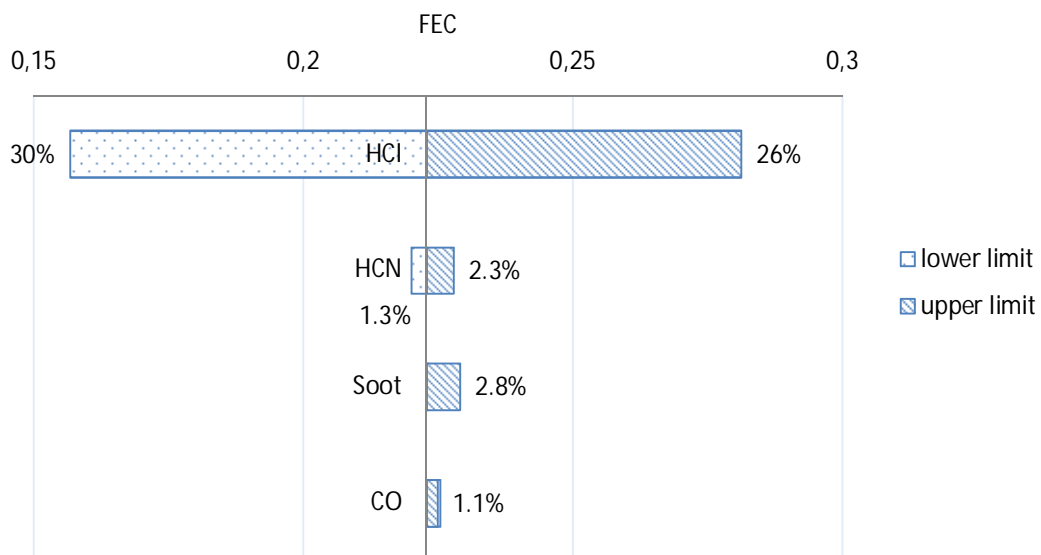


Figure 5.2 Sensitivity of FEC to each yield : Sofa fire

### 5.3 Result for FIC

As discussed in section 4.3, FIC is almost the same value as FEC except some of threshold value used in its formula, so the sensitivity results are also pretty much similar to those of FEC. However, it should be noted that the maximum variation exceeds tenability criteria of 0.3.

Table 5.3 Sensitivity result for FIC : Sofa fire

Species	Uncertainty	Lower limit	Upper limit	Total variation
HCl	±30%	0.17426 (-30%)	0.31256 (+26%)	0.13830 (56%)
HCN	±50%	0.24450 (-1.3%)	0.25319 (+2.3%)	0.00869 (3.5%)
Soot	±18%	0.24791 (+0.1%)	0.25451 (+2.8%)	0.25451 (+2.8%)
CO	±35%	0.25045 (+1.2%)	0.24992 (+0.9%)	0.25045 (+1.2%)

Baseline value for FIC is 0.24760

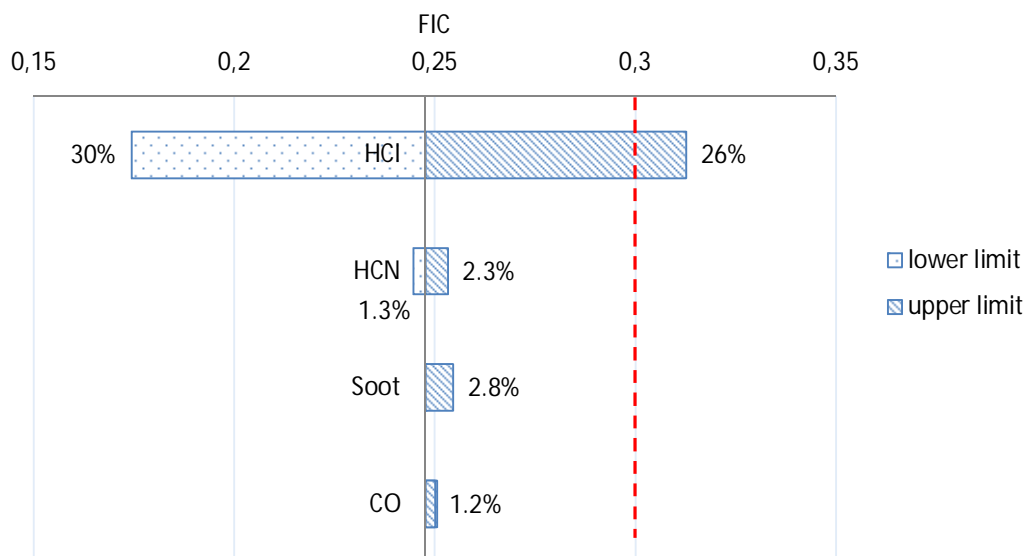


Figure 5.3 Sensitivity of FIC to each yield : Sofa fire

## 5.4 Discussion

The FED results seem to be most sensitive to variation of HCN and CO yield, which is natural since those two factors constitute FED formula eq. (2). FED appears to be not exactly proportional to variation of CO concentration though because its total variation is just 14% while CO yield varies 70% in total. Also, it can be noted that its sensitivity to HCN is almost 5 times more than CO in this simulation. This is due to the fact that HCN concentration has an exponential effect in the formula, while CO concentration contributes linearly. In addition, the exponential term of HCN concentration accounts for the reason why its effect is not equally proportional to positive and negative direction. On the other hand, HCl and soot yield has very little effect on the FED but it is not zero because their variation makes some changes in stoichiometry reaction, so that the amount of CO and HCN production varies accordingly. As for the result of the FEC, it is observed to be linearly proportional to the HCl variation in both directions, while the concentration of HCN, soot and CO has very little effect on the FEC in the same way as discussed above. Due to the nature of linear formula of FEC, its variation is almost the same amount of HCl variation since there is no other irritant gas species in this simulation. As the FIC is somewhat higher than the FEC by definition, some of occupants are found to be exposed to critical condition in case of upper limit of HCl yield as shown in the figure below. They are counted up to 7 of 446 people.

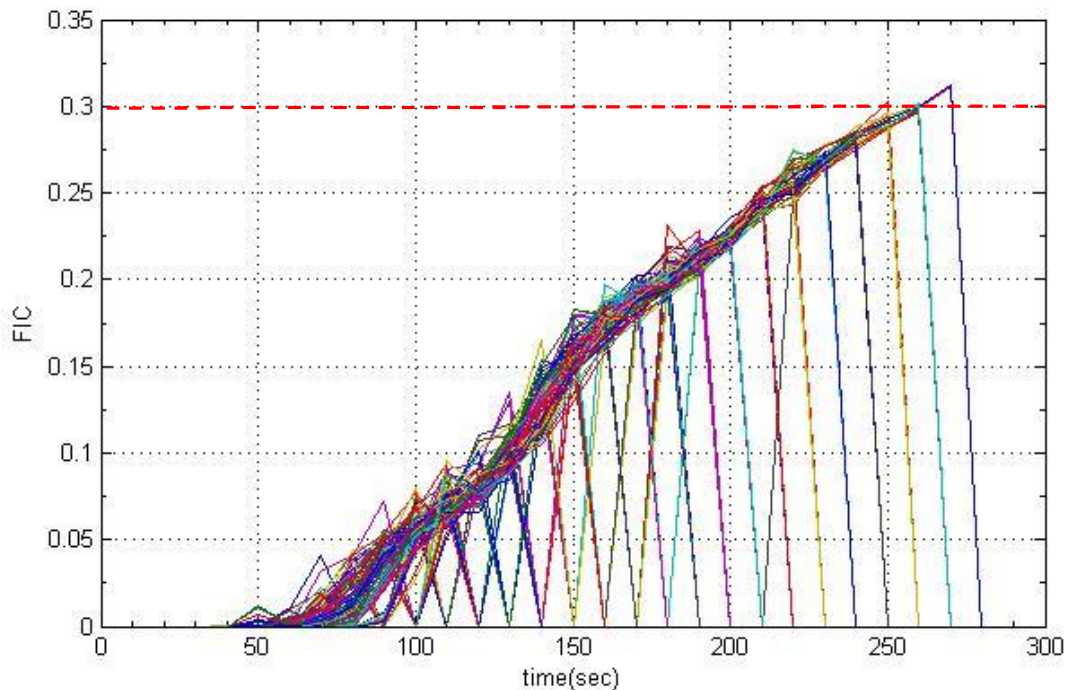


Figure 5.4 FIC for maximum HCl yield : Sofa fire

## 6. Minor Species Effect

Even though minor species such as  $\text{NO}_2$ , Acrolein ( $\text{C}_3\text{H}_4\text{O}$ ) and formaldehyde ( $\text{CH}_2\text{O}$ ) were not detected in the experiment, they were possible to exist since there were fuels containing nitrogen, i.e. polyurethane and wood. The maximum concentrations of those species, which could have been present are given in the Table 2.4. The reaction including all these minor species is so complex in reality that constructing full chemical reaction of it in FDS input would be quite difficult to be done. Therefore, with the pre-flashover yields given in Table 2.4, conversion method for each species has been used to investigate how such species have an effect on FEC level in addition to hydrogen chloride. It is considered to be reasonable since conversion method yields approximately very close result to direct calculation as shown in the section 4.2.2.

### 6.1 Results

The maximum value of total FEC level for both items' fire, and the contribution of each minor irritant gas are compared in the following figure. Maximum value is measured at the time of 270 seconds.

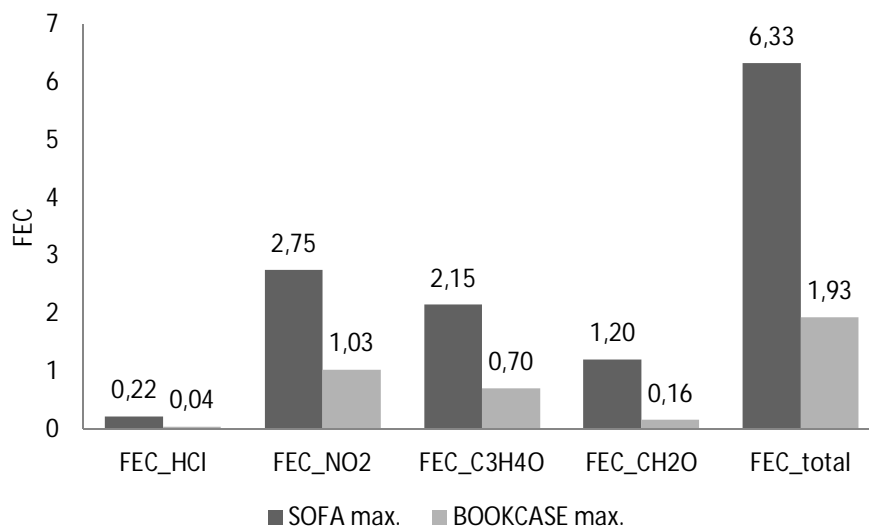


Figure 6.1 Minor species effects on FEC

Because of the very high level of FEC, a large portion of people are exposed to more than the threshold criteria of 0.3 as shown in the following table.

