FIRE CHARACTERISTICS FOR ADVANCED MODELLING OF FIRES

Otto Dvořák

Czech Technical University of Prague - UCEEB, Třinecká 1024, 273 43 Buštěhrad, Czech Republic, otto.dvorak@cvut.cz

ABSTRACT

This paper summarizes the material and fire properties of solid flammable/combustible materials /substances /products, which are used as inputs for the computer numerical fire models. At the same time it gives the test standards for their determination.

KEYWORDS

Material and fire properties of flammable/combustible solid materials: density; specific heat; coefficient of thermal conductivity; thermal inertia; ignition temperature; gross heat of combustion; heat of gasification; heat of reaction; production rate of species; mass loss rate; combustion efficiency; emissivity; flame extinction coefficient; flame spread parameter; input data into mathematical models of fire; ignition; pyrolysis; test standards.

INTRODUCTION

A fire modelling is a progressive discipline of the fire-safety engineering because it is more and more used in practice when designing buildings and their structures, evaluating fire hazards, investigating the causes of fires, the spread of dangerous gases and vapors by flowing etc. Deterministic models are divided into the models of field which include programs FDS [1] SOFIE [2] SMARTFIRE [3], FLUENT [4] FLACS [5] Exodus [10]) and zone models, e.g. BRANZFIRE [6] CCFM [7] CFAST [8] CONTAM [9] and ARGOS [11]. The models predict the behavior of a fire e.g. inside buildings, specifically they describe the gas temperatures, heat flow rates through the openings, heat flows, opacity of smoke, production of selected toxic gases / vapors, the reduction of the strength or the extent of damage of building components and activation time of sprinklers, electrical fire detectors in defined positions (x, y, z) during the time of simulated fire, see the example in Fig. 1.

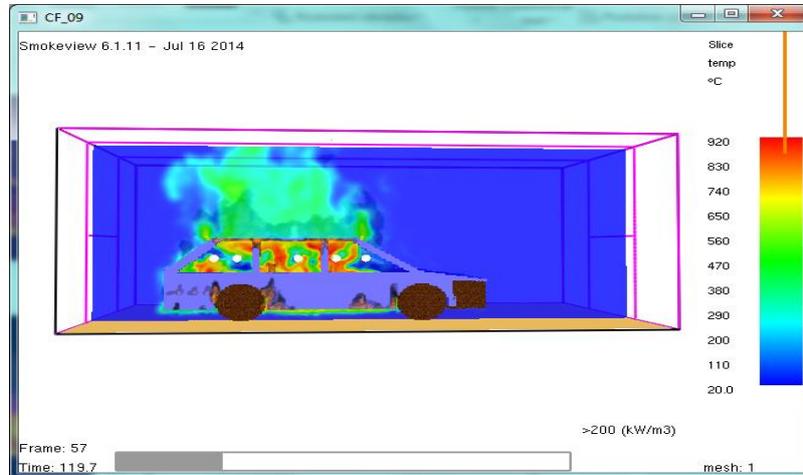

Fig. 1 - Cut of fire temperature field of a car in the 30th second after ignition according to the scenario modelled using the SWs Pyrosim / FDS [47].

Input parameters must be specified for a successful solution of the fire simulation: three-dimensional geometry of a fire field with dimensions of floors, walls, ceilings, openings (doors, windows) and their locations; thermal technical properties of the boundary surfaces of structures (wall, ceiling); position and thermal technical and fire characteristics of flammable/combustible substances/materials incl. burning item; ventilation (forced, natural and combinations thereof); Electronic fire signalization (EPS) and Fixed firefighting systems (SHZ) components and their location. Physical thermal technical and fire characteristics of flammable substances / materials can be determined by laboratory fire tests, or they may be found in the literature. The study of sensitivity to the accuracy of their description is important for quality modelling. Individual values and possibility of their description ability are summarized below.

1. DENSITY

The bulk *density* of a material ρ [kg/m^3] is its mass per unit volume [12]. Density of materials varies for two reasons during heating: releasing the contained volatiles (combustible or non-combustible) and expansioning - volume dilatation (expansion or contraction).

Density of the materials is determined by their weight and volume, see e.g. [13] and [14]. Temperature dependence on density is determined by the temperature changes of a mass with the thermogravimetric analysis, and by volume changes with the dilatometric analysis.

2. SPECIFIC HEAT CAPACITY

The *specific heat capacity* of materials under constant pressure, c_p [kJ/kg.K] is the amount of heat required for rise of the temperature of 1 kg by 1 K [15]:

$$c_{p=}\frac{dq}{dT} = \frac{E}{m\,.\Delta T} \tag{1}$$

where *m* is the mass [kg] of the material, *E* is the amount of supplied heat [kJ], and ΔT is the temperature increment [K].

The apparent specific heat capacity of materials, in which physical-chemical phase transformations proceed at a certain temperature, may be defined as the sum of the inherent specific heat capacity and latent heat required for the temperature increase of 1 kg of material of 1 K. Heat reaction of materials having a tendency to physical-chemical transformations is characterized with specific heat capacity and the competent latent heat in some models, and with the apparent specific heat in other models.

