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SUMMARY

In case of fire dynamics simulation requirements to reliable results are most often very high due to the severe consequences of erroneous results. At the same time it is a well known fact that fire dynamics simulation constitutes rather complex physical phenomena which apart from flow and energy equations require solution of the issues of combustion and gas radiation to mention a few.
This paper performs a sensitivity analysis of a fire dynamics simulation on a benchmark case where measurement results are available for comparison. The analysis is performed using the method of Elementary Effects (Morris method). The parameters considered are selected among physical parameters and program specific parameters. The influence on the calculation result as well as the CPU time is considered. It is found that the result is highly sensitive to many parameters even though the sensitivity varies significantly among them. An importance ranking of the parameters is provided.

INTRODUCTION

In case of fire dynamics simulation requirements to reliable results are most often very high due to the severe consequences of erroneous results. At the same time it is a well known fact that fire dynamics simulation constitutes rather complex physical phenomena which apart from flow and energy equations require solution of the issues of combustion and gas radiation to mention a few. Obviously, the proper solution requires a sufficient physical and numerical description combined with an adequate mesh. However, advanced models and detailed meshes are very costly in terms of manpower, storage and CPU time. At the same time determination of fire scenarios and additional input parameters may be highly uncertain. Thus, to provide reliable results applicable for sound decision support the inclusion of sensitivity analysis is crucial.
The objective of the present work is twofold. Firstly, to investigate if the output parameters (i.e. the results) are sensitive to the expected variation of the input parameters. Secondly, to identify the most important parameters, i.e. to determine what input parameters contribute significantly to the uncertainty of a fire dynamics simulation.

METHODS

Benchmark test case

Sensitivity analysis of a fire dynamics simulation is performed on a benchmark case where measurement results are available for comparison [1]. The benchmark test case corresponds to the steady-state full-scale measurements of a fire scenario in a domestic sized room with one (door shaped) opening, see Figure 1 and Table 1. The walls are made of light materials in order to facilitate a fast steady-state heat balance. The fire is modelled using a methane flame.
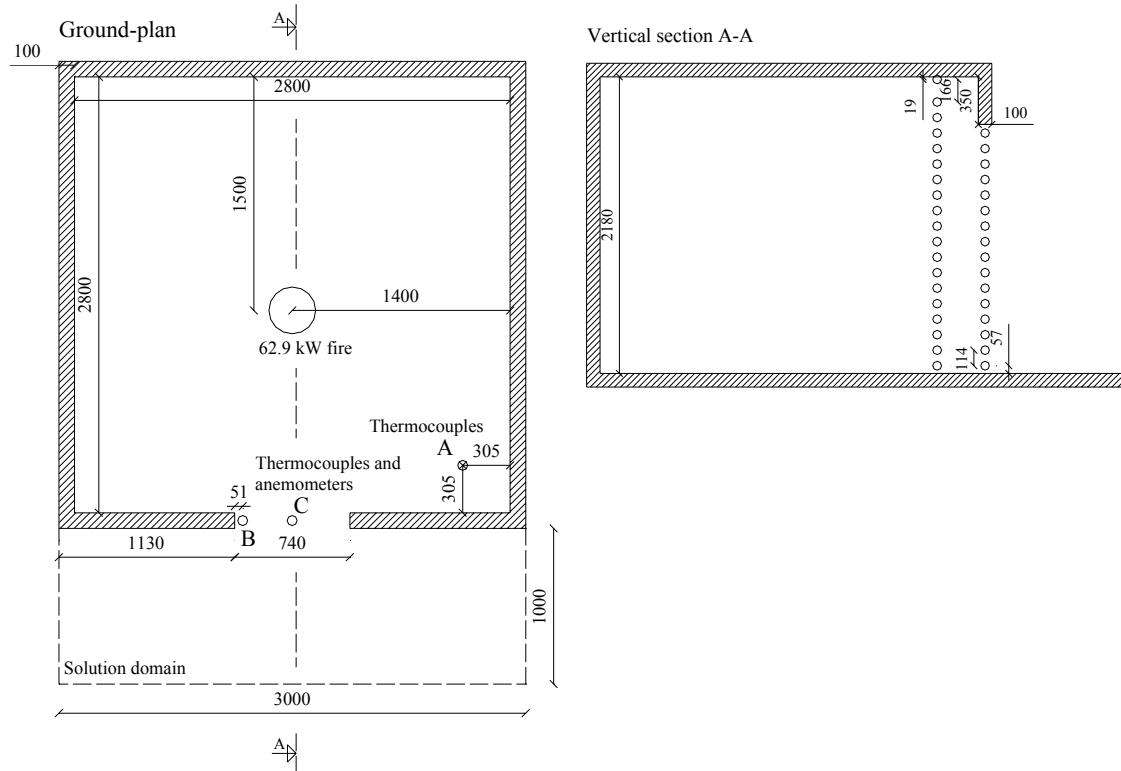
Figure 1. Geometry of the benchmark test case applied in the fire dynamics simulations corresponding to a fire in a domestic sized room with one opening (door). The test case is adopted from [1]. Dimensions in mm.