Table 6.1 People affected by irritant gases

Item	FEC level	Number of people affected
Sofa	$\geq 0.3$	169
	$\geq 1.0$	149
Bookcase	$\geq 0.3$	149
	$\geq 1.0$	107

## 6.2 Discussion

It should be noted that the yields of minor gases used in this simulation are not the experimental measurement but calculated upper limit of existence [4], so the FEC level of these gases are relatively much higher than that of HCl provided in Table 4.4. However, it is still valuable to compare the sofa fire with the bookcase fire and look into the contribution of each species.

It is observed that overall FEC level of the sofa fire is higher than the bookcase fire and  $\text{NO}_2$  is most contributing among three minor species for both items. This is clearly due to the relatively higher production yield of this gas than others, and furthermore due to its relatively lower threshold concentration in denominator of FEC formula. These minor species would play more important role especially for the bookcase fire where HCl yield is considerably lower than the sofa fire.

When these FEC levels are compared with threshold criteria, more than 30% of total people are exposed to tenability limit for both items and a number of people of them are even exposed to complete incapacitation level of 1.0.

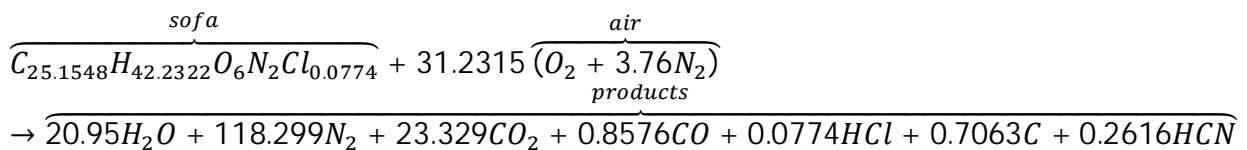
## 7. Post-Flashover Fire

Yields of combustion products are not constant in fact, but variable depending on the ventilation condition at a certain time, namely it is a function of equivalence ratio [19], [20]. In this thesis, FDS simulations are performed basically under the assumption of large-scale, well-ventilated condition with pre-flashover yields. Under-ventilated fire phenomena are quite complex that it is not easy to be calculated by fire simulations [22]. But, it would be necessary to check post-flashover fire since large portion of fire victims comes from post-flashover fires.

### 7.1 Fuel formula

For the comparison with pre-flashover fire, post-flashover yields of each item in Table 2.4 are used for combustion modelling. In this section, it is simulated only for sofa fire because CO and HCl yields of bookcase are the same order of magnitude as sofa except HCN, thus the result for bookcase fire can be easily presumed with the sofa fire results. eq. (8) is reconstructed with post-flashover yield of CO, HCN and HCl as follows.

eq. (12)



### 7.2 Results

The simulation result done by above combustion reaction is summarized as follows.

Table 7.1 FED and FEC level for post-flashover fire : Sofa fire

OUTPUT		Pre-flashover	Post-flashover
FED <sub>CO</sub>	Avg.	0.00153	0.00546
	Max.	0.01169	0.04218
FED <sub>HCN</sub>	Avg.	0.00490	0.07875
	Max.	0.03173	1.16027
FED <sub>total</sub> *	Avg.	0.00660	0.09056
	Max.	0.05091	1.53847
FEC	Avg.	0.01099	0.00370
	Max.	0.22283	0.07271

Above table can be easily analyzed graphically in the figure below.

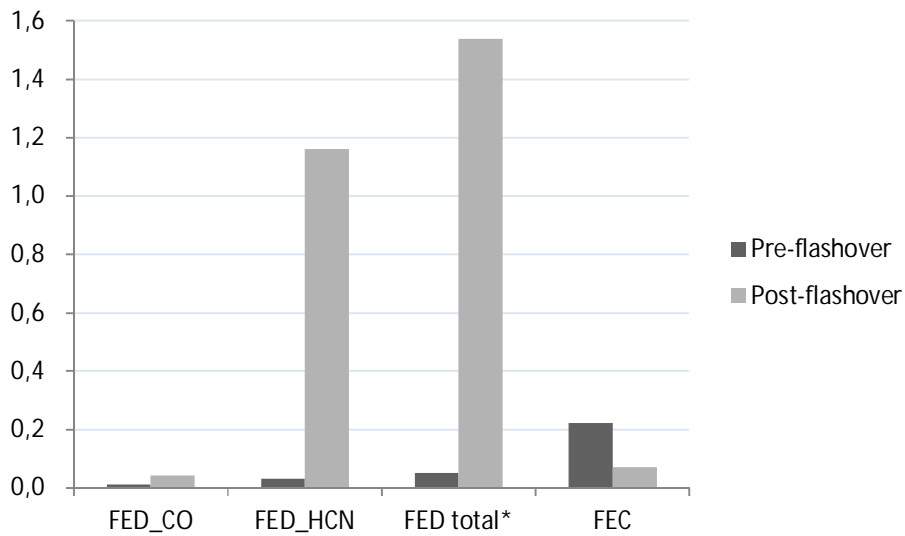


Figure 7.1 comparison of pre- and post-flashover fire for maximum levels

Total FED level for each person is plotted in the figure below and it shows that much more people are exposed to the level exceeding 0.3 and even 1.0.

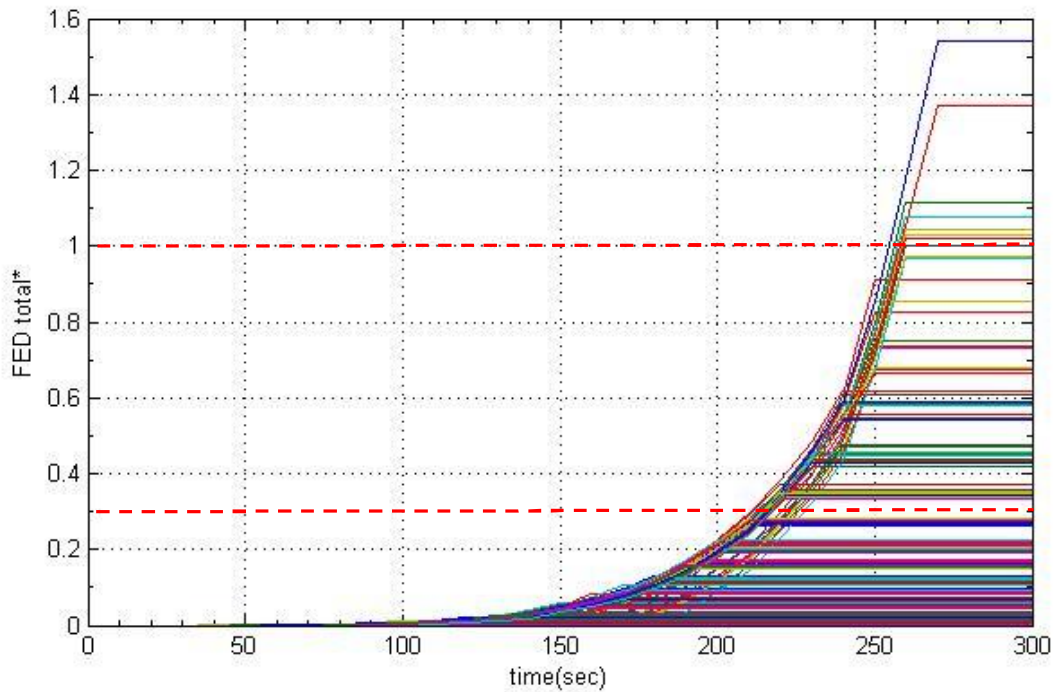


Figure 7.2 FEDtotal\* for post-flashover yield of sofa fire



### 7.3 Discussion

It can be noted that there is a considerable increase in each FED level in case of post-flashover fire, especially remarkable in  $FED_{HCN}$ . Even if both CO and HCN yield is 3 to 4 times higher than their pre-flashover yield, FED level for HCN is increased almost 40 times higher than before due to its exponential effect. This ends up in a total FED level exceeding tenability criteria and even more than the incapacitation level. The numbers of people who are exposed to those levels are given in the table below. On the other hand, it is observed that the FED level becomes lower than the pre-flashover fire due to lower HCl yield. A disproportionate release of fire retardant during the early burning probably accounts for the reason [4].

Table 7.2 People affected by asphyxiant gases : Sofa fire

Item	$FED_{total}^*$	Number of people affected
Sofa	$\geq 0.3$	47
	$\geq 1.0$	7

## 8. Multiple Fuels Fire

If once stoichiometry reaction of each fuel is specified with species yields, it is also possible to combine multiple fuels and predict their combustion products even though yields information of it for the combined fuel is not given, which is enabled by lumped species method. The key assumption made in lumping primitive species is that the new species groups transport and react together. In this section, combined burning of two fuels is investigated with the reaction formulas already determined in the section 4.1.

### 8.1 Modelling of fuel combination

Modelling of combined burning of two items can be readily constructed by putting two chemical reactions together in FDS input as shown below.

```
--- fuel combination ---
&SPEC ID = 'SOFA',      FORMULA = 'C25.474H42.711O6N2C10.237' /
&SPEC ID = 'BOOKCASE', FORMULA = 'C40.1238H68.1857O29.6N0.08C10.0619' /
&SPEC ID = 'OXYGEN',      LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'NITROGEN',    LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'HYDROGEN CHLORIDE', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'WATER VAPOR', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'CARBON MONOXIDE', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'CARBON DIOXIDE', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'SOOT',        LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'HYDROGEN CYANIDE', LUMPED_COMPONENT_ONLY = .TRUE. /

&SPEC ID = 'AIR', BACKGROUND=.TRUE.,
  SPEC_ID(1) = 'OXYGEN', VOLUME_FRACTION(1)= 1,
  SPEC_ID(2) = 'NITROGEN', VOLUME_FRACTION(2)= 3.76 /

&SPEC ID = 'PRODUCTS_SOFA',
  SPEC_ID(1) = 'WATER VAPOR',      VOLUME_FRACTION(1) = 21.205835,
  SPEC_ID(2) = 'NITROGEN',         VOLUME_FRACTION(2) = 121.9270245,
  SPEC_ID(3) = 'CARBON DIOXIDE',   VOLUME_FRACTION(3) = 24.44317625,
  SPEC_ID(4) = 'CARBON MONOXIDE',  VOLUME_FRACTION(4) = 0.247275,
  SPEC_ID(5) = 'HYDROGEN CHLORIDE', VOLUME_FRACTION(5) = 0.237,
  SPEC_ID(6) = 'SOOT',             VOLUME_FRACTION(6) = 0.72121875,
  SPEC_ID(7) = 'HYDROGEN CYANIDE', VOLUME_FRACTION(7) = 0.06233 /

&SPEC ID = 'PRODUCTS_BOOKCASE',
  SPEC_ID(1) = 'WATER VAPOR',      VOLUME_FRACTION(1) = 34.053155 ,
  SPEC_ID(2) = 'NITROGEN',         VOLUME_FRACTION(2) = 152.7236704 ,
  SPEC_ID(3) = 'CARBON DIOXIDE',   VOLUME_FRACTION(3) = 37.94314085 ,
  SPEC_ID(4) = 'CARBON MONOXIDE',  VOLUME_FRACTION(4) = 0.879933214 ,
  SPEC_ID(5) = 'HYDROGEN CHLORIDE', VOLUME_FRACTION(5) = 0.0619 ,
  SPEC_ID(6) = 'SOOT',             VOLUME_FRACTION(6) = 1.283235938 ,
  SPEC_ID(7) = 'HYDROGEN CYANIDE', VOLUME_FRACTION(7) = 0.01749 /
```

```

&REAC ID = 'PUR'
  FUEL = 'SOFA',
  SPEC_ID_NU = 'SOFA','AIR','PRODUCTS_SOFA', NU=-1,-32.16973125,1,
  HEAT_OF_COMBUSTION = 17040., CHECK_ATOM_BALANCE=.TRUE. /

&REAC ID = 'WOOD'
  FUEL = 'BOOKCASE',
  SPEC_ID_NU = 'BOOKCASE','AIR','PRODUCTS_BOOKCASE', NU=-1,-40.60968496,1,
  HEAT_OF_COMBUSTION = 17040., CHECK_ATOM_BALANCE=.TRUE. /

-- 416.5kW/17040(kJ/kg) for each fuel --
&SURF ID='BURNER', SPEC_ID(1)='SOFA', MASS_FLUX(1)=0.0244425, RAMP_MF(1)='PUR',
  SPEC_ID(2)='BOOKCASE', MASS_FLUX(2)=0.0244425, RAMP_MF(2)='WOOD' /

```

Figure 8.1 Input for combined burning of two items

In addition, the portion of each fuel taking part in the combustion should be designated by MASS\_FLUX as shown in the figure above that is the example case of half-and-half combination of sofa and bookcase. And then heat release rate would be specified by RAMP\_MF consistent with single item's fire. The peak heat release rate is still 1MW as before for a fair comparison.

