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# Computer Simulations Using Complex Numerical Pyrolysis and Suppression Models

**Abstract**

This article describes possibilities offered by the existing fire spread and fire suppression models available in the Fire Dynamics Simulator. A theoretical example was provided of a computer analysis using experimental models of pyrolysis and sprinkler models. One of the most important factors that affect results of building safety computer analysis if the heat release rate (HRR) obtained in the model. It may be defined in many ways in computer programmes. Use may be made of the basic method, i.e. a defined value of HRR may be entered, independently of simulation conditions. A more advanced method comprises calculation of HRR from the model by simulating pyrolysis processes. Selection of a method for modelling HRR also defines possibilities related to modelling effects of water suppression. Modelling fire suppression by water must take into account three most important elements: moving of water droplets through the air, transporting the water along the solid surface, and predicting the decreasing of the burning rate. The basic method is to modify HRR curve. More advanced methods allow the user to model decay phase depending on amount of water which reaches fire area.

**Keywords:** pyrolysis modelling, modelling fire suppression, flame spread, CFD simulation, FDS

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# Symulacje komputerowe z wykorzystaniem zaawansowanych modeli numerycznych pirolizy i gaszenia wodą

**Abstrakt**

W niniejszym artykule zaprezentowano możliwości opracowanych modeli rozwoju pożaru i działania tryskaczy, które są dostępne w programie Fire Dynamics Simulator. Przedstawiono

teoretyczny przykład analizy komputerowej z wykorzystaniem eksperymentalnych modeli pirolizy i gaszenia wodą. Jednym z najbardziej istotnych czynników mających wpływ na wyniki analizy komputerowej bezpieczeństwa budynku ma uzyskana w modelu szybkość uwalniania ciepła (z ang. *Heat Release Rate*, HRR). W oprogramowaniu komputerowym może być ona definiowana na wiele sposobów. Można skorzystać z podstawowej metody, czyli wprowadzić określoną wartość HRR, niezależną od warunków symulacji. Bardziej zaawansowany sposób to wyliczanie HRR z modelu poprzez symulowanie procesów pirolizy. Wybór metody modelowania HRR definiuje również możliwości w zakresie modelowania efektów gaszenia wodą. Modelowanie tłumienia ognia przez wodę musi uwzględniać opis trzech zjawisk: transport kropelek wody w powietrzu, przepływ wody wzdłuż stałej powierzchni oraz przewidywanie zmniejszenia się szybkości spalania. Podstawowy sposób to modyfikacja szybkości uwalniania ciepła lub założenie ograniczonej powierzchni pożaru. Bardziej zaawansowane metody pozwalają na modelowanie fazy gaszenia przez program, w zależności od ilości wody, która dociera do strefy spalania.

**Słowa kluczowe:** modelowanie pirolizy, modelowanie gaszenia, rozwój pożaru, symulacje CFD, Fire Dynamics Simulator

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## Комп›ютерне моделювання з використанням передових чисельних моделей піролізу та гасіння водою

**Анотація**

У цій статті представлені можливості розробки моделей розвитку пожежі та роботи спринклерних систем, які доступні у програмі Fire Dynamics Simulator. Наведено теоретичний приклад комп'ютерного аналізу з використанням експериментальних моделей піролізу та гасіння водою. Одним з найважливіших факторів, що впливає на результати комп'ютерного аналізу безпеки будівлі, є отриманий у моделі рівень викиду тепла (*Heat Release Rate*, HRR). Його можна визначати багатьма способами в комп'ютерному опрограмуванні. Можна використати основний метод, тобто ввести конкретне значення HRR, незалежне від умов моделювання. Більш досконалим методом є обчислення HRR шляхом моделювання процесів піролізу. Вибір методу моделювання HRR також визначає можливості моделювання ефектів гасіння водою. При моделюванні гасіння вогню водою необхідно врахувати опис трьох явищ: транспортування крапель води

у повітрі, приплив води вздовж твердої поверхні та прогнозування зниження рівня горіння. Основний метод – це зміни рівня виділення тепла або встановлення обмеженої поверхні пожежі. Більш досконалі методи дозволяють моделювати фазу гасіння за допомогою програми залежно від кількості води, яка доходить до зони горіння.

**Ключові слова:** моделювання піролізу, моделювання гасіння, розвиток пожежі, моделювання CFD, Fire Dynamics Simulator

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## 1. Introduction

The use of computer-based fire models is increasingly popular in assisting the designing of fire protection systems. The major part of analyses that use of computer simulations are based on the assumption of the so-called design fire. In such an assumption the heat release rate, i.e. the HRR curve, is defined as a component of input data for simulations. In numerous cases fire safety engineers need to assess the functioning effectiveness of the sprinkler system. As a rule the applied models assume only a change in the rate of the release of heat from a fire by adopting a limited fire surface. However, the FDS programme [1] allows the adoption of a simplified water extinguishing model, which had been developed pursuant to studies carried out by H.Z. Yu, J.L. Lee and H.C. Kung [2]. Reducing the fire severity as an effect of the impact of water has been presented in equation No. 1:

$$\dot{Q} = \dot{Q}_0 e^{-k(t-t_0)} \tag{1}$$

where:
$\dot{Q}$ – fire severity in time t [kW]
$t_0$ – time of sprinkler activation (commencement of fire suppression) [s]
$\dot{Q}_0$ – fire severity while sprinkler is being activated (commencement of fire suppression) [kW]
k – fire suppression constant [s].