Table 1. Data applied for the benchmark test case.

Parameter	Data
Room size	2.18 m x 2.8 m x 2.8 m
Wall thickness	0.1 m
Wall parameters (assumed)	Density: 1035 kg/m^3
	Heat capacity: 823 J/kgK
	Conductivity: 0.072 W/mK
Opening size	H x W = 1.83 m x 0.74 m
Fire heat release	62.9 kW (steady-state), circular ø 0.3 m
External temperature	29 °C (maintained)

Fire dynamics simulation

Modelling smoke movement in case of fire is complex and demanding in terms of CPU time. The process is highly transient by nature; there is a significant interaction between the fire and the surrounding room; radiation plays an important role; a combination of forced flow and buoyancy induced flow leads to mixed convection; etc. [2, 3]. Thus, smoke transport modelling in case of fire is a task that requires great skill and a proper model. For instance, it is found that the choice of turbulence model is important [2, 3].

The fire dynamics simulations in this paper are made by the special application fire simulation CFD code FDS version 4.06 (Fire Dynamics Simulator, NIST, USA) [4]. The reason for choosing FDS for the simulations is the fact that it is widely used for fire dynamics simulation, probably partly due to the possibility of free download. Even though some results may obviously be program specific most overall conclusion are assumed to apply for other CFD software codes as well.

Sensitivity analysis

The purpose of the paper is to investigate what parameters are most important, to focus attention and resources in an optimal way during the fire dynamics simulations. This is done by means of sensitivity analysis that studies how the variation of the model output can be apportioned qualitatively or quantitatively to different sources of variation.

Two overall classes of sensitivity analysis exist, namely local and global analysis. The typical local analysis may usually comprise variation of one variable at a time e.g. by computing partial derivatives or changing a parameter within certain limits all other things being equal. A global sensitivity analysis is characterised by evaluating individual factors varying all other factors as well. Idealistically, the sensitivity analysis should quantify and apportion the total uncertainty related to the model applied for the fire dynamics simulation. However, due to the complexity of the CFD model as outlined above and the duration of each simulation this procedure is not possible in practise. Thus, a screening method is applied in stead to identify the parameter subset the controls most of the output variability including a ranking of the parameters. This could be seen either as a standalone investigation or as part of a more elaborate work where the most important parameters are identified at the initial stage for further investigation.

The screening method of Elementary Effects [5, 6] is applied in this work. The method, which can be seen as an extension of a derivative-based screening method, can be characterised as a screening method with global characteristics. The method has been applied in several areas of building sciences e.g. natural night ventilation [7] and thermal building simulation [8].