## 8.2 Results

Three different combinations of sofa and bookcase in the same fire position have been simulated and the results are presented in the figures below. As mentioned before, it is not possible to determine FED level by the conversion method since there is no experimental yield data available for this combined burning case. Therefore, the FED results are predicted by only direct calculation of mass fraction output from FDS.

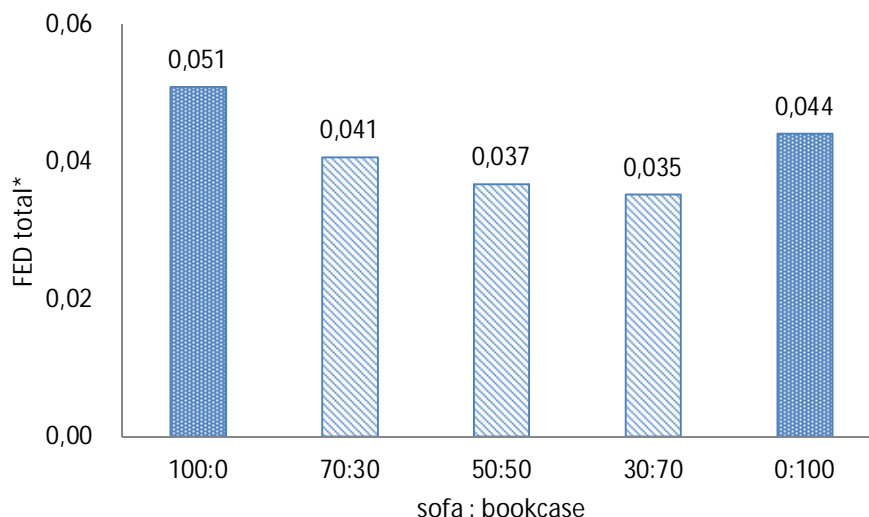


Figure 8.2 Maximum *FED total\** for various combinations of items

Also for the same reason, direct output of FIC is only available, while FEC is not.

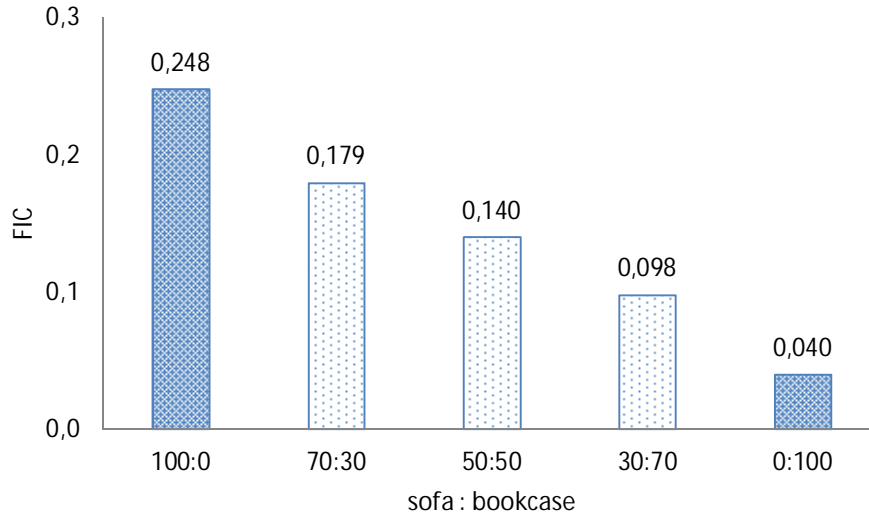


Figure 8.3 Maximum FIC for various combinations of items

In the above figures, the dark bars at both ends represent the cases for single sofa fire and single bookcase fire respectively which are already presented in the section 4.

### 8.3 Discussion

It can be noted that  $FED_{total}^*$  levels for combined burning items are not in between two single items' fire cases but even lower than the single bookcase fire, while FIC level is varying almost linearly in between the two single items' fire results. This is due to the fact that FED level is not a linear function of concentration because of the HCN term. Though the mass flux portion of sofa decreases linearly, the overall FED level decreases exponentially. On the other hand, FIC and FEC are linear functions of species concentration.

When sofa and bookcase are involved in a fire at the same time, it means that polyurethane, wood and PVC is burning together in terms of material composition. As these materials are very common in ordinary building fire, it would be very useful to predict toxicity effect of the fire case including these three representative materials if only each material's composition in the fuel mixture is known.

## 9. Grid Dependency

In order to look into the influence of grid resolution on the final FED and FEC results, a grid sensitivity study has been performed as follows.

### 9.1 Mesh Refinement

All the simulations in this thesis were performed by the mesh structure given in the section 2.2.3. So far 3.3 million cells have been used as the standard mesh. Even though the space nearby fire source used fine grid, atrium and the balcony was still modelled with medium grid (see Table 2.5). As the grid consists of different mesh sizes, refinement is also partially applied, not entirely or uniformly. The most important area of interest is the balcony of the first floor where the FED and FEC is calculated, thus firstly the mesh including the balcony is refined to the fine mesh of 5cm and then the whole atrium is refined as such for the comparison. The detailed mesh information generated is given in the Appendix 14.3. For this processing, MATLAB script should be modified accordingly as well.

Table 9.1 mesh refinement

Resolution	N	2N	4N
No. of cells	3.3M	6.2M	13M
No. of processors	8	16	16
No. of meshes	10	17	31
No. of fine mesh [5cm]	5	13	29
No. of medium mesh [10cm]	3	3	1
No. of coarse mesh [20cm]	2	1	1

Table 9.2 mesh description

Resolution	Fine mesh	Medium mesh	Coarse mesh
N	nearby fire & plume	atrium, balcony	kitchen & serving below the balcony*
2N	nearby fire & plume balcony	atrium below the balcony*	kitchen & serving
4N	nearby fire & plume balcony, atrium	below the balcony*	kitchen & serving

\* on the ground floor

The kitchen and serving area is not refined because it is not in the way of smoke spread to the balcony nor important due to its proximity to the secondary exit (see Figure 2.10).

## 9.2 Result

Grid dependency check was performed for the sofa fire case. This work is computationally quite demanding and could be done by running 16 processors at once in Alarik cluster of LUNARC system. The computing time is not linearly proportional as the number of cells is doubled. The deviation between two grids appears to be very small as shown in the following table. Due to such a small deviation, further data processing for 4N grid case is omitted in the table below.

Table 9.3 Grid dependency result : Sofa fire

OUTPUT		N*	2N	Deviation
FED <sub>total</sub>	Avg.	0.00660	0.00658	0.3%
	Max.	0.05089	0.04975	2.3%
FED <sub>total</sub> *	Avg.	0.00660	0.00658	0.3%
	Max.	0.05091	0.04977	2.3%
FEC	Avg.	0.01099	0.01098	0.1%
	Max.	0.22283	0.21680	2.8%
FIC	Avg.	0.01221	0.01220	0.1%
	Max.	0.24760	0.24090	2.8%
computing time		4days	11days	-

\* result from Table 4.2 and Table 4.4

Following figures show the DEVC outputs of FDS6 for each grid, which were measured at the landing of the main stair on the balcony of the first floor (see Figure 2.11).

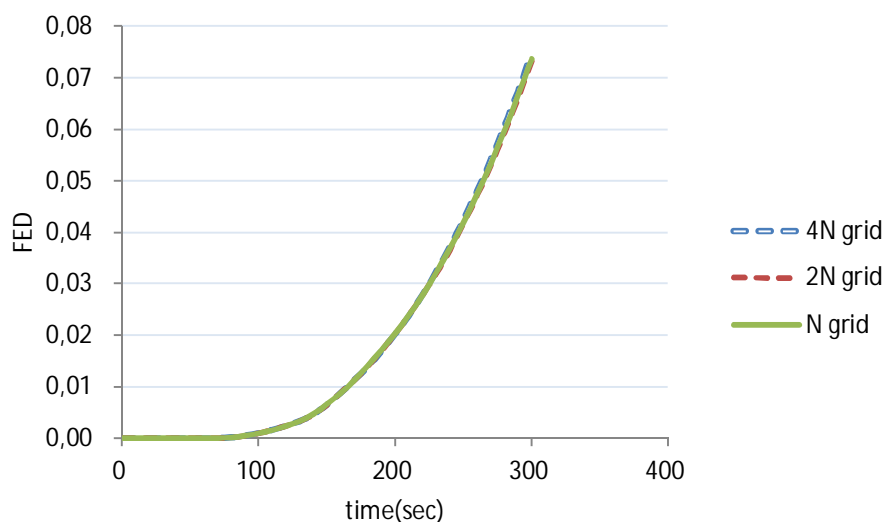


Figure 9.1 FED output of FDS6

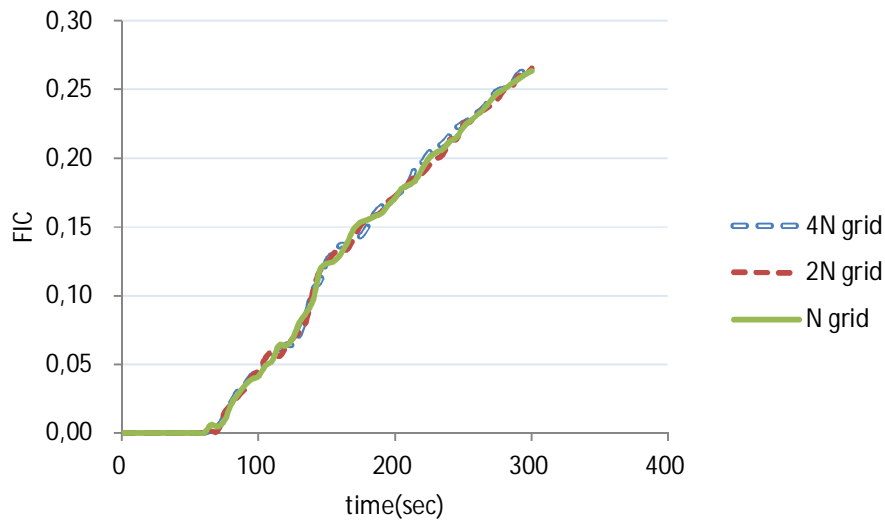


Figure 9.2 FIC output of FDS6

### 9.3 Discussion

By refining the balcony area, the total number of computational cells is doubled and the computing time takes almost 3 times longer than that of standard grid. In case of 4N grid for refining atrium as well, the computing time was 20 days. The computing time is not exactly proportional to the increase of cells because the whole grid is not uniform and the refinement is applied partially. Despite of this refinement, the difference in the final results seems to be very little, namely the maximum level of FED and FEC for each person shows less than only 3 % deviation. This means that the standard grid which has been used in this thesis is not so sensitive to a finer grid that it is quite a reasonable setup in terms of the computing time and grid dependency. Even though the whole atrium is refined to fine mesh, which means almost the entire building is modelled with fine mesh, the final results do not show any significant difference in the above two figures.