Specific heat capacity is measured generally using Differential Scanning Calorimetry (DSC). The sample and reference material are heated at a constant rate with the resistance heating apparatus [16].

3.   THERMAL CONDUCTIVITY

Heat conduction corresponds to a movement of heat in the material due to the temperature gradient. Modelling a heat conduction requires knowledge of the *Thermal conductivity* λ [W/m.K], of materials which is defined as [15]:

$$\lambda = \frac{\vec{q}}{-(\frac{dT}{dx})} \quad . \tag{2}$$

where $\vec{q}$ is the rate of steady flow of heat conduction per unit area in the *x*-direction [W/m²], and *(dT/dx)* is a temperature gradient in the x-direction. Thermal conductivity depends on the moisture content, temperature, porosity, density and microstructure of the material. Some models neglect those dependencies and prefer to use a constant value for the thermal conductivity.

There are two methods for measuring the thermal conductivity of solids: a method of steady state and a transient state method. Method of steady state uses a heat source to maintain a constant temperature gradient across the sample. It is slow and we often need several days to determine the thermal conductivity at several temperatures [17]. Transient state method is classified generally as a method of a "hot drive" [18]. It is measured by the rate of rise of temperature of electrically-heated sample lines in the ambient of sample at a given temperature. This method is much faster than the steady-state method.

4.   THERMAL INERTIA

The *thermal inertia* of the material $, \lambda$ ρ *c* [J²/s.m⁴.K²]*,* is a product of the thermal conductivity $\lambda,$ (see para. 3 above), the density ρ (see para. 1 above) and the specific heat capacity c_p (see para. 2 above). It is used when modelling the transient heating of solid substances/materials. The greater thermal inertia, the longer it takes to reach temperatures of the flow of contained volatiles.

 Modelling problems can occur, especially when the solids degrade thermally rapidly, for example, when the flame is spreading on the surface, therefore it is useful to establish an *effective thermal inertia of materials*, λ ρ *c*. The effective thermal inertia is determined by analyzing igniting data by an auxiliary source of ignition when exposed to radiant heat [19], [15].

5.   IGNITION TEMPERATURE

Ignition of solid fuels is defined as the start of flame combustion in the gaseous phase [20]. When the solid material is exposed to the external heat, it starts to decompose thermally /pyrolyze at the certain time. Fuel vapors are mixed with air in the boundary layer. Shortly after, a pyrolysis

rate may already be sufficient to achieve the LEL and the mixture may ignite under certain conditions. There are two types of ignition: with auxiliary piloted ignition and without the auxiliary source. Flame combustion of the gas mixture is initiated with a small ignition source when igniting with the auxiliary piloted ignition. Piloted ignition may be a small gas burner flame, an electric spark or a hot wire. A solid surface shall achieve a sufficiently high temperature at which the combustion reactions take place to ignite without the auxiliary source. It is difficult to predict when the solid fuel ignites at a certain heat flux. A critical surface temperature when igniting is often used as a criterion for ignition. This critical temperature is the *ignition temperature*. It is higher without auxiliary piloted ignition than with this source. But the ignition temperature is the material property and it does not change with heat flux density for each type of ignition.

Ignition temperature [°C] can be determined in several ways. In the Czech Republic there are commonly determined: - flash points and ignition temperatures of solid combustible materials with the method according to Setchkin, see [21] - ignition temperatures of flammable gases and vapors with the test method that simulates the risk of ignition from hot surfaces, see [22]. Further there are published the test methods that measure: - surface temperatures when testing ignitability by using very fine thermocouples attached to the surface of a sample [19]. This method is difficult because it is difficult to control the fine thermocouples and ensure good contact with the surface to be measured, - the temperatures of the surface of a material sample using an infrared pyrometer targeted to a small area of the surface. In this case the disadvantage is that the heat radiation is measured and the surface temperature is not. Thermal radiation is partly emission and partly a reflection from the test surface. As the surface characteristics (emissivity, reflectivity and absorption) change during the exposure, it is not easy to calculate the surface temperatures from the pyrometer record; - another way is to check the surface temperature by the application of the theory of ignition in a series of measured test results (various times to ignition at different heat fluxes). Then the ignition temperature is obtained from the heat balance equations at the critical density of the radiant flux and for the steady state. We must mention the test standard setting the ignitability of building products using a radiant heat source [23].

6.   GROSS HEAT OF COMBUSTION

The heat energy releases in all reactions of combustion/burning. *Combustion heat*, Δh_c [kJ/kg] is defined as the amount of heat generated by the complete combustion of fuel unit, see e.g. [24].