The method determines the so-called elementary effect EE of a model $y = y(x_1,\ldots,x_k)$ with input factors x_i. The Elementary Effect for the ith input factor in a point $\mathbf{x}$ is

$$EE(x_1,\ldots,x_k) = \frac{y(x_1,x_2,\ldots,x_{i-1},x_i + \Delta,x_{i+1},\ldots,x_k) - y(x_1,\ldots,x_k)}{\Delta} \qquad (1)$$

A number of elementary effects EE_i of each factor are calculated within the factor's range of variation. The method comprises a number of individually randomised one-factor-at-a-time simulations where all factors are varied within their input space in a way that spans the entire input space to form an approximate global sensitivity analysis [5, 6].

The model sensitivity to each factor is evaluated by the mean value and the standard deviation of the elementary effects

$$\mu = \sum_{i=1}^{r} |EE_i| / r \qquad (2)$$

$$\sigma = \sqrt{\sum_{i=1}^{r} (EE_i - \mu)^2 / r} \qquad (3)$$

where μ is the mean value of the absolute values of the elementary effects determining if the factor is important, and σ is the standard deviation of the elementary effects which is a measure of the sum of all interactions of x_i with other factors and of all its nonlinear effects. r is the number of elementary effects investigated for each factor. The results are presented as graphs in Figure 4 where each output factor is shown as a function of μ and σ.

Choice of input and output parameters

An initial subjective "pre-screening" of the numerous input parameters is based on physical understanding, experience, literature, etc. Tables 2 and 3 list the selected parameters and the assumed variation. Figure 2 shows the variation related to fire geometry and location.

Table 2. Input parameter variation applied for the sensitivity analysis (specified in Table 5).

Physical parameters	Variation (compared with benchmark)
Heat release	70%, 100% or 130%
Fire geometry (see Figure 2)	Quadratic or Rectangular
Fire location (see Figure 2)	Centred, Wall or Corner
Fuel type (see Table 3)	Methane, Wood or Polyurethane
Initial and external temperatures (°C)	24, 29 or 34
Opening size (door width adjusted)	75%, 100% or 125%
Program parameters	Variation
Solid angles (grid size of radiation model)	60, 104 or 200
Radiation model	No radiation, Grey gas or 9-Band
Smagorinsky constant	0.10, 0.20 or 0.25

Table 3. Fuel types applied in the simulations.

Name of fuel	Methane	Wood	Polyurethane
Chemical expression	CH_4	$C_{34}H_{62}O_{25}$	$C_{63}H_{71}NO_{21}$
Molecular weight of fuel [g/mol]	16	87	130.3
Stoichiometric coefficient for O_2 [-]	2	3.7	7.025
Stoichiometric coefficient for CO_2 [-]	1	3.4	6.3
Stoichiometric coefficient for H_2O [-]	2	3.1	3.55
Fraction of soot from fuel [g/g]	0.01	0.01	0.10
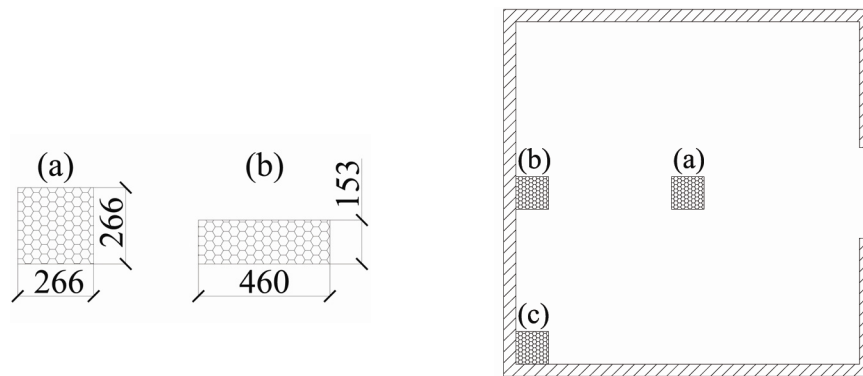
Figure 2. Variation applied for the sensitivity analysis regarding fire geometry (left, dimensions in mm) and fire location (right).

The parameters are divided in physical parameters - comprising fire characteristics, room characteristics and external boundary conditions – as well as program parameters that influence the numerical solution process.

The variations of the physical parameters, taking the benchmark test case as a starting point, are chosen to be as realistic as possible to provide reasonable evaluation of the influence on the output.