The "k" constant may be determined on the basis of studies conducted by D. Madrzykowski and R.L. Vettori [3], as well as according to data developed by Evans [4].

The calculated value is entered to the FDS programme as the "a" constant, calculated according to formula 2:

$$k(t) = a\, m_w\,(t) \tag{2}$$

where:
$m_w$ – mass of water per surface unit [kg/m$^2$]

However, for the above mentioned method also assumed is the fire model based on the so-called "gas burner concept" [1].

On the other hand, one of basic phenomena that occur during the flame spread is the thermal decomposition reaction. In a more advanced model data may be entered for the pyrolysis reaction, i.e. the decomposition of material under the impact of temperature in anaerobic conditions [1]. The phenomenon of thermal decomposition is related to mass loss, which is associated with an increase in released heat. The total power released from the pyrolysis reaction depends on the reaction heat of the tested material and combustion heat. The phenomenon of decomposition takes place once a certain temperature has been reached, the so-called reference temperature. Another vital parameter is also the temperature range/scope, at which mass decomposition takes place. The course of pyrolysis differs for each type of material. Given the above, in the present publication only takes into account the combustion of polyurethane foam, a frequent component of items and elements of furnishings in premises.

At present the most notable study that sums up the hitherto state of studies and presents new digital modelling methods related to the combustion of polyurethane foam is the work of Denis Pau: *Comparative Study on Combustion Behaviours of Polyurethane Foams with Numerical Simulations using Pyrolysis Models* [5]. The objective of publication [5] was to enhance the presently available knowledge related to thermal decomposition and combustion of given types of polyurethane foam. Modelling of such combustion is complicated, because high temperature makes foam decompose not only into gasesous forms of toluene diisocyanate (jointly called TDI), but also liquid polyol. The thermal decomposition process of foam progresses in two stages:

- first reaction: polyurethane foam → molten fraction (polyol) + gas (isocyanate),
- second reaction: molten fraction (polyol) → carbonised fraction + gas (polyol, $H_2CO$, $H_2O$ and $CH_4$)

During the implementation of doctoral dissertation [5] laboratory testing was conducted to obtain a precise determination of physical properties of selected types of polyurethane foam. The tested properties were as follows: viscosity, proper heat, conductivity, combustion heat, reaction heat, reference temperature, speed of reaction and activation energy. The activation energy, a pre-exponential factor, as well as the reaction order for the first and second reaction, has been determined with the use of thermal gravimetric analysis (TGA). Parameters set out by the measurement apparatus were used to define the kinetics of thermal decomposition reaction according to the equation:

$$\frac{d(m/m_0)}{dt} = A\exp\left(\frac{-E}{RT}\right)(m/m_0) \tag{3}$$

where:
m – temporary mass of sample
$m_0$ – initial mass of sample
A – pre-exponential factor
E – activation energy
R – gas constant
T – reaction temperature

Reaction heat ($\Delta h_r$) was determined based on an analysis of changes of heat and mass of the sample, tested with the use of the method of differential scanning calorimetry (DSC). Physical and thermal properties of polyurethane foam, such as the heat conductivity factor, were determined using a non-stationary method (hot disk). Combustion of a sample of polyurethane foam was carried out in a cone calorimeter. Tests were carried out of the processes of combustion and thermal decomposition of specific types of polyurethane foam. The performed testing allowed the description of physical and chemical processes that take place during the process of pyrolysis. In addition a set of data was worked out to describe combustion properties of selected types of polyurethane foam. The precise determination of physical properties of the combustible material, such as density, heat conductivity, proper heat, reaction heat or temperature at which the mass loss rate is the highest (the so-called reference temperature), is of key importance in computer modelling of flame propagation. It is necessary to enter the above mentioned data to make full use of advanced models of pyrolysis and combustion implemented in the Fire Dynamics Simulator programme [1].

Dissertation [5] allowed the development of a scheme for entering input data to the pyrolysis model. The scheme takes into account a two-stage course of the decomposition

reaction of polyurethane foam. The publication author compared two methods of setting out reaction parameters to the model: advanced model making use of genetic algorithms and the direct determination of parameters of materials used in the conducted testing. During entering of adjusted coefficients, an enhancement was ascertained in precision of the model for simulation of combustion in the cone calorimeter. However, the ultimate objective of the dissertation was making a comparison of the model with studies performed at a bigger scale. Reducing the value of activation energy $E$ and/or increasing the value of pre-exponential factor $A$ leads to a reduction in the intensity of thermal decomposition of the material. The author has proven the necessity of reducing the activation energy value in the model to gain results comparable with the testing conducted in the furniture calorimeter. Ultimately the model was validated successfully with respect to obtained HRR curves during an experiment involving combustion of a panel of polyurethane foam [5, 6].

## 2. Methods and tools

A detailed analysis necessary to obtain results included in the present article was made with the use of the Fire Dynamics Simulator programme version 5.5.3 [7] and 6.7.0 [1]. This programme was developed by the NIST (National Institute of Standards and Technology), situated in the United State. FDS is a computer tool designated for fire modelling. The programme enables analyses of the transport of heat and combustion products generated as a result of the fire, as well as heat exchange, convection and radiation. Also possible is modelling the activation of smoke and heat deetectors, operation of sprinkler systems, including also the impact of water droplets on the flames [1].