Gross heats of combustion are measured by the combustion bomb calorimetry [30]. A known amount of fuel is burned completely in an apparatus comprising pure oxygen. The gross heat of combustion is calculated from a known mass of fuel and a temperature increase after subtracting of the dissolving heat and the heat of formation of H_2SO_4 and HNO_3. The *net heat of combustion* is obtained by subtracting the latent heat of evaporation of water caused by burning of hydrogen (contained in the combustible material) and moisture contained in the original sample. *Effective heat of combustion* is determined e.g. by the conical calorimetry [25], which measures the mass loss rate and the heat release rate. *Effective heat of combustion*, $\Delta h_{c,eff}$ [kJ/kg] is the ratio between heat flux $\dot{q}$ [kW] and the mass loss rate, $\dot{m}$ [kg/s]):

$$\Delta h_{c,eff} = \frac{\dot{q}}{\dot{m}} \tag{3}$$

----

7. HEAT OF GASIFICATION

Heat of gasification of material Δh_g [kJ/kg] is equal to the heat that must be supplied so as the unit quantity of material converts to the gaseous volatiles [15]:

$$\Delta h_g = \frac{\dot{q}_{net}}{\dot{m}} \qquad (4)$$

where $\dot{q}_{net}$ is the absorbed heat flux in the material [kW/m^2] and $\dot{m}$ is the mass loss rate of material [kg/m^2.s].

For burning sample the absorbed heat flux directed to the material is equal to the sum of heat fluxes of radiation and convection from the flame and external heat flux (from the radiant heat emitters in small-scale tests) minus the heat losses by radiation from the surface. These properties are dependent on the surface temperature, which is very difficult to measure. The cone calorimetry [25] is used to determine Δh_g in connection with the measurement of the surface temperature. For some materials the surface temperature is approximately constant and independent of the exposure conditions. A graph of the dependence of the mass loss rate on the external radiant heat flux density is nearly linear for this type of materials. Then the Δh_g values can be estimated as the inverse of the slope of the regression line extending across points of the measured data. Unfortunately surface temperatures are not constant for most materials (materials that char and materials with high production of smoke). In this case the modified equation for the Δh_g is used and the time-dependent curve of the heat of gasification is obtained instead of one of its values.

8. REACTION HEAT

Reaction/(pyrolysis heat, Δh_p [kJ/kg] is the energy emitted or consumed during pyrolysis or the thermal degradation of the material [15]. It can be also defined as the difference between the enthalpy of the starting material and the reaction enthalpy of the pyrolysis products. In the calculations of reaction heat it is supposed that the products are present at the thermal decomposition temperature and the original material is present at ambient temperature. The reaction heat of a small sample, which is subjected to the prescribed thermal conditions, is measured by a laboratory test. The reaction heat or the corresponding change of the enthalpy is usually the input parameter in the balance equations of energy for solid materials, which are degraded thermally. Reaction heat is used in the mode where the temperature profile in a solid material, which is heated, is calculated. Generation of internal energy term may be described in several different ways depending on the used model. A common way is to multiply the reaction heat Δh_p [kJ/kg] with the local decomposition rate [kg/m^3.s] thereby obtaining a member of the generation of energy. Instead of the reaction heat it is possible to use a specific heat capacity and the enthalpy of formation and the computer program calculates the enthalpy and the corresponding reaction heat. Some models do not have a term with the reaction heat, because they assume that the change of the real energy is zero.

The most common experimental method for measuring the reaction heat is the Differential Scanning Calorimetry (DSC) [16]. A small amount of sample (mg) is placed in the apparatus and it is subjected to the thermal degradation by a specific exposure to heat in the time. Heat is supplied to a sample and an inert reference material and both materials are maintained at the same temperatures. Added heat is recorded and it is assumed that it is equal to the heat loss or heat gain as a result of the endothermic or exothermic reactions. These results are influenced by several factors: e.g. particle size and heating rate. Thus, these results for such small samples cannot be considered as the representative behavior of materials in practice. DSC methods can be used for measuring the specific heat capacity of materials and enthalpy associated with the

----

physical processes such as evaporation and desorption. The value of the reaction heat Δh_p is generally considered to be negative for exothermic reactions and positive for endothermic reactions.

Another method used for determining is the Differential Thermal Analysis (DTA) and the Thermogravimetry (TA) [26]. Temperature differences between the sample and the reference material are measured as a function of temperature and the reaction heat is calculated from these results.

9. PRODUCTION RATE OF SPECIES

Combustion species are substances that result in the actual combustion process [20]. As a result of complex chemical reactions that take place during the fire, it is not possible to predict the *production rate of species* only from one chemical reaction. Therefore, we must rely on experimental data.

Some experimental devices record the formation of the different products. The Cone calorimeter, the furniture calorimeter and experiments in the fire room measure certain products with specific gas analyzers. Concentrations of O_2, CO, CO_2 and hydrocarbons are often measured in these fire tests. The yield for individual measured products can be achieved according to the following relationship with experimental measurements and assuming that the production rate of species is proportional to the mass loss rate of a fuel:

$$Y_j = \frac{\int_0^t \dot{G}_j \, dt}{\int_0^t \dot{G}_f \, dt} \tag{5}$$

where

Y_j is the yield of products j [kg/kg]; $\dot{G}_f$ is the formation rate of fuel vapors per unit surface area [kg/m^2.s] and it is equal to the mass loss rate $\dot{m}$; $\dot{G}_j$ is the rate of formation of products j from the unit surface area [kg/m^2.s].