## 10. Conclusions

The main findings, conclusions and future work to be needed are summarized as follows.

1. FED and FEC calculation results of FDS5 are compared with FDS6 by the conversion method and it is concluded that FDS5 overestimates about 10% higher than FDS6 on average in case of the cable fire performed in previous studies. The possible reason can be found in the enhanced combustion model of FDS6, i.e. "partially-Stirred Batch Reactor Model" for soot and carbon monoxide formation on which conversion method is based.
2. In order to evaluate FED and FEC level for the fire of common building furniture, a mixture of different two materials is formulated as a single fuel and its stoichiometry reaction is constructed. For the exact calculation of FED, CO<sub>2</sub> concentration check process and hyperventilation factor was added to MATLAB code. By preliminary simulation, it was found that it makes approximately 16% increase in maximum total FED for the sofa fire case.
3. For the sofa fire and bookcase fire, the results of conversion method were well verified by direct calculation from output of FDS6, which was not possible in the previous version of FDS. For the verification, HCN mass fraction and FIC output are retrieved from the simulation result of FDS6. The comparison of both results shows quite good agreement when all the combustion products are specified in the reaction formula. This means that as of FDS6 it is possible to calculate FED and FEC without conversion factor if only the stoichiometry reaction formula of fuel is fully constructed with every species yield involved.
4. When comparing the sofa fire with the bookcase fire, the former showed higher FED and FEC levels than the latter due to its higher HCN and HCl yield. Both FED and FEC levels of furniture fires remain below tenability criteria but sensitivity analysis reveals that FIC level of sofa fire can exceed 0.3 when taking measurement uncertainties into account. Also it was found that FED level is much more sensitive to increasing variance of HCN yield than decreasing of it.
5. For both the sofa fire and the bookcase fire, mainly the visibility issue appears to be the first criteria for the determination of tenability condition in this case study, although all the other assessment parameters remain below the criteria.
6. The FEC level of a halogenated cable fire is higher than sofa fire due to its high HCl yield but the FED level is the other way around. Despite of higher CO yield of the cable fire by an order of magnitude, the FED level of the sofa fire is even higher than that of the cable fire by an order of magnitude because of the exponential effect of the HCN concentration on the FED which is not included in the cable fire.



7. Considering minor species which is not detected in the experimental measurement, the conversion method is still a good alternative to investigate the contribution of those species instead of constructing quite complex reaction formula involving all of them. In this case study of furniture fire,  $\text{NO}_2$  is most influential among them.
8. When it comes to post-flashover conditions, the FED level appears to be quite dominant for tenability assessment rather than FEC as CO and HCN formation is increasing when the fire is under-ventilated, while HCl yield behaves in the other way around or independent of ventilation [7], [20]. Exponential increase of  $\text{FED}_{\text{HCN}}$  coupled with hyperventilation effect accounts for this high level of FED, and thus some people are found to be exposed to critical conditions.
9. With chemical reactions formulated for each single item, it is possible to predict FED and FEC level for the combination of multiple items. Combined fires involving sofa and bookcase with a few compositional variations were demonstrated, which imply most common materials in typical building fires, i.e. polyurethane, wood and PVC.
10. The medium mesh of the balcony area and the atrium was refined to the fine mesh for the grid dependency check. The result shows that despite of doubled mesh cells and 4 times more cells, the final results of the FED and FEC are not sensitive to the finer mesh, thus the original grid is concluded to be a reasonable setup for this case study.

## 11. Further Research

This thesis has been performed with the results of a single evacuation simulation package, SIMULEX and there are several complicated procedures to get the final results of FED and FEC implying combination of evacuation result and FDS result in a way of post-processing, which takes more time and efforts. It would be interesting to perform these calculations with other evacuation simulation package, for example FDS+EVAC, and compare the results with each other.

FDS+EVAC has an advantage in that it can combine CFD and evacuation simulation in one package without post-processing. This thesis also intended to compare the result with it but it was not possible because as of April 2014, FDS+EVAC is still based on FDS5, so it is not yet officially updated to provide FED per person including HCN term and FIC as built-in OUTPUTs. If it is renewed being consistent to FDS6, it is expected to provide more opportunities to do further comparable research with this thesis on determination of FED and FEC level in the building fires.

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Bjarne Husted            *Associate professor, Lund University*

Jonathan Wahlqvist      *PhD student, Lund University*

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## 14. Appendices

FDS input scripts used for CFD simulations and MATLAB codes for FED and FEC calculation are provided as follows.

### 14.1 FDS input scripts

#### 14.1.1 Sofa fire

Sofa fire in EC3 (mpi setup)

```
&HEAD CHID='s6', TITLE='Sofa' / fine grid run

--- meshes ---

&MESH IJK= 72, 40,144, XB= 1.8, 5.4, 6.2, 8.2, -0.2, 7.0 , MPI_PROCESS=0 / Mesh 1 410,000 cells
&MESH IJK= 72, 40,144, XB= 1.8, 5.4, 8.2, 10.2, -0.2, 7.0 , MPI_PROCESS=1 / Mesh 2 410,000 cells
&MESH IJK= 54,120, 72, XB= 0.0, 5.4, 10.2, 22.2, -0.2, 7.0 , MPI_PROCESS=2 / Mesh 3 460,000 cells
&MESH IJK= 54,128, 72, XB= 0.0, 5.4, 22.2, 35.0, -0.2, 7.0 , MPI_PROCESS=3 / Mesh 4 500,000 cells
&MESH IJK= 72, 72, 80, XB= 5.4, 9.0, 4.6, 8.2, 3.0, 7.0 , MPI_PROCESS=4 / Mesh 5 410,000 cells
&MESH IJK= 72, 72, 80, XB= 5.4, 9.0, 8.2, 11.8, 3.0, 7.0 , MPI_PROCESS=5 / Mesh 6 410,000 cells
&MESH IJK= 36,250, 40, XB= 5.4, 9.0, 11.8, 36.8, 3.0, 7.0 , MPI_PROCESS=6 / Mesh 7 360,000 cells
&MESH IJK= 36, 80, 96, XB= 0.0, 1.8, 6.2, 10.2, -0.2, 4.6 , MPI_PROCESS=7 / Mesh 8-1 270,000 cells
&MESH IJK= 18,162, 16, XB= 5.4, 9.0, 4.6, 37.0, -0.2, 3.0 , MPI_PROCESS=8 / Mesh 8-2 50,000 cells
&MESH IJK= 54, 60, 15, XB= 9.0, 19.8, 0.0, 12.0, -0.2, 2.8 , MPI_PROCESS=9 / Mesh 8-3 50,000 cells

--- simulation time ---

&TIME T_END=300.0 /

--- default values and models ---

&MISC SURF_DEFAULT='WALL1', SUPPRESSION=.FALSE. / Important! No suppression included.

&MISC RESTART=.TRUE. /

--- My fuel ---

&SPEC ID = 'SOFA', FORMULA = 'C25.474H42.711O6N2CI0.237' /
&SPEC ID = 'OXYGEN', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'NITROGEN', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'HYDROGEN CHLORIDE', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'WATER VAPOR', LUMPED_COMPONENT_ONLY = .TRUE. /
```

```

&SPEC ID = 'CARBON MONOXIDE', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'CARBON DIOXIDE', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'SOOT',          LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'HYDROGEN CYANIDE', LUMPED_COMPONENT_ONLY = .TRUE. /

&SPEC ID = 'AIR', BACKGROUND=.TRUE.,
  SPEC_ID(1) = 'OXYGEN', VOLUME_FRACTION(1)= 1,
  SPEC_ID(2) = 'NITROGEN', VOLUME_FRACTION(2)= 3.76 /
&SPEC ID = 'PRODUCTS',
  SPEC_ID(1) = 'WATER VAPOR',    VOLUME_FRACTION(1) = 21.205835,
  SPEC_ID(2) = 'NITROGEN',      VOLUME_FRACTION(2) = 121.9270245,
  SPEC_ID(3) = 'CARBON DIOXIDE', VOLUME_FRACTION(3) = 24.44317625,
  SPEC_ID(4) = 'CARBON MONOXIDE', VOLUME_FRACTION(4) = 0.247275,
  SPEC_ID(5) = 'HYDROGEN CHLORIDE', VOLUME_FRACTION(5) = 0.237,
  SPEC_ID(6) = 'SOOT',          VOLUME_FRACTION(6) = 0.72121875,
  SPEC_ID(7) = 'HYDROGEN CYANIDE', VOLUME_FRACTION(7) = 0.06233 /
&REAC FUEL = 'SOFA',
  SPEC_ID_NU = 'SOFA','AIR','PRODUCTS', NU=-1,-32.16973125,1,
  HEAT_OF_COMBUSTION = 17040., CHECK_ATOM_BALANCE=.TRUE. /
&SURF ID='BURNER', HRRPUA=833., TAU_Q=-120, COLOR='RASPBERRY' /

```

--- Wall, ceiling and floor ---

```

&MATL ID      = 'CONCRETE'
  FYI         = 'Heat transfer - table 2.2'
  CONDUCTIVITY = 1.1
  SPECIFIC_HEAT = 0.92
  DENSITY      = 2100. /
&MATL ID      = 'GLASS'
  FYI         = 'Different sources... (specify)'
  CONDUCTIVITY = 1.1

```

```
SPECIFIC_HEAT = 0.84
DENSITY      = 2400. /
&SURF ID     = 'WALL1'
RGB          = 70,70,150
MATL_ID      = 'CONCRETE'
THICKNESS    = 0.30 /
&SURF ID     = 'WALL11'
RGB          = 70,70,150
MATL_ID      = 'CONCRETE'
THICKNESS    = 0.30
TRANSPARENCY=0.0 /
&SURF ID     = 'WALL2'
RGB          = 200,200,200
MATL_ID      = 'CONCRETE'
THICKNESS    = 0.30 /
&SURF ID     = 'WALL22'
RGB          = 200,200,200
MATL_ID      = 'CONCRETE'
THICKNESS    = 0.30
TRANSPARENCY=0.0 /
&SURF ID     = 'WINDOW'
RGB          = 180,200,240
MATL_ID      = 'GLASS'
TRANSPARENCY = 0.3
THICKNESS    = 0.02 /
&SURF ID     = 'CEILING'
RGB          = 240,230,210
MATL_ID      = 'CONCRETE'
THICKNESS    = 0.30
FREE_SLIP    = .TRUE. / FDS6 !!!
```