The application makes use of the *Computational Fluid Dynamics* method (CFD). The programme solves numerically the form of the Navier-Stokes equations. The modelling comprises flows of relatively small velocities (i.e. lower than the speed of sound $< 300$ m/s) and incompressible fluids, i.e. gases, in the case of which it is possible to omit density changes at small flow velocities. The FDS programme enables modelling of turbulences, both with the use of the DNS method (Direct Numerical Simulation), as well as the LES technique (Large Eddy Simulation). The DNS method is not used in engineering applications due to the necessity of applying large computational capacity. The most frequently used LES method assumes that the biggest flow scales (eddies) are calculated directly from transport equations. Insignificant eddy movements are modelled at a certain approximation or omitted [8].

In the analysis use was made of a regular cubic mesh with side length of 10 × 5 cm. The mesh dimensions have been chosen pursuant to dissertation [5] and guidelines of NUREG published also in the FDS6 User's Guide [1]. The calculation of the time leap in the FDS programme is done maintaining the CFL criterion (formula No. 4).

$$CFL = \delta t \frac{||\mathbf{u}||}{\delta x} < 1 \tag{4}$$

The time leap is calculated in an automatic way in accordance with one of three schemes related to standardisation methods of the velocity vector. The default scheme for the applied 6.7.0 version is the $L_\infty$ scheme:

$$\frac{||\mathbf{u}||}{\delta x} = max\left(\frac{|u|}{\delta x}, \frac{|v|}{\delta y}, \frac{|w|}{\delta z}\right) + |\nabla \cdot \mathbf{u}| \tag{5}$$

The equation of radiation transport for grey gas is solved with the use of FVM – *Finite Volume Method*. This method divides the entire radiation spectrum into a few frequency intervals (typically 6) and makes use of them in the full form of radiation transport equations. Those intervals are selected to match spectrum bands of substances present in the set. A part of the flux of the fire severity emitted as radiation is constant and is one of the simulation parameters. A default value of radiation fraction of 35% was assumed that conforms to combustion of the major part of plastics [1].

Use was made of the *mixing-controlled* combustion model (combustion takes place in the gaseous phase). This model assumes that the stechiometric composition of a flammable mixture is defined by a mass fraction of combustible gases and combustion products and air. It is also assumed that combustion takes place immediately after mixing and is single-phase and complete. In addition the percentage of generated carbon oxide is constant and arises from initial assumptions of the simulation, and not from real combustion conditions. Those assumptons allow achieving correct results for fires controlled by fuel, such as for example in the assumed simulations [1]. Polyurethane foam has been adopted as a combustibe material. Flammable properties were compiled in table 1.

**Table 1. Parameters of combustion reactuion in the gaseous phase used in the simulation**

| | |
|---|---|
| heat of combustion [kJ/kg] | 26200 |
| mass fraction of smoke | 0.13 |

**Continued Table 1.**

| | |
|---|---|
| mass fraction of carbon oxide | 0.01 |
| ratio of atoms of carbon: hydrogen : oxygen (scenario no. 1) | 1 : 1.75 : 0.25 |
| ratio of atoms of carbon: hydrogen : oxygen : nitrogen (scenario no. 2) | 1 : 1.77 : 0.31 : 0.06 |
| mass extinction coefficient $K_m$ [$m^2$/kg] | 8700 |

Source: [9]

Table 2 presents values assumed for modelling the thermal decomposition reaction of polyurethane foam.

**Table 2. Values of particular materials adopted for simulations of pyrolysis of polyurethane foam**

| property of material | adopted values | | |
|---|---|---|---|
| λ [W/mK] | T ≤ 222°C<br>0.049 | 222°C ≤ T ≤ 310°C<br>0.049–0.186 | T ≥ 310°C<br>0.186 |
| $C_p$ [J/kgK] | T ≤ 222°C<br>2996 | 222°C ≤ T ≤ 310°C<br>2996–2053 | T ≥ 310°C<br>2053 |
| ρ [kg/$m^3$] | 297 | | |
| $d$ [mm] | 10.40 mm | | |
| $E_1$ [kJ/mol] | 58.2 | | |
| $A_1$ [$s^{-1}$] | $6.82 \times 10^4$ | | |
| $n_1$ | 0.00 | | |
| $\Delta hr_1$ [J/g] | 1357 | | |
| $E_2$ [kJ/mol] | 159.9 | | |
| $A_2$ [$s^{-1}$] | $1.25 \times 10^7$ | | |

**Continued Table 2.**

| | |
|---|---|
| $n_1$ | 0,00 |
| $\Delta hr_2$ [J/g] | 218 |
| $\Delta h_{c,eff}$ [MJ/kg] | 25 |

Source: [5]