The program parameters are obviously linked to the specific software applied for the simulations, however, still assumed to provide a rough indication on the overall influence. The number of solid angles applied in the radiation model (default value of 104) and the choice of radiation model (gray gas being default) are especially important to fire dynamics simulation where radiation from surfaces as well as gas is known to be important. The turbulence is modelled using Large Eddy Simulation that applies the Smagorinsky constant (default value 0.20). The Smagorinsky constant has been found to influence the results in earlier work and is therefore included in the investigation.

Investigation of grid independence has been undertaken and it is found that a reasonable grid independent result is found for approximately 260,000 grid points which is applied for all simulations.

The output parameters outlined in Table 4 are chosen to represent important parameters that are either crucial as to the influence of preserving lives in case of a real fire (temperatures, radiation, smoke layer height) as well as parameters closely linked to the flow characteristics (same parameters and velocity). Apart from physical parameters the CPU-Time is included to provide an indication of the "cost" of the simulation e.g. in case of varying number of solid angles, etc.

Table 4. Output parameters considered (results found in Table 6).

Physical parameters
Temperature at corner (at 1 m height and 2 m height)
Radiation at corner (at 1 m height and 2 m height)
Smoke layer temperature
Velocity at door opening (outflow max. and inflow max.)
Smoke layer height (three methods: NFPA, FDS and visual evaluation)
Program parameters
CPU-Time

The smoke layer height is evaluated by three different methods: The built-in method in FDS based on temperature assuming two-zone behaviour of the fire scenario [4]. The method of NFPA (National Fire Protection Association, USA) which is also based on the temperature distribution and an empirical interpolation constant [9]. Finally, visual inspection of the output visualised in the FDS graphical output tool "Smokeview". It is obvious that all three methods work the best in case of an "ordinary" fire with strong vertical temperature and smoke (soot) gradients. In case of a fire with a low rate of heat release the two former methods may fail [10].

RESULTS

The input parameter distributions applied in a total of 40 CFD simulations (determined according to the method of Elementary Effects) are shown in Table 5. The corresponding output is found in Table 6. On the basis of the input and the output the elementary effects (equation 1) are calculated and the corresponding mean value and standard deviations are used to create the graphs shown in Figure 4.

Figure 3 provides an example of the transient solution regarding temperature and velocity at a certain location to indicate the principle of generation of steady-state results. The time-varying case is stopped when the behaviour of the output parameters is reasonably steady-state. Then a mean value of sufficient time-duration is taken as the steady-state result.
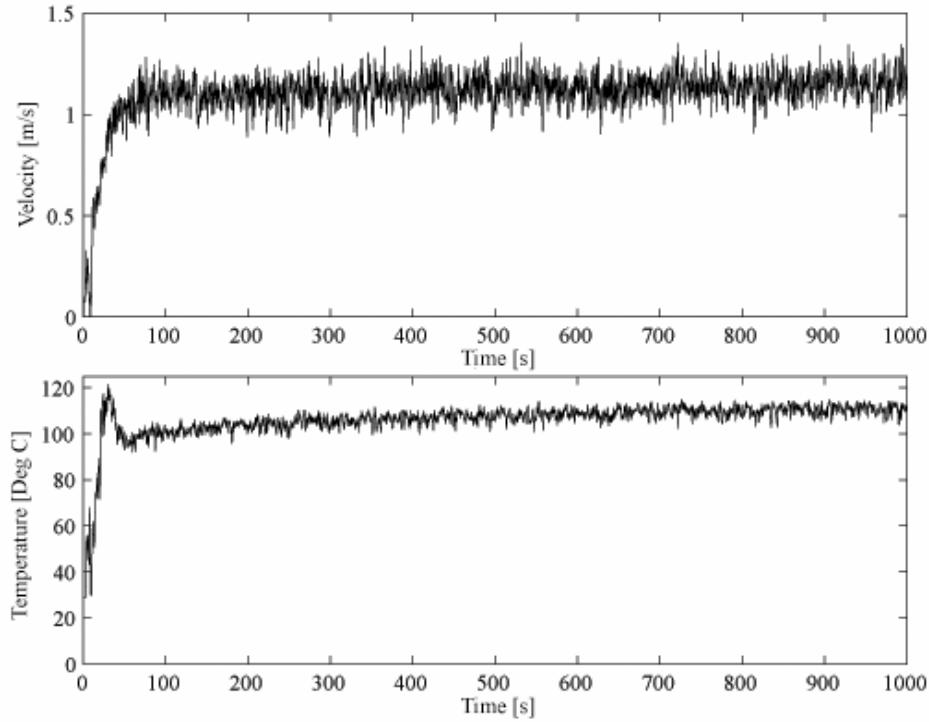
Figure 3. Example of output from the fire dynamics simulations. Time series of velocity (top) and temperature (bottom). The results presented in Table 6 are taken as average values at steady-state conditions at the end of each transient simulation.