Product yields Y_j can be used for predicting the formation of species:

$$\dot{G}_j(t) = Y_j . \dot{G}_f(t) = Y_j . \dot{m} \tag{6}$$

The value Y_j may vary during the time depending on the combustion conditions. In this case it is necessary to define Y_j as a function of time and not as an average value of time as expressed above. Instantaneous value Y_j at time t * is given by the following formula:

$$Y_j (t^*) = \frac{\dot{G}_j(t^*)}{\dot{G}_f(t^*)} \tag{7}$$

This approach simplifies the problem of prediction of the production rate of species in a fire. Great attention must be paid to the experimental methods used to obtain the data. Several variables affect the production rate of species, e. g. fuel type, geometry of the fuel and retroaction of heat radiation on the surface of the fuel. It is also a function of ventilation in the fire room and can be changed orderly up among the conditions of lack of air and excess air conditions. Useful apparatuses for this type of experiments: cone calorimeter [25], and furniture calorimeter and room / corner test [27], [28], large–scale verification test [29].

----

10. MASS LOSS RATE

Most of the fuels in a fire are burning in a gas phase by a flame. *Mass loss rate* $\dot{m}$ of a fuel is equal to the rate at which the fuel gasification takes place [25], [45]. In a laboratory test the m*ass loss rate* of samples $\dot{m}$ in [kg/s] or [kg/m^2.s] is measured under the prescribed temperature conditions. Mathematical models of fire inside the room can predict the thermal environment in defined positions and the mass loss rate only on large surfaces, if the surface spread of flame is accurately calculated. It is common to divide the surface into small parts/segments, so that the heat flux to each part can be regarded as the same. Algorithms of flame spread (in both directions) in the model are determined, when a certain part / segment ignites. After ignition, this model uses the speed of a mass loss determined in the whole range of densities of radiation heat fluxes in the laboratory or large-scale tests. The mathematical model must also consider the orientation of the fuel. This is achieved by the exposure because the orientation affects predominantly retroaction of flame to fuel and consequently the exposure on interfaces solid fuel/gas.

Procedures in models are based on the mass loss rate data of large surfaces obtained by calorimetric measurements in rows of levels of densities of radiant fluxes. The mass loss rate of a part of material can be expressed as follows:

$$\dot{m} = \frac{\dot{q}_e + \dot{q}_f - \dot{q}_l}{\Delta h_g} \tag{8}$$

where $\dot{m}$ is the mass loss rate per unit area [kg/m^2.s], $\dot{q}_e$ is the outer radiant heat flux [kW/m^2], $\dot{q}_f$ is the heat flux from the flame [kW/m^2], $\dot{q}_l$ are heat losses from the surface [kW/m^2] and Δh_g is the heat of gasification [kJ/kg]. The surface temperature of the burning material is constant and stable, and m can be obtained at constant $\dot{q}_e$ that proofs the material has a sufficient thickness. Constants $(\dot{q}_f - \dot{q}_l)$ and Δh_g are obtained from the intersection and the slope of the curve of the dependence of $\dot{m}$ on $\dot{q}_e$. Many materials do not behave in this way, but approximations on average values $(\dot{q}_f - \dot{q}_l)$ and Δh_g is still acceptable. It was found that the flame radiation is a linear function of the concentration of O$_2$ and therefore it is possible to separate $\dot{q}_f$ from $\dot{q}_l$ by a correlation of the mass loss data derived from a wide range of density values of radiant heat flux and O$_2$ concentration. Carbonizing materials, e.g. wood, do not have constant values $(\dot{q}_f - \dot{q}_l)$ and Δh_g even if $\dot{q}_e$ is constant. In this case $\dot{m}$ can be calculated with a model based on exposure and exposure history by interpolation by series of charts of the rate of mass loss obtained in a cone calorimeter at constant $\dot{q}_e$.

Useful apparatus for the measurement in question - for large surfaces in a laboratory scale using a cone calorimeter [25], - for the data from the large-scale tests using the room-corner test, furniture calorimeter and large-scale test [27], [28] a [29].

11. HEAT RELEASE RATE

Realistic calculations of a fire influence require knowledge of the burning rate. This can be expressed as a mass rate of generation of volatiles (products generated by the reaction) or as the *heat release rate* (heat flow rate) with SI units in [W] or [kW] [25].

The heat release rate cannot be predicted from a measurement of material properties. It is a function of the thermal environment, and the volatility of the fuel and combustion efficiency of volatiles. The heat release rate is expressed by the formula

$$\dot{q} = \dot{m} \, \chi \, \Delta h_{c,net} \tag{9}$$

where $\Delta h_{c,net}$ is the *net heat of combustion* of volatiles [kJ/kg], χ is the *combustion efficiency* and $\dot{m}$ is the mass loss rate of fuel [kg/s]. Assuming that the heat is released by a reaction where only H_2O, CO_2 and CO are generated, and O_2 is consumed completely, the heat release rate can be calculated from the following equation:

$$\dot{q} = \frac{\Delta h_v}{\dot{k}_{CO_2}} . D_{O_2} \tag{10}$$

$$\dot{q} = \frac{\Delta h_v}{\dot{k}_{CO_2}} . G_{CO_2} + \frac{\Delta h_v - \Delta h_{CO}}{\dot{k}_{CO}} . G_{CO} \tag{11}$$