Polyurethane foam has been introduced to FDS via the OBST function as a cuboid element consisting of two layers: foam of defined properties (upper layer with a thickness of a single computational cell) and default INERT material (lower layer, the remaining part of the drawn-in block). The adopted resolution of the computational grid is 5 cm. The ignition source, i.e. a linear burner, has been defined as a vertical flat element placed against the border of foam block. The element has properties of INERT. A boundary condition that specifies the heat release rate has been assigned to the defined surface. A constant of fire severity HRRPUA = 500 kW/m$^2$ has been assumed, which for a burner surface of 0.050 m$^2$ assures a total capacity of 25 kW. Dimensions of the burner of 5 cm × 10 cm are identical to dimensions of the foam block border. Using the function of STRETCH_FACTOR=1 a uniform resolution of the computational grid for the heat transfer model in the element was assured. The FDS programme calculates as default the grid resolution in constant elements from the formula $\sqrt{\lambda/\rho C_p}$. Using the function of CELL_SIZE_FACTOR=0.43 an adjustement was made of the default value dso that the resolution equalled to 0.1 mm. Also assumed was a default parameter for the function BACKING=VOID, on the presumption that the reverse side of the material adheres to the air void at ambient temperature. In the REAC function, which defines parameters for combustion reaction in the gaseous phase, adopted was the FORMULA=$C_{1.00}H_{1.77}O_{0.31}N_{0.06}$ (foam type: NFR-SB-31) [5].

In the FDS programme [1] a fire suppression curve consistent with equation (1) may be obtained by entering to the input file of the E_COEFFICIENT parameter in the function of &SURF (fire surface). The programme will then compute the course of the burning out curve depending on the mass of water that reaches the assumed fire area. Calculation of the burning out phase is made with the use of the expotential function on the presumption that the density of fire severity [kW/m$^2$] decreases pursuant to dependence No. 6:

$$q(t) = q_0(t)\, e^{-\int k(t)dt} \tag{6}$$

where:
$q(t)$ – heat release rate per surface unit, without water inflow [kW/m$^2$]
$k(t)$ – function reflecting the mass of water, which falls on a surface unit [kg/m$^2$]

Parameter $k(t)$ may be expressed by formula 7:

$$k(t) = am_W(t) \tag{7}$$

where:
$a$ – experimentally determined constant that depends on the type of material, storage and sprinkling intensity [s$^{-1}$]

The "$a$" constant was entered to the input file via the E_COEFICCIENT function [1]. The calculations have been made for the sprinkling intensity of 0.041 mm/s [4].

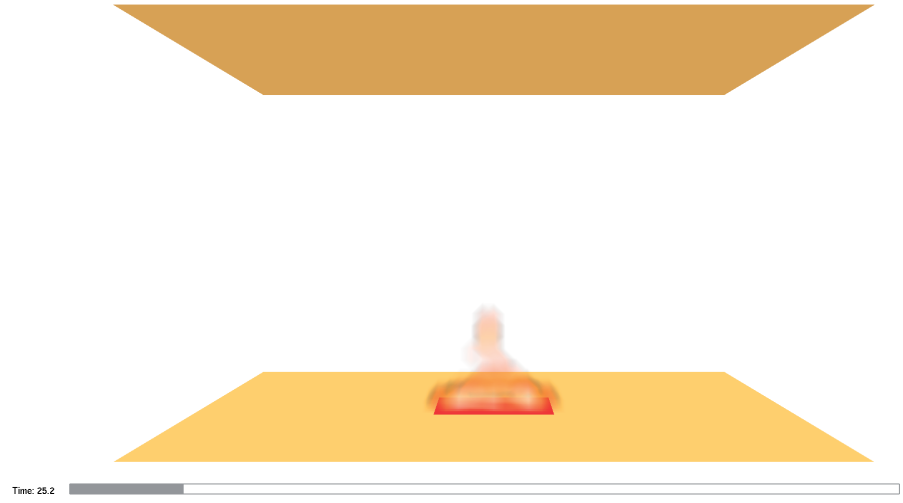
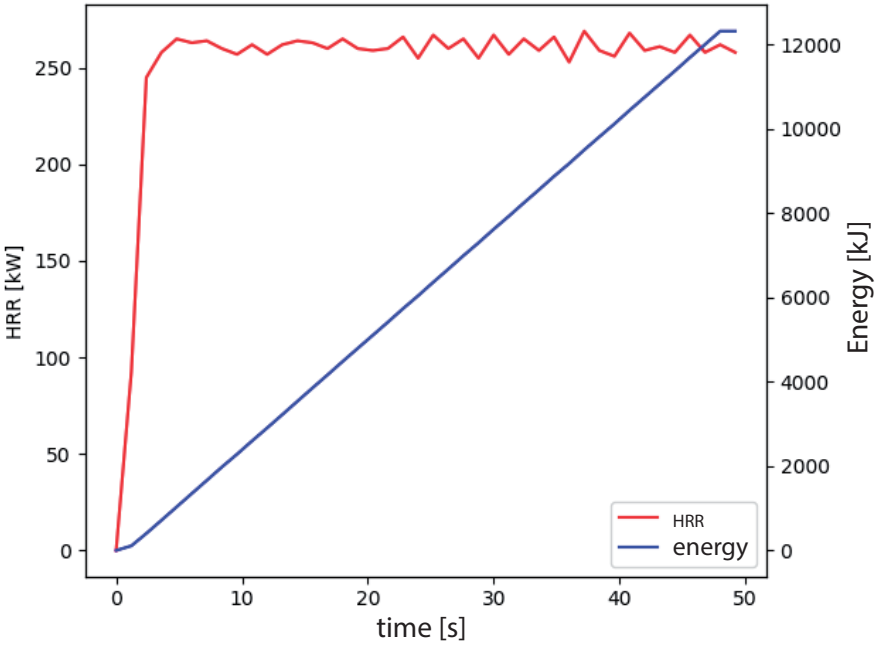
To verify the pyrolysis and fire suppression model, four simulations were carried out in the Fire Dynamics Simulator programme:

- simulation No. 1: modelling of a fire with the use of a simplified pyrolysis model,
- simulation No. 2: fire suppression modelling using the E_COEFFICIENT parameter,
- simulation No. 3: modelling of a fire with the use of an advanced pyrolysis model,
- simulation No. 4: modelling interactions of the advanced pyrolysis and fire suppression model.