DISCUSSION

The graphs in Figure 4 provide the basis for evaluation of the sensitivity of each of the output parameters subject to variation of the input parameters. The broken lines on each graph facilitate the evaluation. If a point lies above the broken line there is a reasonable probability that the factor acts in a nonlinear way or that it is correlated with other parameters and cannot be treated as an independent parameter.

Overall it is seen that several parameters indicate a nonlinear behaviour and/or correlation with other input parameters. This may be important to consider if further analysis is undertaken. It indicates that the behaviour of a certain parameter may depend significantly on the "status" of other parameters which stresses the importance of global sensitivity analysis.

The *temperature at the corner* (especially at a height of 2 m) is highly influenced by the heat release, fire location, opening area, fire geometry and the Smagorinsky constant - ranked in order of importance. The influence is found to be very strong for most of the mentioned parameters and should definitely be considered when fire scenarios are evaluated. The same conclusion applies approximately for the *smoke layer temperature*.

The *radiation at the corner* is influenced significantly by the fire geometry, radiation model, opening area, heat release and fire geometry. The importance of the radiation model stresses the existing knowledge that proper modelling of radiation is crucial.

Table 5. Input parameter variation for the sensitivity analysis comprising 40 simulation cases generated according to the variations in Table 2 using the principles of the method of Elementary Effects.

Sim. No.	Heat Release (%)	Fire Geometry	Fire Location	Fuel Type	Solid Angles	Radiation Model	Initial Temp. (Deg C)	Opening Size (%)	Smagorinsky
1	130	b	a	Polyurethane	60	Grey Gas	29	100	0.10
2	130	b	a	Polyurethane	60	No Radiation	29	100	0.10
3	130	a	a	Polyurethane	60	No Radiation	29	100	0.10
4	130	a	b	Polyurethane	60	No Radiation	29	100	0.10
5	130	a	b	Methane	60	No Radiation	29	100	0.10
6	130	a	b	Methane	60	No Radiation	29	125	0.10
7	70	a	b	Methane	60	No Radiation	29	125	0.10
8	70	a	b	Methane	104	No Radiation	29	125	0.10
9	70	a	b	Methane	104	No Radiation	24	125	0.10
10	70	a	b	Methane	104	No Radiation	24	125	0.20
11	70	a	c	Wood	104	9 Band	29	125	0.10
12	70	b	c	Wood	104	9 Band	29	125	0.10
13	70	b	c	Wood	104	9 Band	24	125	0.10
14	70	b	a	Wood	104	9 Band	24	125	0.10
15	70	b	a	Wood	200	9 Band	24	125	0.10
16	70	b	a	Wood	200	No Radiation	24	125	0.10
17	70	b	a	Wood	200	No Radiation	24	75	0.10
18	130	b	a	Wood	200	No Radiation	24	75	0.10
19	130	b	a	Wood	200	No Radiation	24	75	0.25
20	130	b	a	Polyurethane	104	9 Band	24	75	0.25
21	100	a	c	Polyurethane	60	9 Band	29	75	0.25
22	100	a	c	Polyurethane	60	9 Band	29	75	0.25
23	100	a	c	Polyurethane	60	9 Band	29	125	0.25
24	70	a	c	Polyurethane	60	9 Band	29	125	0.25
25	70	b	c	Polyurethane	60	9 Band	29	125	0.25
26	70	b	c	Wood	60	9 Band	29	125	0.25
27	70	b	c	Wood	60	9 Band	34	125	0.25
28	70	b	b	Wood	60	9 Band	34	125	0.25
29	70	b	b	Wood	60	Grey Gas	34	125	0.25
30	70	b	b	Wood	60	Grey Gas	34	125	0.20
31	100	b	c	Polyurethane	60	9 Band	34	75	0.25
32	100	b	c	Polyurethane	60	9 Band	34	100	0.25
33	100	b	c	Wood	60	9 Band	34	100	0.25
34	100	b	c	Wood	60	9 Band	34	100	0.20
35	100	b	c	Wood	60	9 Band	29	100	0.20
36	100	b	b	Wood	60	9 Band	29	100	0.20
37	100	b	b	Wood	104	9 Band	29	100	0.20
38	100	b	b	Wood	104	Grey Gas	29	100	0.20
39	130	b	b	Wood	104	Grey Gas	29	100	0.20
40	130	a	b	Wood	104	Grey Gas	29	100	0.20