where $\dot{q}$ is the *heat release rate* per unit area [kW/m²], $\Delta h_{v,}$ is the *net heat of combustion* of perfect combustion of materials [kJ/kg], Δh_{CO} is the *gross heat of combustion* of CO [kJ/kg], D_{O_2} is the *rate of oxygen consumption* per unit of surface area [kg/m²s], k_{CO_2} is the *maximum possible yield of* CO_2 [kg/kg], k_{CO} is the *maximum possible yield* of CO [kg/kg], G_{CO_2} is the CO_2 *formation rate* [kg/m²s] and G_{CO} is the *rate of formation of CO* [kg/m².s]. Most of the apparatuses measuring the heat release rate use oxygen calorimetry principle: a cone calorimeter [25], and furniture calorimeter and room/corner test [27], [28], Large-Scale Validation Test [29]. When applying data in the models of a fire room, it is appropriate to take into account the limits of ventilation and the back flow of heat from the upper layer of smoke and from the walls.

12. PYROLYSIS TEMPERATURE

If the solids are exposed to external heat, they start to decompose at a certain *pyrolysis temperature* T_p [°C] or [K] [34], [45]. Pyrolysis is defined as the thermal decomposition under oxygen absence [30]. Certain types of plastics (e.g. PMMA) burn more or less like liquids. Phase transformation (of solid to liquid) occurs on the surface and the solid residues do not occur here. Other materials, such as wood, do not evaporate completely but produce carbon residues. The charred layer increases during time and a thermal decomposition occurs in a greater depth below the surface. For both types of materials, the thermal decomposition is described with combination of chemical reactions by Arrhenius-type equations for all components of the fuel:

$$\frac{\partial \rho}{\partial t} = \sum_{i=1}^{i=j} A_i \left(\rho_i - \rho_{ic} \right)^{n_i} \exp\left(-\frac{E_i}{RT} \right) \tag{12}$$

where ρ is the *density* [kg/m³], t is the *time* [s], ρ_i is *the density of component i* [kg/m³], ρ_{ic} [kg/m³] is a *finite density of component i* (the char rest), n_i is the *reaction order* for component i , A_i is *pre-exponential factor* for a component i, E_i is the *activation energy* for component i [J/mol·K] and T is the *temperature* [K]. Modelling of the pyrolysis using Arrhenius-type equations is not easy even in the case when the fuel contains about one component. It is difficult to find kinetic parameters A, n and E. During heating at rates that are typical for fire conditions, many building materials begin to decompose thermally already at a certain lower temperature at which the thermal decomposition is negligible. This temperature is controlled by the activation energy. The thermal decomposition occurs in a relatively narrow temperature interval. This is due to the fact that after the beginning of the heat decomposition the rate increases rapidly and the temperature increases only by a few degrees. At the same time a fuel is consumed and a density member approaches rapidly to zero. It may be assumed that the material begins to decompose immediately at the pyrolysis temperature T_p.

Pyrolysis temperature T_p of some materials can be found in the literature, or it is determined by thermogravimetric analysis, e. g. [26]. The essence of this method is the measurement of the rate of a mass loss rate of a small amount of material during heating at constant speed. Arrhenius´s equations are used to correlate the data. As explained above, the thermal decomposition takes place within a small temperature interval. T_p can be estimated as the average of this interval. It differs from the *surface ignition temperature* T_{ig} when igniting with the auxiliary piloted ignition, but they are often very close to each other for some materials and T_{ig} can be used as an estimate for T_p.

13. AIR/FUEL RATIO

Air/fuel ratio, φ is the amount of air $m_v\ [kg]$ required for combustion of fuel amount m_p [kg] according to the following relationship [20]:

$$\varphi = \frac{m_v}{m_p} \tag{13}$$

The so-called *fuel-air equivalent ratio* is often used as the mass fraction of the fuel/oxygen to fuel/oxygen ratio needed to form a stoichiometric mixture, see formula [14]:

$$\Phi = \frac{m_p/m_{O_2}}{(m_p/m_{O_2})st} \tag{14}$$

Stoichiometric combustion means the combustion in which the $\Phi = 1$.

Efficient air/fuel ratio used in some mathematical models of fire is greater than or equal to the stoichiometric air/fuel ratio. Air/fuel ratio is used in fire models to calculate the burning rate and the heat release rate. It is a dimensionless and specific for each fuel.

The stoichiometric fuel-air ratio can be calculated from the stoichiometry of the reaction equations, but this is not often possible, since elemental composition of the fuel is unknown. It is determined most commonly by calculating the ratio of the amount of energy released by combustion of unit mass of air when exhausting its oxygen content and from the gross heat of combustion [30].

14. COMBUSTION EFFICIENCY

Effective heat of combustion is smaller than the *net heat of combustion* due to incomplete combustion of fuel vapor. *Combustion efficiency* (or burning efficiency) χ explains imperfect combustion / burning [30]:

$$\chi = \frac{\Delta h_{c,eff}}{\Delta h_{net}} \tag{15}$$

where $\Delta h_{c,eff}$ is the *effective heat of combustion* [kJ/kg] and Δh_{net} is the *net heat of combustion* [kJ/kg]. Combustion efficiency is in the range from 0.4 to 0.9 for most hydrocarbons. It can be measured using a cone calorimeter [25], or bomb calorimetry [30].