## 3. Results of simulations

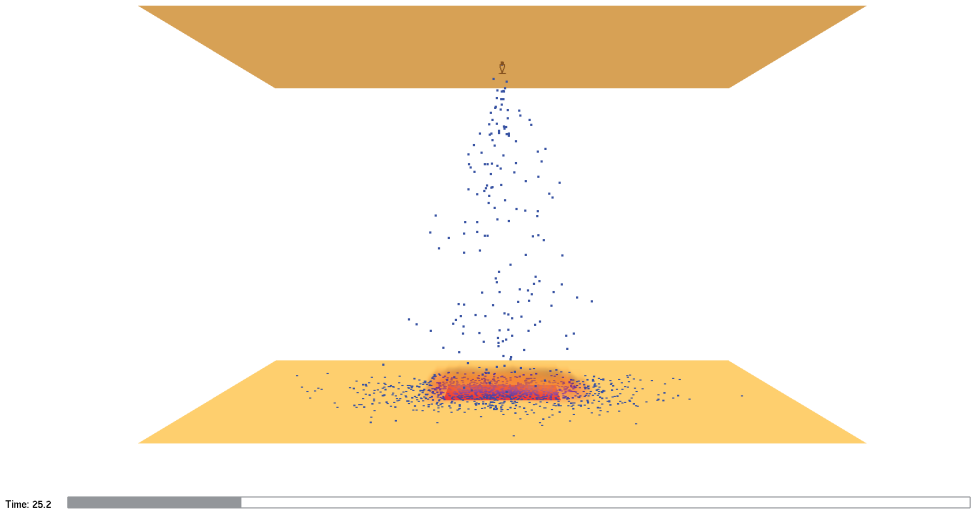
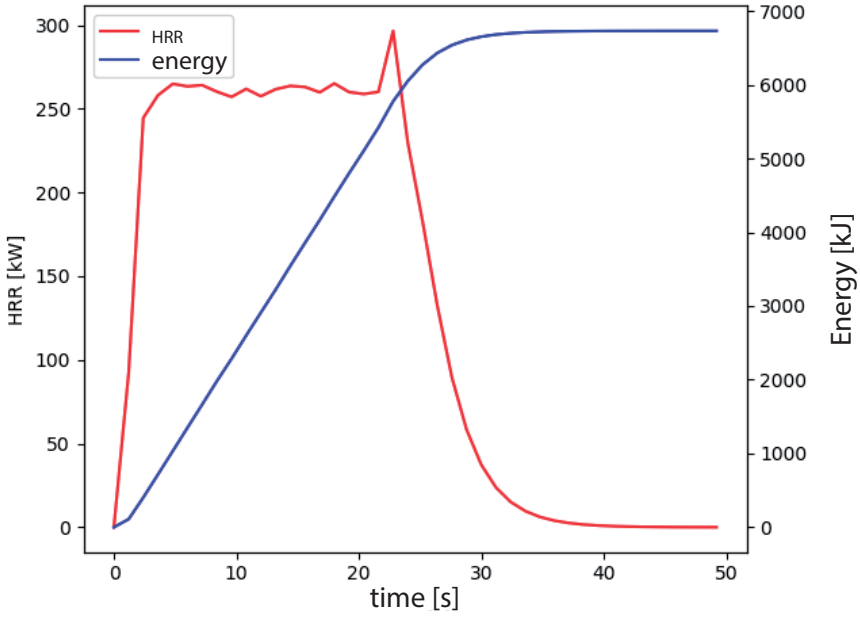
Tables 3, 4, 5 and 6 contain a specification of results obtained from the conducted simulations. Graphics contained in the tables show a visualisation of calculations and diagrams of energy release from the modelled fire. The view from simulations had been executed in the Smokeview programme, which is generally used for needs of making graphical interpretations of results obtained in the FDS programme [1]. The diagrams were generated with the use of a script written in the Python programming language. The script plotted results from .csv files generated by the FDS programme.

**Table 3. Results obtained in simulation No. 1**

| Visualisation at 25 s of calculations |
|---|
|   |
| Diagram of heat release rate |
|   |