Table 6. Output results corresponding to input parameters defined in Table 5.

| Sim. No.	Temperature at Corner [°C] Height 2 m	Height 1 m	Radiation at Corner [W/m²] Height 2 m	Height 1 m	Smoke Layer Temp. [°C]	Velocity at Door Opening [m/s] Outflow Max.	Inflow Max.	Smoke Layer Height [m] NFPA	FDS	Visual	CPU Time [hours]
1	124.00	84.20	4.42	4.80	115.00	1.87	0.93	0.76	0.34	0.24	15.97
2	115.00	59.90	1.89	1.89	104.00	1.71	0.83	0.98	0.93	0.17	13.83
3	105.00	42.30	1.89	1.89	94.00	1.68	0.75	0.88	0.56	0.31	13.67
4	184.00	31.10	1.89	1.89	162.00	1.84	0.48	1.52	1.07	0.81	20.37
5	205.00	32.00	1.89	1.89	179.00	2.02	0.51	1.50	1.05	1.06	20.23
6	191.00	29.10	1.89	1.89	170.00	1.66	0.33	1.58	1.20	1.13	20.44
7	126.00	29.10	1.89	1.89	115.00	1.34	0.31	1.54	1.19	1.13	26.26
8	126.00	29.10	1.89	1.89	115.00	1.34	0.31	1.54	1.19	1.13	15.84
9	118.00	24.10	1.77	1.77	107.00	1.33	0.30	1.56	1.18	1.18	26.01
10	151.00	24.00	1.77	1.77	155.00	1.40	0.22	1.78	1.35	1.24	13.38
11	109.00	30.70	3.37	2.56	105.00	1.04	0.21	1.52	1.39	1.24	52.63
12	103.00	30.90	3.25	2.56	99.40	1.07	0.24	1.44	1.29	1.21	49.57
13	97.30	25.70	3.05	2.40	93.80	1.08	0.23	1.46	1.32	1.24	49.81
14	72.90	41.10	2.97	3.02	66.30	1.24	0.62	1.00	0.46	0.90	32.20
15	72.20	38.70	2.87	2.92	65.50	1.24	0.61	1.14	0.49	1.00	79.95
16	66.50	32.60	1.77	1.77	59.60	1.17	0.57	1.24	0.56	0.86	9.47
17	120.00	96.70	1.77	1.77	112.00	2.07	1.59	0.74	0.21	0.29	11.04
18	175.00	139.00	1.77	1.77	161.00	2.57	1.92	0.80	0.20	0.24	17.01
19	189.00	127.00	1.77	1.77	166.00	2.88	1.99	0.66	0.25	0.32	9.62
20	181.00	129.00	1.77	1.77	168.00	2.88	2.02	0.62	0.25	0.06	9.51
21	183.00	44.80	7.70	3.69	155.00	2.16	0.93	1.42	0.94	0.93	38.89