&SURF ID = 'FLOOR'

RGB = 70,50,40

MATL\_ID = 'CONCRETE'

THICKNESS = 0.30 /

&SURF ID = 'PILLAR'

RGB = 0,0,0

MATL\_ID = 'CONCRETE'

THICKNESS = 0.30 /

--- Burner : Sofa ---

&OBST XB= 2.6, 4.6, 6.4, 6.6, 0.0, 1.0, COLOR='ORANGE RED' / back rest

&OBST XB= 2.6, 4.6, 6.6, 7.2, 0.0, 0.4, COLOR='ORANGE RED' / seat

&OBST XB= 2.4, 2.6, 6.4, 7.2, 0.0, 0.8, COLOR='ORANGE RED' / arm rest

&OBST XB= 4.6, 4.8, 6.4, 7.2, 0.0, 0.8, COLOR='ORANGE RED' / arm rest

&VENT XB= 2.6, 4.6, 6.6, 6.6, 0.4, 1.0, SURF\_ID='BURNER' / Fire on the back rest

--- Obstacles of the primary room (large room) ---

- Floors -

&OBST XB= 0.0, 9.0, 4.6, 37.0, -0.2, 0.0, SURF\_ID='FLOOR' / floor

&OBST XB= 6.4, 8.8, 4.8, 36.6, 2.6, 3.0, SURF\_IDS='FLOOR','WALL2','CEILING' / mid floor1

&OBST XB= 5.6, 6.4, 4.8, 6.2, 2.6, 3.0, SURF\_IDS='FLOOR','WALL2','CEILING' / mid floor1

&OBST XB= 0.0, 5.4, 30.4, 34.6, 0.0, 1.0, SURF\_ID='FLOOR' / floor stair

- Pillars -

&OBST XB= 6.8, 7.0, 6.2, 6.4, 0.0, 5.8, SURF\_ID='PILLAR' / pillar

&OBST XB= 6.8, 7.0, 12.2, 12.4, 0.0, 5.8, SURF\_ID='PILLAR' / pillar

&OBST XB= 6.8, 7.0, 18.2, 18.4, 0.0, 5.8, SURF\_ID='PILLAR' / pillar

&OBST XB= 6.8, 7.0, 24.2, 24.4, 0.0, 5.8, SURF\_ID='PILLAR' / pillar

&OBST XB= 6.8, 7.0, 30.2, 30.4, 0.0, 5.8, SURF\_ID='PILLAR' / pillar

&OBST XB= 1.6, 1.8, 12.2, 12.4, 0.0, 4.4, SURF\_ID='PILLAR' / pillar

&OBST XB= 1.6, 1.8, 18.2, 18.4, 0.0, 4.4, SURF\_ID='PILLAR' / pillar

&OBST XB= 1.6, 1.8, 24.2, 24.4, 0.0, 4.4, SURF\_ID='PILLAR' / pillar



- Walls -

&OBST XB= 5.6, 9.0, 4.6, 4.8, 0.0, 6.8, SURF\_ID='WALL22' / wall6 VISUALIZATION!!!

&HOLE XB= 7.6, 8.6, 4.59, 4.81, 3.0, 5.0 / hole in wall8

&OBST XB= 8.8, 9.0, 4.8, 36.6, 0.0, 6.8, SURF\_ID='WALL11' / wall7 VISUALIZATION!!!

&HOLE XB=8.79, 9.01, 6.4, 10.2, 0.0, 2.2 / hole in wall7 - between large room and sales area

&OBST XB= 7.0, 9.0, 36.6, 37.0, 0.0, 6.8, SURF\_ID='WALL22' / wall8

&HOLE XB= 7.6, 8.6, 35.79, 37.01, 3.0, 5.0 / hole in wall8

&OBST XB= 0.0, 0.2, 6.4, 30.2, 0.0, 1.4, SURF\_ID='WALL22' / wall9 VISUALIZATION!!!

&OBST XB= 0.0, 0.2, 6.4, 30.2, 1.4, 3.6, SURF\_ID='WINDOW' / wall10 (window)

&OBST XB= 0.0, 3.6, 30.2, 30.4, 0.0, 6.8, SURF\_ID='WALL2' / wall11

&OBST XB= 1.6, 1.8, 30.4, 33.2, 1.0, 6.8, SURF\_ID='WALL2' / wall12

&HOLE XB=1.59, 1.81, 30.6, 31.6, 1.0, 3.0 / hole in wall12

&OBST XB= 3.4, 3.6, 30.4, 33.2, 1.0, 6.8, SURF\_ID='WALL2' / wall13

&HOLE XB=3.39, 3.61, 30.6, 31.6, 1.0, 3.0 / hole in wall13

- Inactive boxes (flow) -

&OBST XB= 0.0, 3.6, 33.2, 37.0, 0.0, 6.8, SURF\_ID='WALL2' / box1

&OBST XB= 3.6, 7.0, 34.6, 37.0, 0.0, 6.8, SURF\_ID='WALL2' / box2

&OBST XB= 0.0, 5.6, 4.6, 6.4, 0.0, 6.8, SURF\_ID='WALL2' / box3

&OBST XB= 6.8, 8.8, 4.8, 36.6, 5.8, 6.8, SURF\_ID='CEILING' / bar (on top of the inner row of pillars etc)

- Ceilings -

&OBST XB= 6.4, 9.0, 4.6, 37.0, 6.8, 7.0, SURF\_ID='CEILING' / ceiling2

&OBST XB= 6.0, 6.4, 4.6, 37.0, 6.6, 7.0, SURF\_ID='CEILING' / ceiling1

&OBST XB= 5.6, 6.0, 4.6, 37.0, 6.4, 7.0, SURF\_ID='CEILING' / ceiling2

&OBST XB= 5.2, 5.6, 4.6, 37.0, 6.2, 7.0, SURF\_ID='CEILING' / ceiling3

&OBST XB= 4.8, 5.2, 4.6, 37.0, 6.0, 7.0, SURF\_ID='CEILING' / ceiling4

&OBST XB= 4.4, 4.8, 4.6, 37.0, 5.8, 7.0, SURF\_ID='CEILING' / ceiling5

&OBST XB= 4.0, 4.4, 4.6, 37.0, 5.6, 7.0, SURF\_ID='CEILING' / ceiling6

&OBST XB= 3.6, 4.0, 4.6, 37.0, 5.4, 7.0, SURF\_ID='CEILING' / ceiling...

&OBST XB= 3.2, 3.6, 4.6, 37.0, 5.2, 7.0, SURF\_ID='CEILING' / ceiling...

&OBST XB= 2.8, 3.2, 4.6, 37.0, 5.0, 7.0, SURF\_ID='CEILING' / ceiling...

&OBST XB= 2.4, 2.8, 4.6, 37.0, 4.8, 7.0, SURF\_ID='CEILING' / ceiling...

&OBST XB= 2.0, 2.4, 4.6, 37.0, 4.6, 7.0, SURF\_ID='CEILING' / ceiling...

&OBST XB= 1.6, 2.0, 4.6, 37.0, 4.4, 7.0, SURF\_ID='CEILING' / ceiling...

&OBST XB= 1.2, 1.6, 4.6, 30.2, 4.2, 7.0, SURF\_ID='CEILING' / ceiling...

&OBST XB= 0.8, 1.2, 4.6, 30.2, 4.0, 7.0, SURF\_ID='CEILING' / ceiling...

&OBST XB= 0.4, 0.8, 4.6, 30.2, 3.8, 7.0, SURF\_ID='CEILING' / ceiling...

&OBST XB= 0.0, 0.4, 4.6, 30.2, 3.6, 7.0, SURF\_ID='CEILING' / ceiling...

&OBST XB= 0.0, 1.6, 30.2, 37.0, 6.8, 7.0, SURF\_ID='CEILING' / ceiling...

--- Obstacles of the secondary mesh (kitchen) ---

- Floors -

&OBST XB= 9.0, 19.8, 0.0, 12.0, -0.2, 0.0, SURF\_ID='FLOOR' / floor

- Walls -

&OBST XB= 9.0, 19.8, 6.2, 6.4, 0.0, 2.8, SURF\_ID='WALL2' / wall1 - between kitchen and sales area

&HOLE XB=11.8, 16.8, 6.19, 6.41, 1.0, 2.2 / hole in wall1 - between kitchen and sales area

&OBST XB= 18.2, 18.4, 0.0, 2.2, 0.0, 2.8, SURF\_ID='WALL2' / wall2 - between kitchen and outdoors

&HOLE XB=18.19, 18.41, 1.0, 2.0, 0.0, 2.0 / hole in wall1 - between kitchen and sales area

&OBST XB=16.4, 18.2, 0.0, 0.2, 0.0, 2.8, SURF\_ID='WALL2' / wall3 - between kitchen and outdoors

&OBST XB=19.6, 19.8, 3.8, 12.0, 0.0, 2.8, SURF\_ID='WALL2' / wall4 - between kitchen and outdoors

&OBST XB= 9.0, 19.6, 11.8, 12.0, 0.0, 2.8, SURF\_ID='WALL2' / wall5 - between kitchen and outdoors