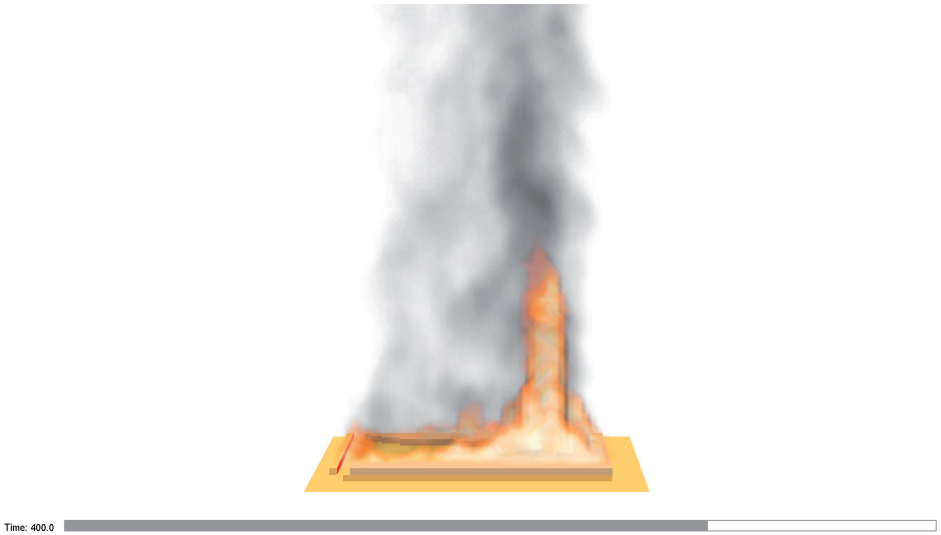
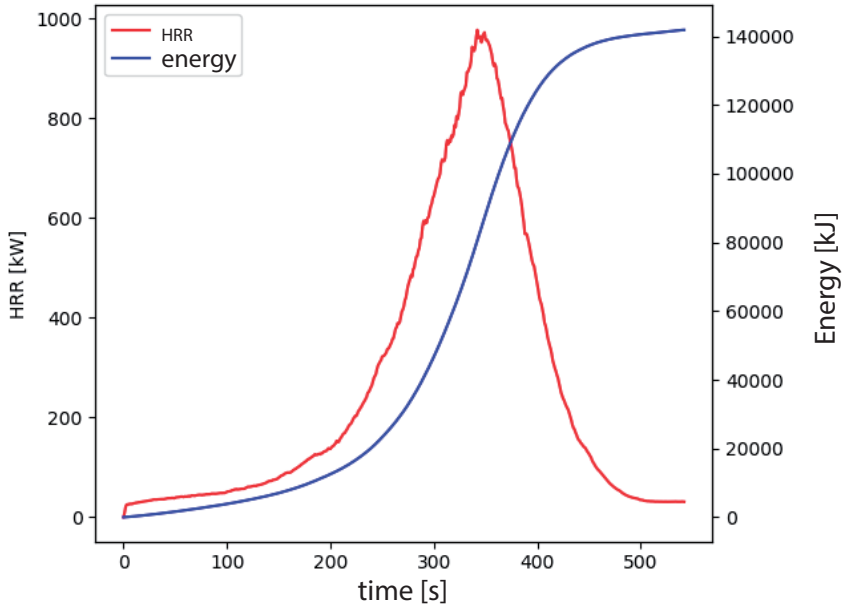
Source: [5]

**Table 4. Results obtained in simulation No. 2**

| Visualisation at 25 s of calculations |
| --- |
|   |
| Diagram of heat release rate |
|   |

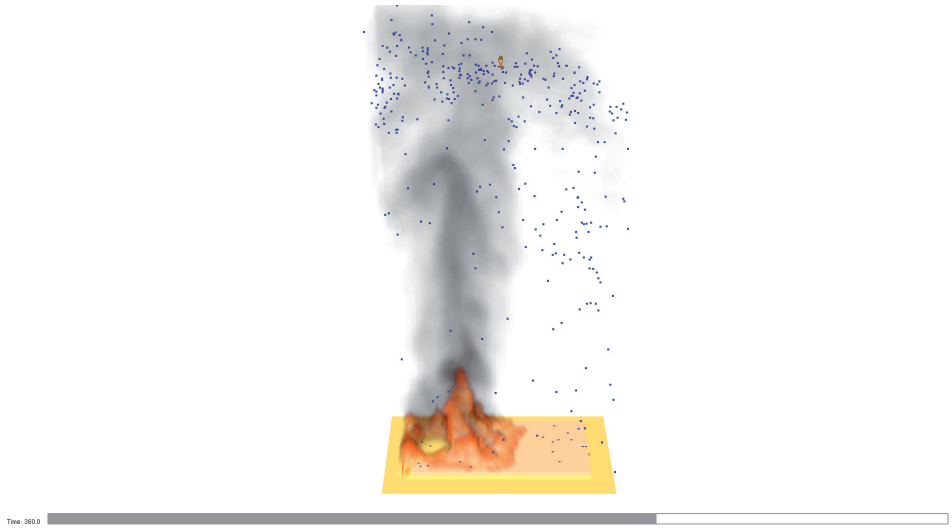
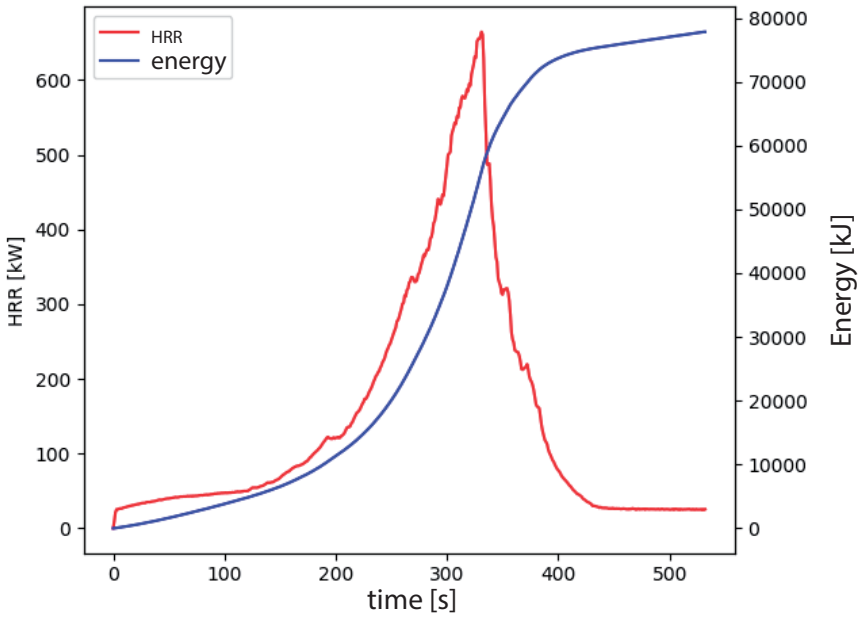
Source: [5]