22	182.00	45.60	7.69	4.53	153.00	2.15	0.94	1.42	0.93	0.94	43.08
23	155.00	32.80	5.88	4.31	154.00	1.09	0.27	1.68	1.56	1.00	48.82
24	124.00	31.70	4.34	3.33	119.00	0.93	0.26	1.68	1.53	1.24	29.36
25	117.00	31.50	3.95	2.98	110.00	0.96	0.23	1.68	1.47	1.18	26.45
26	115.00	31.40	3.93	2.90	116.00	1.00	0.21	1.74	1.48	1.29	27.53
27	121.00	36.30	4.16	3.07	127.00	0.99	0.20	1.74	1.54	1.24	27.35
28	116.00	37.30	3.95	3.02	118.00	1.02	0.27	1.78	1.42	1.15	27.84
29	119.00	37.10	3.80	3.01	120.00	1.05	0.28	1.82	1.46	1.29	10.00
30	109.00	36.80	3.71	2.99	114.00	1.03	0.57	1.84	1.43	1.29	11.25
31	173.00	52.70	7.36	4.11	147.00	2.14	1.08	1.56	0.80	0.81	30.37
32	156.00	40.10	6.01	3.98	135.00	1.28	0.37	1.68	1.29	1.13	38.26
33	162.00	39.60	5.96	3.83	147.00	1.29	0.34	1.68	1.36	1.21	30.51
34	162.00	39.50	5.91	3.83	145.00	1.29	0.34	1.62	1.33	1.18	45.84
35	161.00	34.20	5.72	3.65	142.00	1.31	0.34	1.64	1.34	1.22	35.52
36	140.00	36.20	4.95	3.37	128.00	1.38	0.40	1.70	1.25	1.18	35.37
37	138.00	35.40	4.94	3.46	130.00	1.39	0.40	1.74	1.26	1.20	40.29
38	142.00	36.00	4.65	3.49	131.00	1.41	0.40	1.68	1.26	1.20	13.35
39	164.00	38.70	5.67	4.02	149.00	1.55	0.45	1.64	1.25	1.22	14.69
40	219.00	44.90	9.90	5.62	193.00	1.97	0.53	1.68	1.17	1.13	38.73
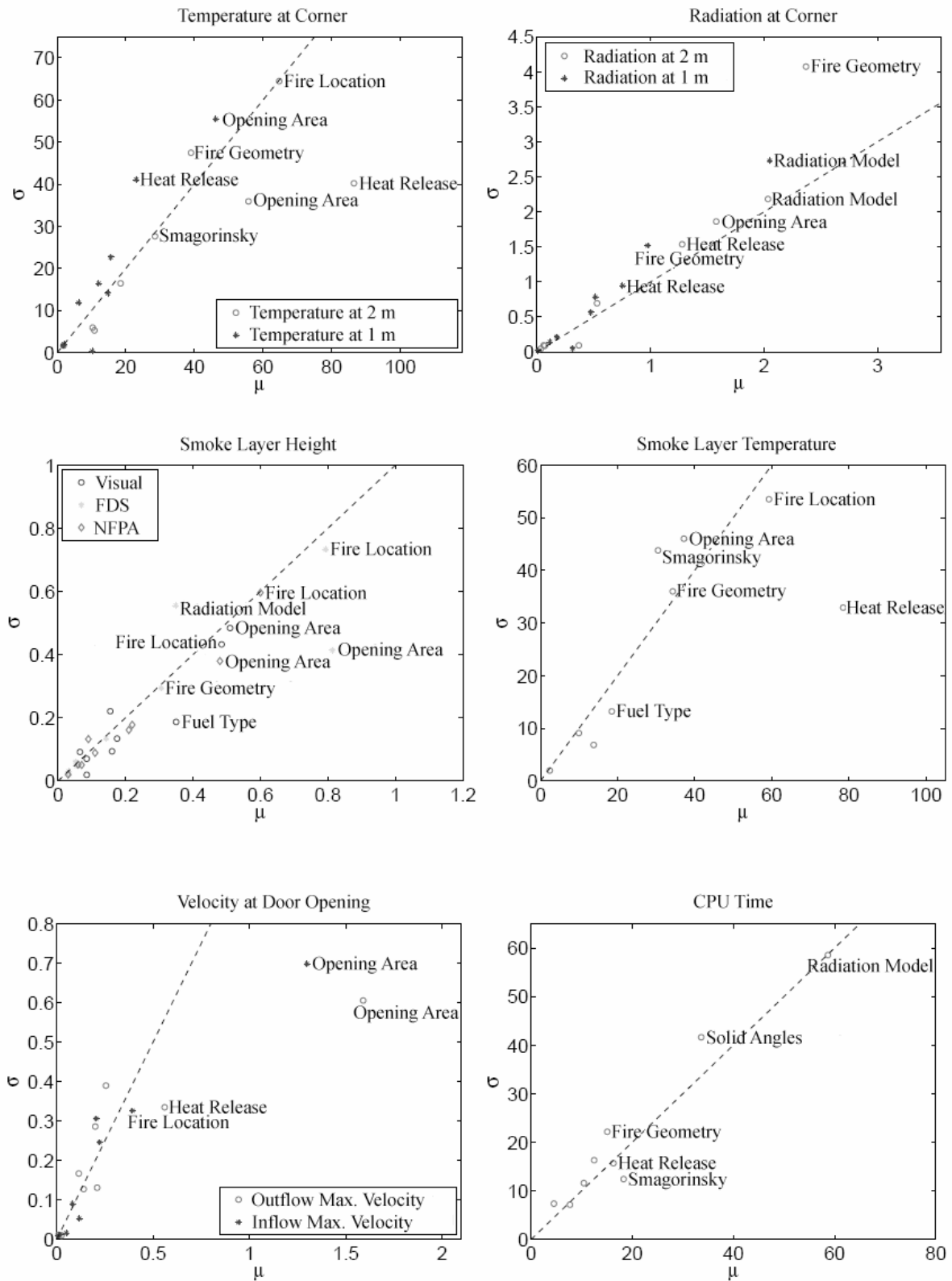
Figure 4. Presentation of results from the screening sensitivity analysis (based on data from Tables 5 and 6) using the method of Elementary Effects. μ and σ are the mean value and the standard deviation of the elementary effects, respectively. The broken lines indicate where μ equals σ to facilitate easy evaluation of the results.