- Inactive boxes (flow) -

&OBST XB= 9.0, 11.8, 0.0, 6.2, 0.0, 2.8, SURF\_ID='WALL2' / box4

&OBST XB=11.8, 13.4, 0.0, 4.0, 0.0, 2.8, SURF\_ID='WALL2' / box5

&OBST XB=13.4, 16.4, 0.0, 2.2, 0.0, 2.8, SURF\_ID='WALL2' / box6

&OBST XB= 9.0, 12.8, 10.8, 12.0, 0.0, 2.8, SURF\_ID='WALL2' / box7

&OBST XB=18.2, 19.8, 2.2, 3.8, 0.0, 2.8, SURF\_ID='WALL2' / box8

- Ceilings -

&OBST XB= 9.0, 19.8, 0.0, 12.0, 2.6, 2.8, SURF\_ID='CEILING' / ceiling10

--- Outer vents ---

&VENT XB=19.8, 19.8, 0.0, 2.2, 0.0, 2.4, SURF\_ID='OPEN', COLOR='VIOLET' / atm1

&VENT XB= 0.0, 0.0, 30.4, 33.2, 1.0, 6.8, SURF\_ID='OPEN', COLOR='VIOLET' / atm2

--- Outputs ---

-- devc det --

&DEVC ID='SD\_1 T', QUANTITY='TEMPERATURE', XYZ= 5.8, 9.0, 6.2 /

&DEVC ID='SD\_2 T', QUANTITY='TEMPERATURE', XYZ= 5.8, 11.0, 6.2 /

&DEVC ID='SD\_1 r', QUANTITY='DENSITY', XYZ= 5.8, 9.0, 6.2 /

&DEVC ID='SD\_2 r', QUANTITY='DENSITY', XYZ= 5.8, 11.0, 6.2 /

&DEVC ID='SD\_1 CO MF', SPEC\_ID='CARBON MONOXIDE', QUANTITY='MASS FRACTION', XYZ= 5.8, 9.0, 6.2 /

&DEVC ID='SD\_2 CO MF', SPEC\_ID='CARBON MONOXIDE', QUANTITY='MASS FRACTION', XYZ= 5.8, 11.0, 6.2 /

&DEVC ID='SD\_1 SOOT MF', SPEC\_ID='SOOT', QUANTITY='MASS FRACTION', XYZ= 5.8, 9.0, 6.2 /

&DEVC ID='SD\_2 SOOT MF', SPEC\_ID='SOOT', QUANTITY='MASS FRACTION', XYZ= 5.8, 11.0, 6.2 /

&DEVC ID='1.CO2 VF', SPEC\_ID='CARBON DIOXIDE', QUANTITY='VOLUME FRACTION', XYZ= 7.7, 12.0, 4.6 /

&DEVC ID='2.CO2 VF', SPEC\_ID='CARBON DIOXIDE', QUANTITY='VOLUME FRACTION', XYZ= 7.7, 34.0, 4.6 /

&DEVC ID='HD\_1', PROP\_ID='Acme Heat', XYZ= 5.8, 9.0, 6.2 /

&PROP ID='Acme Heat', QUANTITY='LINK TEMPERATURE', RTI=0.5, ACTIVATION\_TEMPERATURE=33. / CIBSE Guide 10.6.3

&DEVC ID='SD\_1', PROP\_ID='Acme Smoke Detector', XYZ= 5.8, 9.0, 6.2 /

&PROP ID='Acme Smoke Detector', QUANTITY='CHAMBER OBSCURATION', LENGTH=1.8, ACTIVATION\_OBSCURATION=3.24 /

&DEVC ID='SD\_2', PROP\_ID='Acme Smoke Detector', XYZ= 5.8, 11.0, 6.2 /

&PROP ID='Acme Smoke Detector', QUANTITY='CHAMBER OBSCURATION', LENGTH=1.8, ACTIVATION\_OBSCURATION=3.24 /

&DEVC ID='FED1', QUANTITY='FED', XYZ= 7.7, 12.0, 4.6 /

&DEVC ID='FED2', QUANTITY='FED', XYZ= 7.7, 34.0, 4.6 /

&DEVC ID='FIC1', QUANTITY='FIC', XYZ= 7.7, 12.0, 4.6 /

&DEVC ID='FIC2', QUANTITY='FIC', XYZ= 7.7, 34.0, 4.6 /

-- slcf 1 --

&SLCF XB= 6.4, 8.8, 4.8, 36.6, 4.0, 5.0, QUANTITY='TEMPERATURE' / Soot slice

&SLCF XB= 6.4, 8.8, 4.8, 36.6, 4.0, 5.0, QUANTITY='DENSITY' / Soot slice

&SLCF XB= 6.4, 8.8, 4.8, 36.6, 4.0, 5.0, SPEC\_ID='CARBON MONOXIDE', QUANTITY='MASS FRACTION' / CO slice

&SLCF XB= 6.4, 8.8, 4.8, 36.6, 4.0, 5.0, SPEC\_ID='SOOT', QUANTITY='MASS FRACTION' / Soot slice

&SLCF XB= 6.4, 8.8, 4.8, 36.6, 4.0, 5.0, SPEC\_ID='CARBON DIOXIDE', QUANTITY='VOLUME FRACTION' / CO2 slice

&SLCF XB= 6.4, 8.8, 4.8, 36.6, 4.0, 5.0, QUANTITY='FIC' / FIC slice

&SLCF XB= 6.4, 8.8, 4.8, 36.6, 4.0, 5.0, SPEC\_ID='HYDROGEN CYANIDE', QUANTITY='MASS FRACTION' / HCN slice

-- slcf 2 --

&SLCF XB= 5.41, 6.4, 33.0, 34.6, 4.0, 5.0, QUANTITY='TEMPERATURE' / Soot slice

&SLCF XB= 5.41, 6.4, 33.0, 34.6, 4.0, 5.0, QUANTITY='DENSITY' / Soot slice

&SLCF XB= 5.41, 6.4, 33.0, 34.6, 4.0, 5.0, SPEC\_ID='CARBON MONOXIDE', QUANTITY='MASS FRACTION' / CO slice

&SLCF XB= 5.41, 6.4, 33.0, 34.6, 4.0, 5.0, SPEC\_ID='SOOT', QUANTITY='MASS FRACTION' / Soot slice

&SLCF XB= 5.41, 6.4, 33.0, 34.6, 4.0, 5.0, SPEC\_ID='CARBON DIOXIDE', QUANTITY='VOLUME FRACTION' / CO2 slice

&SLCF XB= 5.41, 6.4, 33.0, 34.6, 4.0, 5.0, QUANTITY='FIC' / FIC slice

&SLCF XB= 5.41, 6.4, 33.0, 34.6, 4.0, 5.0, SPEC\_ID='HYDROGEN CYANIDE', QUANTITY='MASS FRACTION' / HCN slice

-- slcf 3 --

&SLCF XB= 1.8, 5.39, 30.4, 34.6, 2.0, 3.0, QUANTITY='TEMPERATURE' / Soot slice

&SLCF XB= 1.8, 5.39, 30.4, 34.6, 2.0, 3.0, QUANTITY='DENSITY' / Soot slice

&SLCF XB= 1.8, 5.39, 30.4, 34.6, 2.0, 3.0, SPEC\_ID='CARBON MONOXIDE', QUANTITY='MASS FRACTION' / CO slice

&SLCF XB= 1.8, 5.39, 30.4, 34.6, 2.0, 3.0, SPEC\_ID='SOOT', QUANTITY='MASS FRACTION' / Soot slice

&SLCF XB= 1.8, 5.39, 30.4, 34.6, 2.0, 3.0, SPEC\_ID='CARBON DIOXIDE', QUANTITY='VOLUME FRACTION' / CO2 slice

&SLCF XB= 1.8, 5.39, 30.4, 34.6, 2.0, 3.0, QUANTITY='FIC' / FIC slice

&SLCF XB= 1.8, 5.39, 30.4, 34.6, 2.0, 3.0, SPEC\_ID='HYDROGEN CYANIDE', QUANTITY='MASS FRACTION' / HCN slice

-- slcf temp (convergence) --

&SLCF PBY= 30.1, QUANTITY='TEMPERATURE' / Temperature slice at stairs

&SLCF PBY= 25.9, QUANTITY='TEMPERATURE' / Temperature slice at mid-point

&SLCF PBY= 20.9, QUANTITY='TEMPERATURE' / Temperature slice at mid-point

&SLCF PBY= 15.9, QUANTITY='TEMPERATURE' / Temperature slice at mid-point

&SLCF PBY= 10.9, QUANTITY='TEMPERATURE' / Temperature slice at mid-point

&SLCF PBY= 5.9, QUANTITY='TEMPERATURE' / Temperature slice at mid-point

-- dump line -- the rate at which output files are written

&DUMP DT\_SL3D=10.0, DT\_SLCF=10.0, DT\_DEVC=5.0, DT\_PL3D=15.0, WRITE\_XYZ=.TRUE. ,  
PLOT3D\_QUANTITY(5)='MASS FRACTION', PLOT3D\_SPEC\_ID(5)='CARBON MONOXIDE' /

&TAIL /

#### 14.1.2 Bookcase fire (fuel and burner part only)

--- My fuel ---

&SPEC ID = 'BOOKCASE', FORMULA ='C40.1238H68.1857O29.6N0.08CI0.0619' /

&SPEC ID = 'OXYGEN', LUMPED\_COMPONENT\_ONLY = .TRUE. /

&SPEC ID = 'NITROGEN', LUMPED\_COMPONENT\_ONLY = .TRUE. /

&SPEC ID = 'HYDROGEN CHLORIDE', LUMPED\_COMPONENT\_ONLY = .TRUE. /

&SPEC ID = 'WATER VAPOR', LUMPED\_COMPONENT\_ONLY = .TRUE. /

&SPEC ID = 'CARBON MONOXIDE', LUMPED\_COMPONENT\_ONLY = .TRUE. /

&SPEC ID = 'CARBON DIOXIDE', LUMPED\_COMPONENT\_ONLY = .TRUE. /

&SPEC ID = 'SOOT', LUMPED\_COMPONENT\_ONLY = .TRUE. /

&SPEC ID = 'HYDROGEN CYANIDE', LUMPED\_COMPONENT\_ONLY = .TRUE. /

&SPEC ID = 'AIR', BACKGROUND=.TRUE.,

SPEC\_ID(1) = 'OXYGEN', VOLUME\_FRACTION(1)= 1,

SPEC\_ID(2) = 'NITROGEN', VOLUME\_FRACTION(2)= 3.76 /

&SPEC ID = 'PRODUCTS',

SPEC\_ID(1) = 'WATER VAPOR', VOLUME\_FRACTION(1) = 34.053155 ,

SPEC\_ID(2) = 'NITROGEN', VOLUME\_FRACTION(2) = 152.7236704 ,

SPEC\_ID(3) = 'CARBON DIOXIDE', VOLUME\_FRACTION(3) = 37.94314085 ,

SPEC\_ID(4) = 'CARBON MONOXIDE', VOLUME\_FRACTION(4) = 0.879933214 ,

SPEC\_ID(5) = 'HYDROGEN CHLORIDE', VOLUME\_FRACTION(5) = 0.0619 ,

SPEC\_ID(6) = 'SOOT', VOLUME\_FRACTION(6) = 1.283235938 ,

SPEC\_ID(7) = 'HYDROGEN CYANIDE', VOLUME\_FRACTION(7) = 0.01749 /

&REAC FUEL = 'BOOKCASE',

SPEC\_ID\_NU = 'BOOKCASE','AIR','PRODUCTS', NU=-1, -40.60968496 , 1,

HEAT\_OF\_COMBUSTION = 17040., CHECK\_ATOM\_BALANCE=.TRUE. /

```
&SURF ID='BURNER', HRRPUA=833., TAU_Q=-120, COLOR='RASPBERRY' /
--- Burner : Bookcase ---
&OBST XB= 3.2, 3.8, 6.4, 6.6, 0.0, 2.0, COLOR='BURNT SIENNA',
  SURF_ID6='INERT','INERT','INERT','BURNER','INERT','INERT' / Fire in bookcase
```