**Table 5. Results obtained in simulation No. 3**

| Visualisation at 400 s of calculations |
|---|
|   |
| Diagram of heat release rate |
|   |

Source: [5]

**Table 6. Results obtained in simulation No. 4**

| Visualisation at 50 s of calculations |
|---|
|  |
| Diagram of heat release rate |
|  |



Source: [5]

## 4. Discussion of results

Table No. 3 presents results of simulation No. 1, during which a fire was modelled with the use of a simplified pyrolysis model. The presented method is used by fire safety engineers for modelling design fires. The input file contained only a determination of the maximum constant fire severity, and fuel was released from a surface of 1 $m^2$. Consequently in simulation No. 1 a gas burner has been designed from which the assumed amount of fuel is released. Next at the time of mixing with oxygen fuel became immediately combusted.

Table No. 4 presents results of simulation No. 2, during which sprinkler activation has been modelled. Assumptions for the model were the same as in simulation No. 1. In addition the programme also calculated the course of the burning out curve depending on the mass of water that reaches the assumed fire surface. Calculation of the burning out phase was consistent with equation No. 6. The diagram presented in table No. 2 shows that in the 22$^{nd}$ s an increase of the fire severity takes place. This is the moment of interaction of water droplets with the fuel. A leap of the fire severity is only of a temporary nature, and in the 24$^{th}$ second this severity falls, according to the assumed burning out model. The fire severity in the 35$^{th}$ s of the simulation amounts to ca. 5 kW, and in the 50$^{th}$ s of calculations reaches the value of 0 kW.

Table No. 5 presents results of simulation No. 3, during which a fire was modelled with the use of an advanced pyrolysis model. The simulation was carried out to reproduce results obtained in study [5]. The maximum fire severity is reached in 350 s of the simulation and amounts to ca. 970 kW. After that time a decrease in the fire severity takes place as an effect of burning out of the material (polyurethane foam).

Table No. 6 presents results of simulation No. 4, during which an attempt was made at modelling the interaction of an advanced pyrolysis model with the fire suppression model using water released from the operating sprinkler. Assumptions for the combustion of polyurethane foam were the same as in simulation No. 3. In this case the maximum power was achieved after 330 s and amounted to ca. 665 kW. After that time a reduction of the fire severity took place as an effect of water reaching the modelled combustion zone. The impact of water droplets led to intensification of the pyrolysis reaction, and consequently also to reducing the amount of combusted fuel in the gaseous phase. It should be emphasised that the fire severity had not been reduced to 0 kW. This is due to the fact that a gas burner with a power of 25 kW has been modelled with the use of a simplified purolysis model. What is more, no E_COEFFICIENT parameter has not been assigned to the burner surface.

## 5. Conclusions

When modelling a fire in the FDS, a differentiation should be made into modelling of combustion in the gaseous phase from modelling of pyrolysis or thermal decomposition of the material. Pyrolysis is decomposition or transformation of a compound that leads to the formation of pyrolytic gases under the impact of heat. Pyrolysis is the first stage of a chemical reaction that occurs in the combustion process of numerous solid fuels, such as wood, textiles, paper and plastics. Combustion in a gaseous phase refers to exothermal chemical reaction taking place between the gaseous fuel and oxygen, which is accompanied by the release of heat and light in the form of a flame. This means that pyrolysis of fuel in the solid phase causes the generation of combustible pyrolytic gases. A visible flame is not created due to combustion of solid fuel, but as an effect of the reaction of flammable pyrolytic gases with oxygen that are released from this material. In the FDS programme fire is a specific border condition, which is applied on a given surface. The program enables adopting two ways for defining a fire. The first one of them is the determination of the heat release rate from the surface, i.e. HRR. The second approach consists of a precise determination of properties of combustibles and modelling their combustion. In this case the combustion rate depends on the heat that affects the surface of studied material, in such a way causing the release of combustible pyrolytic gases. Defining of a design fire with precisely specified parameters and modelling pyrolysis of a solid consist of computing in the programme the release of the appropriate amount of specified (single type) of fuel in a gaseous state, which burns in a defined fire zone. On the other hand, in a real fire there is a great amount of combustible gases that originate from diverse materials. Combustible gases being released from a fire area predefined in the programme become mixed with fuel and burn. There is no need to determine the source of ignition as the combustion model assumes that fuel undergoes combustion at the moment of its mixing with oxygen. Consequently it may be imagined that each cell of the computational grid contains a virtual spark plug that initiates ignition once the sufficient temperature is achieved along with the appropriate ratio of fuel and oxygen concentrations. During the combustion process heat and smoke are released. The simulation allows the definition of many type of combustibles, yet modelling may be done only for one type of fuel in a gaseous state. Consequently it is necessary to define chemical properties of fuel that have a dominating share in the combustion reaction. The model has been simplified because solving transport equations for many types of fuels in a gaseous state is a process that requires a considerable computational capacity. FDS calculates automatically the