The *smoke layer height* is another parameter that may be crucial to the security of people in case of a fire. An interesting result is that the sensitivity depends heavily on the method of evaluation of the smoke layer height. Thus, further work on this area should be undertaken to establish proper numerical methods or procedures to evaluate the smoke layer height in accordance with physical measurements. Fire location and opening area are considered important for all three methods. The FDS method considers radiation model and fire geometry important, too. The visual method includes fuel type as an important parameter.

The *velocity at the door opening* is strongly dependent on the opening area, which is not surprising. Heat release and fire location are also found to exert an influence on the velocity even though it is less significant.

CPU-Time is included to assess the cost of the simulations. It is found that the CPU-Time depends significantly on all considered "program parameters", especially the choice of radiation model and number of solid angles. Apart from that choice of Smagorinsky constant, heat release and fire geometry may influence the simulation cost.

In general it is found that the fire dynamics simulations show a very significant sensitivity towards a high number of input parameters. Deviations of 100% of an output parameter in case of "expected" variation of input parameters is not impossible. Unfortunately most input parameters in fire dynamics simulations are by nature quite uncertain. This adverse combination stresses the importance of proper estimation of the uncertainty of fire dynamics simulations. Even though the present results relate to a specific case, evidence seems to underline the statement that fire dynamics simulation results should never be accepted and applied in practise unless proper sensitivity analysis and uncertainty estimation have been carefully undertaken.

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