15. CONVECTIVE HEAT TRANSFER COEFFICIENT

Convective heat transfer relates to the movement of heat (energy) between the solid surface and the surrounding fluid substance due to temperature difference between them. The *convective heat transfer coefficient* α is used for its description. It is defined as [15]:

$$\alpha = \frac{\dot{q}}{\Delta T} = \frac{\dot{Q}}{S \cdot \Delta T} \qquad (16)$$

where $\dot{q}$ is the *heat flux* [W/m²] and ΔT is the *temperature difference* between the surface and the moving fluid [K], $\dot{Q}$ is the *total heat flux* [W] and S is the area [m²]. It depends on the fluid properties (thermal conductivity, density, pressure, viscosity), the nature of the flow of volatiles (velocity, turbulence), and on the geometry of the solid surface.

Selection of an appropriate heat transfer coefficient can be difficult because a large number of variables is needed for its derivation. It can be simplified when the volatile is air. Most of the fire models assume that smoke has similar physical properties as air. For example, the convective heat transfer coefficient between the turbulent air flow and the vertical plane may be simplified as follows:

$$\alpha = 0{,}95 \cdot (\Delta T)^{\frac{1}{3}} \qquad (17)$$

where α is the *convective heat transfer coefficient* [W/m²·K] and ΔT is the *temperature difference* between the vertical surface and the air [K].

Some models use constant heat transfer coefficient commonly. Regardless of the conditions within the hot layer the heat transfer coefficient is set to a constant value of 10 [W/m².K]. Other models express the heat transfer coefficient as a function of temperature of the hot layer. Lower limit is 5 [W/m².K] and the upper one is 50 [W/m².K]. Theory of similarity allows to reduce the number of independent variables using *Prandtl number (Pr)* and *Grashof number* (*Gr*). So α can be calculated from the Nusselt number (*Nu*), which is a function of *Gr* and *Pr*:

$$Nu = \frac{\alpha \cdot D}{\lambda} = C_1 \cdot (Gr \cdot Pr)^x \qquad (18)$$

where: α is the *convective heat transfer coefficient* [W/m².K], *D* is the *characteristic length of the surface* [m], λ is *the thermal conductivity* of the substance [W/m.K], C_1 and *x* are constants, $Pr = v/a$ (v is the *kinematic viscosity* with the unit [m²/s]), *a* is the *thermal conductivity* with the unit [m²/s], $Gr = \beta(T_s - T_o)gD^3)/v^2$, if β is the *coefficient of thermal volumetric expansion* of liquid at constant pressure [[K^{-1}], *g* is the *acceleration of gravity* [m/s²], T_s is *the surface temperature* in [°C] or [K], T_o is the temperature of the surrounding liquid in [°C] or [K]. The assumption that heat transfer is predominantly due to natural convection must be true to use this equation. This does not always apply, for example, if the flame speed and flows through vents are controlled by heat transfer. The equation for the Nusselt number (*Nu)*, which is a function of the Reynolds number (*Re*) and Prandtl number (*Pr*), should be used for the compulsory convection:

$$Nu = \frac{\alpha \cdot D}{\lambda} = C_2 \cdot Re^x \cdot Pr^y \qquad (19)$$

where *C2, x* and *y* are constants.

----

16. EMISSIVITY

Emissivity of materials ε is the ratio of energy emitted per unit area of real material and energy radiated by a black body at the same temperature [20]. It represents the thermal properties of the heat radiation integrated over all wavelengths. It is a dimensionless quantity and its maximum value for a black body is equal to one. There are several standard tests for measuring the emissivity of materials. The test specimen of the material is usually placed in an evacuated chamber and is typically electric-heated to a temperature of interest. The energy dissipated by a material is determined and it is equal to the radiative heat transfer to the surroundings. The emissivity is calculated using this energy and the Stefan-Boltzman equation $I = \varepsilon\,\sigma\,T^4$, where I is the *total radiation* heat release rate [W/m^2], σ is the *Stefan - Boltzmann constant* = 5, 67 x 10^{-8} [Wm^{-2}.K^{-4}] and T is the *thermodynamic temperature* [K], the temperature difference between the vertical surface and the air temperature.

Emissivity can be measured for example by a thermocouple, by an infrared camera TESTO and subsequently by calculation using the following formula (20) or by a spectrometer [31]:

$$\varepsilon = \left(\frac{T_T^n - T_R^n}{T_w^n - T_R^n}\right) \tag{20}$$

where T_T is the *surface temperature* measured by a camera [°C], T_R is the *ambient temperature* (radiation) in [°C], T_w *is* the temperature [°C] measured by a thermocouple, n is the *exponent* expressing the dependence of the heat flux on temperature.