### 14.1.3 Post-flashover sofa fire (fuel part only)

```
--- My fuel ---
&SPEC ID = 'SOFA',    FORMULA = 'C25.1548H42.2322O6N2Cl0.0774' /
&SPEC ID = 'OXYGEN',    LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'NITROGEN',    LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'HYDROGEN CHLORIDE', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'WATER VAPOR',    LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'CARBON MONOXIDE', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'CARBON DIOXIDE', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'SOOT',        LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'HYDROGEN CYANIDE', LUMPED_COMPONENT_ONLY = .TRUE. /
&SPEC ID = 'AIR', BACKGROUND=.TRUE.,
  SPEC_ID(1) = 'OXYGEN', VOLUME_FRACTION(1)= 1,
  SPEC_ID(2) = 'NITROGEN', VOLUME_FRACTION(2)= 3.76 /
&SPEC ID = 'PRODUCTS',
  SPEC_ID(1) = 'WATER VAPOR', VOLUME_FRACTION(1) =      20.9466,
  SPEC_ID(2) = 'NITROGEN', VOLUME_FRACTION(2) =      118.2994344,
  SPEC_ID(3) = 'CARBON DIOXIDE', VOLUME_FRACTION(3) =      23.32934688,
  SPEC_ID(4) = 'CARBON MONOXIDE', VOLUME_FRACTION(4) = 0.857596875,
  SPEC_ID(5) = 'HYDROGEN CHLORIDE', VOLUME_FRACTION(5) = 0.0774,
  SPEC_ID(6) = 'SOOT', VOLUME_FRACTION(6) =      0.70625625,
  SPEC_ID(7) = 'HYDROGEN CYANIDE', VOLUME_FRACTION(7) = 0.2616 /
&REAC FUEL = 'SOFA',
  SPEC_ID_NU = 'SOFA','AIR','PRODUCTS', NU=-1,      -31.23144531, 1,
  HEAT_OF_COMBUSTION = 17040., CHECK_ATOM_BALANCE=.TRUE. /
```

## 14.2 MATLAB script

```
function [] = FDStoFED_FIC_HCN_HV_NO2_sofa(Simulex_out_file, FDS_file_name)

% loads the simulex file and calculates FED and FEC with the FDS files

% ('SC2_30-300.m','sofa_FEC_FED_')

Simulex_matrix = load(Simulex_out_file);

[Nrows,Ncols] = size(Simulex_matrix);

% Set initial parameters...

Npersons = (Ncols-1)/2;

Ntimes = Nrows;

% Define FED matrices

% FED_matrix = zeros(Ntimes, (1+Npersons) );

FED_CO = zeros(Ntimes, (1+Npersons) );

FED_HCN = zeros(Ntimes, (1+Npersons) );

FED_total = zeros(Ntimes, (1+Npersons) );

FED_T = zeros(Ntimes, (1+Npersons) );

% FED calculated from HCN OUTPUT

FED_fds = zeros(Ntimes, (1+Npersons) );

% CO2 volume fraction

CO2 = zeros(Ntimes, (1+Npersons) );

% FIC from FDS OUTPUT

FIC = zeros(Ntimes, (1+Npersons) );

% Define FEC matrices

FEC_NO2 = zeros(Ntimes, (1+Npersons) );

FEC_C3H4O = zeros(Ntimes, (1+Npersons) );

FEC_CH2O = zeros(Ntimes, (1+Npersons) );

FEC_HCl = zeros(Ntimes, (1+Npersons) );

FEC_total = zeros(Ntimes, (1+Npersons) );

% Soot

FEC_Soot = zeros(Ntimes, (1+Npersons) );

Soot = zeros(Ntimes, (1+Npersons) );
```

```

%FDS_filename = FDS_file_name
for k=1:Ntimes
    PersonID = 1;
    time = Simulex_matrix(k,1);
    % Set the time in the matrices
    FED_CO(k,1) = time;
    FED_HCN(k,1) = time;
    FED_total(k,1) = time;
    FED_T(k,1) = time;
    FEC_NO2(k,1) = time;
    FEC_C3H4O(k,1) = time;
    FEC_CH2O(k,1) = time;
    FEC_HCl(k,1) = time;
    FEC_total(k,1) = time;
    FEC_soot(k,1) = time;
    Soot(k,1) = time;
    % New outputs
    CO2(k,1) = time;
    FIC(k,1) = time;
    FED_fds(k,1) = time;
    % old script continues
    Temp_FDS_file_name = [FDS_file_name num2str(time) '.txt'];
    FDS_file = importdata(Temp_FDS_file_name, ',');
    FDS_matrix = FDS_file.data;
    %FDS_matrix=load(Temp_FDS_file_name);
    %[FDS_rows]
    for i=1:Npersons
        x_simulex = Simulex_matrix(k, PersonID*2 );
        y_simulex = Simulex_matrix(k, 1+PersonID*2 );
        x_fds = 6.5 + (y_simulex - 25.7)*0.85;

```



```

y_fds = (53.9-x_simulex);
if x_fds > 6.5 & x_fds < 8.8 & y_fds > 11.9 & y_fds < 36.6
    [rows,dummy1,dummy2] = find( FDS_matrix(:,2) == round(y_fds*10)/10 );
    [max,dummy] = size(rows);
    [row ,dummy1,dummy2] = find( FDS_matrix(rows(1,1):rows(max,1),1) == round(x_fds*10)/10 );
    row=row+rows(1,1)-1;
    % Take the CO and soot scalar, air density and temperature as a starting point
    CO_scalar = FDS_matrix(row,6);
    Soot_scalar = FDS_matrix(row,7);
    air_density = FDS_matrix(row,5);
    Temp = FDS_matrix(row,4) + 273;
    % In addition, take the CO2, FIC and HCN scalar
    CO2_scalar = FDS_matrix(row,8);
    FIC_scalar = FDS_matrix(row,9);
    HCN_scalar = FDS_matrix(row,10);
    % Calculate concentration in kg/m3
    CO_conc = CO_scalar*air_density;
    Soot_conc = Soot_scalar*air_density;
    HCN_conc = HCN_scalar*air_density;
    % Calculate CO2 volume fraction in percent
    CO2_percent = CO2_scalar*100;
    % Calculate concentration in ppm and ideal gas assumption
    CO_ppm = (8.20575e-5*Temp)/(1*28e-3)*CO_conc*1000000;
    NO2_ppm = (8.20575e-5*Temp)/(1*46e-3)*CO_conc*1000000*0.0;
    C3H4O_ppm = (8.20575e-5*Temp)/(1*56e-3)*CO_conc*1000000*0.0;
    CH2O_ppm = (8.20575e-5*Temp)/(1*30e-3)*CO_conc*1000000*0.0;
    HCl_ppm = (8.20575e-5*Temp)/(1*36.5e-3)*CO_conc*1000000*1.25;
    HCN_ppm = (8.20575e-5*Temp)/(1*27e-3)*CO_conc*1000000*0.243056;
    % Calculate HCN concentration in ppm from FDS OUTPUT
    HCN_ppm_fds = (8.20575e-5*Temp)/(1*27e-3)*HCN_conc*1000000;

```

```

if k==1
    % FED
    FED_CO(k,i+1) = CO_ppm/35000*10/60;
    FED_HCN(k,i+1) = exp(HCN_ppm/43)/220*10/60;
    FED_total(k,i+1) = CO_ppm/35000*10/60 + exp(HCN_ppm/43)/220*10/60;
    FED_T(k,i+1) = 1/(4.1e8*(Temp-273)^-3.61)*10/60;
    % FED from HCN OUTPUT
    FED_fds(k,i+1) = CO_ppm/35000*10/60 + exp(HCN_ppm_fds/43)/220*10/60;
    % CO2 volume percent
    CO2(k,i+1) = CO2_percent;
    % FIC
    FIC(k,i+1) = FIC_scalar;
    % FEC
    FEC_NO2(k,i+1) = NO2_ppm/250;
    FEC_C3H4O(k,i+1) = C3H4O_ppm/30;
    FEC_CH2O(k,i+1) = CH2O_ppm/250;
    FEC_HCl(k,i+1) = HCl_ppm/1000;
    FEC_total(k,i+1) = NO2_ppm/250 + C3H4O_ppm/30 + CH2O_ppm/250 + HCl_ppm/1000;
    % soot
    FEC_soot(k,i+1) = Soot_conc/0.8e-3;
    Soot(k,i+1) = Soot_conc;
else
    % FED
    FED_CO(k,i+1) = FED_CO(k-1,i+1) + CO_ppm/35000*10/60;
    FED_HCN(k,i+1) = FED_HCN(k-1,i+1) + exp(HCN_ppm/43)/220*10/60;
    FED_T(k,i+1) = FED_T(k-1,i+1) + 1/(4.1e8*(Temp-273)^-3.61)*10/60;
    % FED from HCN OUTPUT and Conversion coeff. considering Hyperventilation
    if CO2_percent > 2.0
        FED_total(k,i+1) = FED_total(k-1,i+1) + exp(CO2_percent/5)*CO_ppm/35000*10/60 +
        exp(CO2_percent/5)*exp(HCN_ppm/43)/220*10/60;
    end
end

```

```

    FED_fds(k,i+1) = FED_fds(k-1,i+1) + exp(CO2_percent/5)*CO_ppm/35000*10/60 +
exp(CO2_percent/5)*exp(HCN_ppm_fds/43)/220*10/60;
else
    FED_total(k,i+1) = FED_total(k-1,i+1) + CO_ppm/35000*10/60 + exp(HCN_ppm/43)/220*10/60;
    FED_fds(k,i+1) = FED_fds(k-1,i+1) + CO_ppm/35000*10/60 + exp(HCN_ppm_fds/43)/220*10/60;
end
% CO2 volume percent
CO2(k,i+1) = CO2_percent;
% FIC
FIC(k,i+1) = FIC_scalar;
% FEC
FEC_NO2(k,i+1) = NO2_ppm/250;
FEC_C3H4O(k,i+1) = C3H4O_ppm/30;
FEC_CH2O(k,i+1) = CH2O_ppm/250;
FEC_HCl(k,i+1) = HCl_ppm/1000;
FEC_total(k,i+1) = NO2_ppm/250 + C3H4O_ppm/30 + CH2O_ppm/250 + HCl_ppm/1000;
% soot
FEC_soot(k,i+1) = Soot_conc/0.8e-3;
Soot(k,i+1) = Soot_conc;
end
else
    if k==1
        % FED
        FED_CO(k,i+1) = 0;
        FED_HCN(k,i+1) = 0;
        FED_total(k,i+1) = 0;
        FED_T(k,i+1) = 0;
        % FED from HCN OUTPUT
        FED_fds(k,i+1) = 0;
        % CO2 volume percent
        CO2(k,i+1) = 0;

```

```

% FIC
FIC(k,i+1) = 0;

% FEC
FEC_NO2(k,i+1) = 0;
FEC_C3H4O(k,i+1) = 0;
FEC_CH2O(k,i+1) = 0;
FEC_HCl(k,i+1) = 0;
FEC_total(k,i+1) = 0;

% soot
FEC_soot(k,i+1) = 0;
Soot(k,i+1) = 0;
else
% FED
FED_CO(k,i+1) = FED_CO(k-1,i+1);
FED_HCN(k,i+1) = FED_HCN(k-1,i+1);
FED_total(k,i+1) = FED_total(k-1,i+1);
FED_T(k,i+1) = FED_T(k-1,i+1);
% FED from HCN OUTPUT
FED_fds(k,i+1) = FED_fds(k-1,i+1);
% CO2 volume percent
CO2(k,i+1) = 0;
% FIC
FIC(k,i+1) = 0;
% FEC
FEC_NO2(k,i+1) = 0;
FEC_C3H4O(k,i+1) = 0;
FEC_CH2O(k,i+1) = 0;
FEC_HCl(k,i+1) = 0;
FEC_total(k,i+1) = 0;
% soot