combustion rate of solids and fluids, taking into consideration the combustion heat of the given material. If the material being combusted has a different combustion heat (determined in the MATL line) than the combustion heat of the global combustion reaction (determined in the REAC line), then FDS adjusts the amount of released fuel from the given material. FDS makes it possible to define the combustion reaction in the gaseous phase in two ways. As a default the programme makes use of the so-called fraction mixture model, which describes the reaction from the moment of fuel outflow in a gaseous state from a fire surface specified in the programme to the stage at which it becomes burnt. Ths model assumes that the reaction between oxygen and fuel progresses infinitely quickely. Another modelling method is adopting the model of specified reaction rate, in which all particular gases participating in the combustion process are defined. This method is more complex and requires the application of bigger computational capacity of the computer than the model of fraction mixture. As default FDS makes use of a simple model of a fraction mixture and assumes the presence of three reaction parameters: fuel, oxygen and combustion products. This model is suitable for anticipating combustion processes in conditions of sufficient ventilation. To be able to make full use of the model, a chemical equation of the combusted material is defined and mass fractions of soot, CO or hydrogen. The RADIATIVE_FRACTION parameter defines a fraction of energy emitted from a fire by radiation. The radiation value is a function of flame temperature and the chemical composition of fuel. The precise calculation of the radiation value requires a considerable computational capacity. Given the above it is not "the radiation fraction" that is calculated, but rather the value is determined by the user or amounts to 35% for the default value set up in the FDS. The MATL function may be used to determine parameters related to the pyrolysis of solids. In the FDS a relatively simple model has been implemented that describes the progress of multi-stage reactions, related with the combustion of materials consisting of a few components. It turned out that during the combustion process each material may undergo a few reactions that may occur at different temperatures and use up different amounts of heat. Each of those reactions may cause the formation of separate products in the solid phase, fuel in volatile state or water vapour. The heat of combustion, i.e. HEAT_OF_COMBUSTION, is the energy released during the combustion of a given mass of a mixture of fuel with air. This shows that this parameter concerns energy released during combustion of gaseous fuel and is not related with the pyrolysis process. Despite the fact that FDS allows defining various combustibles in a simulation, the programme may only model the combustion of a single fuel in the gaseous phase. As has been mentioned earlier, stechiometry of the dominating reaction is defined by

parameters of the REAC function, i.e. the heat of combustion defined as a parameter of the REAC function refers to combustion of fuel in the gaseous phase. On the other hand, the combustion heat defined in the MATL function refers to combustion of pyrolytic gases. If the combustion heat is a parameter of the MATL function, the FDS programme automatically adjusts the mass loss rate related with the generation of pyrolytic gases. In such a case the adjusted mass loss rate multiplied by the global heat of combustion specified in the REAC line causes a specific rate of heat release from the fire. This suggests that if for example the combustion heat defined as a parameter of the REAC function is two-fold higher than the one defined in the MATL function, then the mass of material subjected to pyrolysis contained in the given cell comprising material becomes reduced according to calculations of the pyrolysis model, while the fuel mass in the volatile state added to the gaseous phase would be reduced by 50%. Unfortunately there is no adopted methodology for entering tested properties of combustible materials to the input file in FDS. There is also a shortage of experimental data and validations with respect to anticipations of flame spreading. Given the above, it is recommended that a simplified method of modelling the combustion development be used by direct introduction of the so-called design fire to the simulation. As had been mentioned above, in this method the fire development curve is set out in a precise way by defining the heat release rate HRR. The HRR value is entered on the basis of data obtained from literature as well as experimental data.

When working out computer analyses related to fire safety it is frequently necessary to allow for the impact of sprinklers on the development of the fire. Water reduces the rate of pyrolysis by cooling the material surface, and by changing chemical reactions connected with the release of pyrolytic gases. In engineering assumptions the process of modelling the fire suppression effect of sprinklers is generally limited to modifying the heat release rate from the fire and adoption of a specific fire surface. The FDS also allows modelling the interaction of fire development with the water fire suppression model. However, it should be emphasised that models of sprinklers implemented to the current version of FDS remain in the experimental phase. For the time being it is impossible to take into consideration for example the formation of a water film, generation of dense streams, local evaporation or water absorption in porous materials etc. [11, 12]. Further, according to study [2], in the majority of cases sprinklers reduce the fire severity, yet quite frequently they are unable to fully extinguish a fire. Also in this respect the model had not been validated. In addition there are certain difficulties in describing the real number of droplets in the Lagrange model [15, 16]. Taking the above into consideration, results of mutual impact of the pyrolysis and fire

suppression model have to be interpreted with great caution. For the time being those models have not been documented yet by the required number of full-scale testing.

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