17 FLAME EXTINCTION COEFFICIENT

The *flame extinction coefficient k* correlates the average parameters of heat radiation, that is the emissivity, flame intensity and temperature for the entire spectrum of wavelengths in a mutual relationship. It is used to calculate the emissivity of the flame in the following empirical equation [45]:

$$E = A\sigma T_f^A (1 - e^{-kl}) \tag{21}$$

where $\dot{E}$ is the *emissive power of a flame* [W], A is the enviloping *area of a flame* [m^2], σ is the Boltzmann constant 5,67x10^{-8} [W/m^2.K^4], T_f is the *flame temperature* [K], k is *the flame extinction coefficient* [m^{-1}] and l is the *optical path length* [m]. The quantity k may also be referred to as *absorption coefficient*, *absorption-emission coefficient* or *effective emission coefficient*.

The coefficient k may be estimated from measurements of *emissivity ε* and the *optical length l* by the relationship:

$$\varepsilon = 1 - e^{-kl} \tag{22}$$

Flame extinction coefficient can be determined by measuring all quantities in equation [45] except for *k*. Fire models usually contain similar empirical equations, but often without detailed specifications.

----

17. FLAME SPREAD PARAMETER

Flame spread r*ate* against the direction of the ambient flow or against gravity is expressible with empirical equation suggested by Deris [23]:

$$v_p = \frac{\varphi}{\lambda \varrho c (T_{ig} - T_s)^2} \tag{23}$$

where v_p is the *flame spread rate* [m/s], φ is the *flame spread parameter* [W^2/m^3], λ is the *thermal conductivity* [W/m·K], ρ is the density [kg/m^3], c is the *specific heat capacity* [J/kg·K], T_{ig} is the surface temperature during ignition [K] and T_s is the surface temperature at the time of contact with the face of the flame [K].

Flame spread parameter, for a certain orientation, and the standard medium in the air is typical for heat transfer from the flame to the fuel in the neighborhood of the lower part of the flame before the flame front. It is a material property.

Flame spread parameter φ can be obtained by a correlation of data of counter-flow flame spread, that is the flame spread rate at different radiant heat flux (or surface temperature). ASTM E1321 [19] describes a method for measuring the characteristics of flame spread.

CONCLUSION

Thermal technical and fire characteristics of materials are important input data determining the quality of predictions from numerical models and should be selected according to specific scenarios of fire. Some models have their own small database of material properties, e.g. SMARTFIRE [3], FLUENT ANSYS [4], BRANZFIRE [6], others for example FDS [1] or SOFIE [2] do not have it. Missing characteristics can be found in the databases available on the Web, see e.g. [36] - [39], in the literature, see e.g. [40] - [44] or determinated by tests with standardized internationally recognized procedures, see the text above incl. [45], [46]. However, the data obtained from the literature or laboratory tests do not guarantee proper behavior of the materials, as in real scale, which can be evaluated by the verification and validation of the calculations from the used mathematical model in comparison with e.g. the data measured during the large-scale fire test. It is the task of fire research, among others to develop. Pyrolysis models applicable to most flammable materials and methodologies for determining material properties as input data for CFD mathematical fire models and to complement relevant databases accessible to all interested parties.

ACKNOWLEDGEMENT

REFERENCES

[1] *http://www.nist.gov/el/firesimsoft.cfm* [online].

[2] *www.cranfield.ac.uk/sme/sofie* [online].

[3] *www.fseg.gre.ac.uk/smartfire* [online].

[4] *www.fluent.com* [online].

[5] *http://www.gexcon.com/flacs-software* [online].

[6] *http://www.branz.co.nz/cms_display.php?sn=74&st=1* [online].

[7] *www.nist.gov/el/fire_research/firesafety* [online].

[8] *http://www.nist.gov/el/firesimsoft.cfm* [online].

[9] *http://www.bfrl.nist.gov/IAQanalysis/software/index.htm* [online].

[10] *http://fseg.gre.ac.uk/exodus/index.html* [online].

[11] w*ww.jensenhughes.com/services/modelling en.dbi-net.dk/argos* [online].

[12] *ČSN ISO 80000 - 4 Veličiny a jednoty- Část 4:Mechanika. 2011.*

[13] *ČSN 490108 Drevo. Zisťovanie hustoty. 1993.*

[14] *ČSN EN ISO 1183 - 1 Plasty- Metody stanovení hustoty nelehčených plastů. Část 1: Inverzní metoda, metoda s kapalinovým pyknometrem a titrační metoda. 2013.*

[15] *ČSN ISO 80000 - 5 Veličiny a jednoty- Část 5:Termodynamika. 2011.*

[16] *ČSN EN ISO 11357 - 4 Plasty – Diferenciální snímací kalorimetrie (DSC)- Část 4: Stanovení měrné tepelné kapacity. 2014.*

[17] *ČSN 727012 - 1 Stanovení součinitele tepelné vodivosti materiálu v ustáleném stavu. Deskové metody. Část 1: Společná ustanovení.*

[18] *ČSN EN ISO 22007 - 2 Plasty - Stanovení tepelné vodivosti a rozptylu tepla – Část 2: Metoda nestacionárního rovinného tepelného zdroje (horkého disku).*

[19] *ASTM E 1321 - 13 Standard Test Method for Determining Material Ignition and Flame Properties. 2013.*