```

```

        FEC_soot(k,i+1) = 0;
        Soot(k,i+1) = 0;
    end
end
PersonID=PersonID+1;
end
end
% FED
save('FED_CO.txt','FED_CO','-ASCII');
save('FED_HCN.txt','FED_HCN','-ASCII');
save('FED_total.txt','FED_total','-ASCII');
save('FED_T.txt','FED_T','-ASCII');
save('FED_fds.txt','FED_fds','-ASCII');
% FEC
save('FEC_NO2.txt','FEC_NO2','-ASCII');
save('FEC_C3H4O.txt','FEC_C3H4O','-ASCII');
save('FEC_CH2O.txt','FEC_CH2O','-ASCII');
save('FEC_HCl.txt','FEC_HCl','-ASCII');
save('FEC_total.txt','FEC_total','-ASCII');
save('FIC.txt','FIC','-ASCII');
% CO2
save('CO2.txt','CO2','-ASCII');
% soot
save('FEC_soot.txt','FEC_soot','-ASCII');
save('Soot.txt','Soot','-ASCII');

```

## 14.3 Mesh refinement details

### 14.3.1 2N case : 17 meshes

--- meshes ---

&MESH IJK= 72, 40,144, XB= 1.8, 5.4, 6.2, 8.2, -0.2, 7.0, MPI\_PROCESS=0 / Mesh 1 410,000 cells 5cm  
&MESH IJK= 72, 40,144, XB= 1.8, 5.4, 8.2, 10.2, -0.2, 7.0, MPI\_PROCESS=1 / Mesh 2 410,000 cells 5cm  
&MESH IJK= 54,120, 72, XB= 0.0, 5.4, 10.2, 22.2, -0.2, 7.0, MPI\_PROCESS=2 / Mesh 3 460,000 cells 10cm  
&MESH IJK= 54,128, 72, XB= 0.0, 5.4, 22.2, 35.0, -0.2, 7.0, MPI\_PROCESS=3 / Mesh 4 500,000 cells 10cm  
&MESH IJK= 72, 72, 80, XB= 5.4, 9.0, 4.6, 8.2, 3.0, 7.0, MPI\_PROCESS=4 / Mesh 5 410,000 cells 5cm  
&MESH IJK= 72, 72, 80, XB= 5.4, 9.0, 8.2, 11.8, 3.0, 7.0, MPI\_PROCESS=5 / Mesh 6 410,000 cells 5cm

<MESH IJK= 36,250, 40, XB= 5.4, 9.0, 11.8, 36.8, 3.0, 7.0 / Mesh 7 360,000 cells 10cm>

----- grid dependency test : 8 sub-meshes -----

&MESH IJK= 36,250, 40, XB= 5.4, 7.2, 11.8, 24.3, 3.0, 5.0, MPI\_PROCESS=6 / Mesh 7-1 360,000 cells 5cm  
&MESH IJK= 36,250, 40, XB= 7.2, 9.0, 11.8, 24.3, 3.0, 5.0, MPI\_PROCESS=7 / Mesh 7-2 360,000 cells 5cm  
&MESH IJK= 36,250, 40, XB= 5.4, 7.2, 24.3, 36.8, 3.0, 5.0, MPI\_PROCESS=8 / Mesh 7-3 360,000 cells 5cm  
&MESH IJK= 36,250, 40, XB= 7.2, 9.0, 24.3, 36.8, 3.0, 5.0, MPI\_PROCESS=9 / Mesh 7-4 360,000 cells 5cm  
&MESH IJK= 36,250, 40, XB= 5.4, 7.2, 11.8, 24.3, 5.0, 7.0, MPI\_PROCESS=10 / Mesh 7-5 360,000 cells 5cm  
&MESH IJK= 36,250, 40, XB= 7.2, 9.0, 11.8, 24.3, 5.0, 7.0, MPI\_PROCESS=11 / Mesh 7-6 360,000 cells 5cm  
&MESH IJK= 36,250, 40, XB= 5.4, 7.2, 24.3, 36.8, 5.0, 7.0, MPI\_PROCESS=12 / Mesh 7-7 360,000 cells 5cm  
&MESH IJK= 36,250, 40, XB= 7.2, 9.0, 24.3, 36.8, 5.0, 7.0, MPI\_PROCESS=13 / Mesh 7-8 360,000 cells 5cm

&MESH IJK= 36,324, 32, XB= 5.4, 9.0, 4.6, 37.0, -0.2, 3.0, MPI\_PROCESS=14 / Mesh 8-2 370,000 cells 10cm

&MESH IJK= 36, 80, 96, XB= 0.0, 1.8, 6.2, 10.2, -0.2, 4.6, MPI\_PROCESS=15 / Mesh 8-1 270,000 cells 5cm

&MESH IJK= 54, 60, 15, XB= 9.0, 19.8, 0.0, 12.0, -0.2, 2.8, MPI\_PROCESS=15 / Mesh 8-3 50,000 cells 20cm

### 14.3.2 4N case : 31 meshes

--- meshes --- grid dependency test

&MESH IJK= 72, 40,144, XB= 1.8, 5.4, 6.2, 8.2, -0.2, 7.0, MPI\_PROCESS=0 / Mesh 1 410,000 cells 5cm  
&MESH IJK= 54,120, 72, XB= 0.0, 2.7, 10.2, 16.2, -0.2, 3.4, MPI\_PROCESS=0 / Mesh 3-1 460,000 cells 5cm

&MESH IJK= 72, 40,144, XB= 1.8, 5.4, 8.2, 10.2, -0.2, 7.0, MPI\_PROCESS=1 / Mesh 2 410,000 cells 5cm  
 &MESH IJK= 54,120, 72, XB= 2.7, 5.4, 10.2, 16.2, -0.2, 3.4, MPI\_PROCESS=1 / Mesh 3-2 460,000 cells 5cm  
 &MESH IJK= 54,120, 72, XB= 0.0, 2.7, 16.2, 22.2, -0.2, 3.4, MPI\_PROCESS=2 / Mesh 3-3 460,000 cells 5cm  
 &MESH IJK= 54,120, 72, XB= 2.7, 5.4, 16.2, 22.2, -0.2, 3.4, MPI\_PROCESS=3 / Mesh 3-4 460,000 cells 5cm  
 &MESH IJK= 54,120, 72, XB= 0.0, 2.7, 10.2, 16.2, 3.4, 7.0, MPI\_PROCESS=4 / Mesh 3-5 460,000 cells 5cm  
 &MESH IJK= 72, 72, 80, XB= 5.4, 9.0, 4.6, 8.2, 3.0, 7.0, MPI\_PROCESS=4 / Mesh 5 410,000 cells 5cm  
 &MESH IJK= 54,120, 72, XB= 2.7, 5.4, 10.2, 16.2, 3.4, 7.0, MPI\_PROCESS=5 / Mesh 3-6 460,000 cells 5cm  
 &MESH IJK= 72, 72, 80, XB= 5.4, 9.0, 8.2, 11.8, 3.0, 7.0, MPI\_PROCESS=5 / Mesh 6 410,000 cells 5cm  
 &MESH IJK= 54,120, 72, XB= 0.0, 2.7, 16.2, 22.2, 3.4, 7.0, MPI\_PROCESS=6 / Mesh 3-7 460,000 cells 5cm  
 &MESH IJK= 36,250, 40, XB= 5.4, 7.2, 11.8, 24.3, 3.0, 5.0, MPI\_PROCESS=6 / Mesh 7-1 360,000 cells 5cm  
 &MESH IJK= 54,120, 72, XB= 2.7, 5.4, 16.2, 22.2, 3.4, 7.0, MPI\_PROCESS=7 / Mesh 3-8 460,000 cells 5cm  
 &MESH IJK= 36,250, 40, XB= 7.2, 9.0, 11.8, 24.3, 3.0, 5.0, MPI\_PROCESS=7 / Mesh 7-2 360,000 cells 5cm  
 &MESH IJK= 54,128, 72, XB= 0.0, 2.7, 22.2, 28.6, -0.2, 3.4, MPI\_PROCESS=8 / Mesh 4-1 500,000 cells 5cm  
 &MESH IJK= 36,250, 40, XB= 5.4, 7.2, 24.3, 36.8, 3.0, 5.0, MPI\_PROCESS=8 / Mesh 7-3 360,000 cells 5cm  
 &MESH IJK= 54,128, 72, XB= 2.7, 5.4, 22.2, 28.6, -0.2, 3.4, MPI\_PROCESS=9 / Mesh 4-2 500,000 cells 5cm  
 &MESH IJK= 36,250, 40, XB= 7.2, 9.0, 24.3, 36.8, 3.0, 5.0, MPI\_PROCESS=9 / Mesh 7-4 360,000 cells 5cm  
 &MESH IJK= 54,128, 72, XB= 0.0, 2.7, 28.6, 35.0, -0.2, 3.4, MPI\_PROCESS=10 / Mesh 4-3 500,000 cells 5cm  
 &MESH IJK= 36,250, 40, XB= 5.4, 7.2, 11.8, 24.3, 5.0, 7.0, MPI\_PROCESS=10 / Mesh 7-5 360,000 cells 5cm  
 &MESH IJK= 54,128, 72, XB= 2.7, 5.4, 28.6, 35.0, -0.2, 3.4, MPI\_PROCESS=11 / Mesh 4-4 500,000 cells 5cm  
 &MESH IJK= 36,250, 40, XB= 7.2, 9.0, 11.8, 24.3, 5.0, 7.0, MPI\_PROCESS=11 / Mesh 7-6 360,000 cells 5cm  
 &MESH IJK= 54,128, 72, XB= 0.0, 2.7, 22.2, 28.6, 3.4, 7.0, MPI\_PROCESS=12 / Mesh 4-5 500,000 cells 5cm  
 &MESH IJK= 36,250, 40, XB= 5.4, 7.2, 24.3, 36.8, 5.0, 7.0, MPI\_PROCESS=12 / Mesh 7-7 360,000 cells 5cm  
 &MESH IJK= 54,128, 72, XB= 2.7, 5.4, 22.2, 28.6, 3.4, 7.0, MPI\_PROCESS=13 / Mesh 4-6 500,000 cells 5cm  
 &MESH IJK= 36,250, 40, XB= 7.2, 9.0, 24.3, 36.8, 5.0, 7.0, MPI\_PROCESS=13 / Mesh 7-8 360,000 cells 5cm  
 &MESH IJK= 54,128, 72, XB= 0.0, 2.7, 28.6, 35.0, 3.4, 7.0, MPI\_PROCESS=14 / Mesh 4-7 500,000 cells 5cm  
 &MESH IJK= 36,324, 32, XB= 5.4, 9.0, 4.6, 37.0, -0.2, 3.0, MPI\_PROCESS=14 / Mesh 8-2 370,000 cells 10cm  
 &MESH IJK= 54,128, 72, XB= 2.7, 5.4, 28.6, 35.0, 3.4, 7.0, MPI\_PROCESS=15 / Mesh 4-8 500,000 cells 5cm  
 &MESH IJK= 36, 80, 96, XB= 0.0, 1.8, 6.2, 10.2, -0.2, 4.6, MPI\_PROCESS=15 / Mesh 8-1 270,000 cells 5cm  
 &MESH IJK= 54, 60, 15, XB= 9.0, 19.8, 0.0, 12.0, -0.2, 2.8, MPI\_PROCESS=15 / Mesh 8-3 50,000 cells 20cm