[20] *ČSN EN ISO 13943 Požární bezpečnost. Slovník. 2011.*

[21] *ČSN 64 0149 Stanovení vznětlivosti materiálů. 2010.*

[22] *ČSN EN 14 522 Stanovení teploty vznícení plynů a par. 1977.*

[23] *ISO 5657 Reaction to fire tests – Ignitability of building products using a radiant heat source. 1997.*

[24] *ČSN EN ISO 1716 Zkoušení reakce výrobků na oheň. Stanovení spalného tepla.*

[25] *ISO 5660 - 1 Reaction to fire test- Heat release, smoke production and mass loss rate – Part1: Heat release rate (cone calorimeter method) and smoke production rate (dynamic measurement). 2014.*

[26] *ISO 11358 Plastics – Thermogravimetry of polymers. 2014.*

[27] *ISO 9705 - 1 Reaction to fire tests – Room corner test for wall and ceiling lining products- Part 1: Test method for a small room configuration. 2016.*

[28] *ČSN EN 13823+A1 Zkoušení reakce stavebních výrobků na oheň – Stavební výrobky kromě podlahových krytin vystavené účinku jednotlivého hořícího předmětu. 2015.*

[29] *ČSN EN 14390 Požární zkouška – Velkorozměrová ověřovací zkouška výrobků pro povrchové úpravy. 2007.*

----

[30] ČSN ISO 1928 *Stanovení spalného tepla kalorimetrickou metodou v tlakové nádobě a výpočet výhřevnosti. 2010.*

[31] PAVELEK M. a E. JANOTKOVÁ. Termovizní měření emisivit stavebních materiálů. In: *XXIX. mezinárodní konference Hydro-Termo.* 2010. Rožnov pod Radhoštěm, s. 223-226. ISBN 978-80-248-2244-0

[32] *ISO/TS 5658 - 1*: 2006 *Reaction to fire tests – Speed of flame – Part 1: Guidance on flame spread.*

[33] DVOŘÁK O. a L. ŠEVČÍK. Možnosti stanovení efektivní výhřevnosti metodou kónické kalorimetrie. *Kalorimetrický seminář .*2007. hotel Medlov u Nového Města na Moravě.

[34] CELBA K., O. DVOŘÁK, P. BURSÍKOVÁ a L. ŠEVČÍK. Využití metody kónické kalorimetrie ke stanovení základních tepelně technických charakteristik hořlavých materiálů pro potřebu matematického modelování. *Sborník přednášek mezinárodní konference PO 2005.* 2005. Ostrava: VŠB-TUO, 2005, s. 69-78.

[35] deRIS,J. N.: Spread of Laminar Diffusion Flame*,* In: *12th Int. Symposium on Combustion.* 1969, pp. 241 – 252.

[36] *http://uchi.vscht.cz/index.php/cs/studium/uplatneni-absolventu/e-tabulky).*

[37]*www.firebid.uned.edu/burning-database.php* [online].

[38] *www.firebid.uned.edu/material-database.php* [online].

[39] *http://www.nist.gov/srd/onlinelist.cfm* [online].

[40] DVOŘÁK O. a A. DUDÁČEK: *Zpráva o výsledcích požární zkoušky v rodinném domku v Bohumíně dne 19. 11. 2009.* Praha, Ostrava: TÚPO MV-GŘ HZS PRAHA a FBI VŠB-TU OSTRAVA, 2010, 51 s.

[41] DVOŘÁK O. a DUDÁČEK A.: *Zpráva o výsledcích požární zkoušky v rodinném domku v Kamenné u Milína dne 8. 10. 2010.* Praha, Ostrava: TÚPO MVGŘ HZS PRAHA a FBI VŠB-TU OSTRAVA, 2010, 30 s.

[42] DVOŘÁK O. a kol. Vývoj a validace požárních modelů pro stanovení vývinu/šíření tepla a kouře, toxických plynů, tlakových vln pro simulaci/interpretaci scénářů požárů/výbuchů a jejich ničivých účinků. *Závěrečná výzkumná zpráva o výsledcích řešení dílčího výzkumného úkolu DVÚ č. 2 výzkumného projektu VD20062010A07.* Praha: MV-GŘ HZS ČR, TÚPO, únor 2011, 141 s.

[43] KOZUBKOVÁ M., BOJKO M., ZAVILA O.: *Zpráva řešení modelování požáru daného tepelným výkonem a chemickou reakcí.* Ostrava: VŠB – TUO, 2009, 45 s.

[44] KOZUBKOVÁ M.: *Numerické modelování proudění FLUENT I. c2003.* Ostrava: VŠB-TU, 6. 1. 2005, 116 s. Dostupné z: http://www.338.vsb.cz/seznam.htm *[Online].*

[45] *ASTM E 1591 – 13 Standard Guide for Obtaining Data for Fire Growth Models.* 2013.

[46] *ASTM E 1623 – 14 Standard Test Method for Determination of Fire and Thermal Parameters of Materials, Products and Systems Using an Intermediate Scale Calorimeter.* 2014.

[47] DVOŘÁK, O. a kol. *Zpráva o výsledcích velkorozměrové zkoušky s automobilem FABIA Combi 1.2 TDI.* Praha: ČVUT Praha, UCEEB, TÚPO, 2015, 72 s.