Mathematical Modeling of Fire Dynamics

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Abstract— Computer based compartment fire models can be classified as zone models or field models. A zone model is normally made up of two zones (a hot upper layer and a cooler lower layer). However, in post-flashover models, a one zone model is acceptable. These assume the whole compartment is at a uniform temperature and gas concentration. Mass and energy balances are enforced for each layer, with additional models describing other physical processes appended as differential or algebraic equations as appropriate. The rapid growth of computing power and the corresponding maturing of computational fluid dynamics (CFD) has led to the development of CFD based "field" models applied to fire research problems. The use of CFD models has allowed the description of fires in complex geometries and the incorporation of a wide variety of physical phenomena.

The differential equations are solved numerically by dividing the physical space where the fire is to be simulated into a large number of rectangular cells. Within each cell the gas velocity, temperature, etc., are assumed to be uniform; changing only with time. The accuracy with which the fire dynamics can be simulated depends on the number of cells that can be incorporated into the simulation. This number is ultimately limited by the computing power available. Present day, single processor desktop computers limit the number of such cells to at most a few million. This means that the ratio of the largest to smallest length scales that can be resolved by the computation (the "dynamic range" of the simulation) is on the order of 100. In a real life building fire situation we are dealing with dimensions of the order of tens of meters, and the combustion processes take place at length scales of 1 mm or less. This, in turn, requires parallel processing and therefore a very lengthy computation time for each time step. On the other hand, the "fuel" in most fires was never intended as such. Thus, the mathematical modeling of the physical and chemical transformations of real materials as they burn is in very early stages of development. The end result of all these numerical computations is the input data for the following very complex structural analysis, therefore, the simplifications and approximation of the structural fire load is absolutely essential.

Keywords **— fire simulation; irradiative heat transfer**

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I. Introduction

The purpose of this study is to examine some differences and amalgamations between combined effects on a structural system from multiple fires and "local" explosions. Here are some areas of similarities and differences between fire and explosion.

1. Both of them have periods of ignition ("growth period" in case of fire). However, non-dimensional parameters are different.
2. Both of them have a self ignition period ("flash-over" in case of fire). However, again, non-dimensional parameters characterizing self ignition are different.
3. Thermodynamics (combination of conduction, radiation and convection) can be described by similar parameters in both cases.
4. Hydrodynamics of both processes are described by using so-called "opening factor F" in case of fire, and similar parameter "K_v" used in formula (1) of this article. This is the most important parameter in both cases.
5. The type of fire that may occur is defined by the amount of combustible materials and the size and locations of the windows in the building. Based on heat release rate the fire can be classified as slow, medium and fast.
6. The total energy released during "local explosion" or building fire has a quasi-dynamic effect on structural system, depending on the period of ignition or the flash-over period in case of fire.
7. The temperature time curves as a function of the opening factor K_v ("F" – in case of fire) had been developed.

Gas, vapor, or dust explosions are described in many research papers published over the years as well as different special journals and magazines. The problem of evaluation of critical regimes thought of as regimes separating the regions of explosive and non-explosive ways of thermo-positive chemical reactions are the main mathematical problem.

II. INTERNATIONAL CODE REQUIREMENTS REVIEW

The aim of structural fire engineering design is to ensure that structures do not collapse when subjected to high temperatures in fire. Traditional prescriptive methods of design based on fire resistance testing require steel elements of construction to stay below a critical temperature, typically 550°C, for the fire resistance period of the structure. This has led to extensive use of passive fire protection to limit the heating of the structural elements (boards, sprays) at considerable cost (up to 20% of the total construction cost). Design of structures for fire still relies on single element behavior in the fire resistance test. The future of structural fire design has to be evaluated in terms of the whole performance based design of structures for fire. This should include natural fire exposures, heat transfer calculations and whole frame structural behavior; recognizing the interaction of all elements of the structure in the region of the fire and any cooler elements outside the boundary of the compartment. Prescriptive fire grading and design methods based on heating single elements in the fire resistance test over-simplify the whole fire design process. The real problem can be addressed by performance based design methods where possible fire scenarios are investigated and fire temperatures are calculated based on the compartment size, shape, ventilation, assumed fire load and thermal properties of the compartment boundaries. The temperatures achieved by the connected structure can then be determined by heat transfer analysis. Traditional steel fire design has been based upon fire resistance testing, although fire resistance by calculation has also been implemented for many years. Factors affecting structural behavior in fire are described, such as material degradation at elevated temperatures, restrained thermal expansion, thermal bowing and the degree of redundancy available when the structure acts as a whole. Each factor is addressed separately, but in an integrated structure exposed to fire they will all interact to generate more complex structural behavior. Standard fire tests are conducted worldwide and are defined by the International Standards Organization in ISO 834 [1]. Standard fire tests in the United Kingdom are defined in BS 476: Parts 20-23: Fire tests on building materials and structures [2]. The fire resistance test has been criticized by many researchers over many years. One major criticism is that the temperature of the furnace gases do not represent the fire exposure to the element under test because the fire exposure is dependent on the physical properties of the furnace. The construction shape influences the degree of turbulence and thus convective heat transfer. However, most significantly, the thermal inertia of the wall linings affects the irradiative heat transfer to the element under test. Furnaces also differ in the fuel adopted. They may be gas or oil fired. Another criticism of the standard temperature-time curve is that it bears little resemblance to a real fire temperature-time history. It has no decay phase and as such does not represent any temperature-time histories of "real" fires. Analysis of a small number of room fire tests revealed that fire load was an important factor in determining fire severity. It has been suggested that fire severity could be related to the fire load of a room and expressed as an area under the temperature-time curve. The severity of two fires is equal if the area under the temperature-time curves is equal (above a base line of 300°C). Thus any fire temperature-time history could be compared to the standard curve. This approach obviously has limited applicability with respect to structural design. The direct scaling between the heating effect of real fires and a standard fire is impossible because heat transfer, when dominated by radiation, depends upon irradiative heat flux on T^4. The structural engineer is obviously interested to know not only the temperature-time relationship but the second derivation of such function, which creates the acceleration and therefore the dynamic forces that are acting on the structural system on top of static forces due to temperature elongations. The real fire test normally is presented by the double-curvature temperature-time function, while the standard test is presented by a single-curvature function, and that makes a whole difference for structural design. On top of that, the real fire computer simulations [3] of the temperature-time curves have “small” oscillations along the curve, that are creating additional dynamic forces. The area under the temperature-time curve obviously doesn’t provide the answer to all these questions.

The Eurocodes are a collection of the most recent methodologies for design. Eurocode 3: Design of Steel Structures, Part 1.2: Structural fire design and Eurocode 4: Design of steel and composite structures, Part 1.2: Structural fire design were formally approved in 1993 [4]. Each Eurocode is supplemented by a National Application Document (NAD) appropriate to the country. It details safety factors and other issues specific to that country. All Eurocodes are presented in a limit state format where partial safety factors are used to modify loads and material strengths. EC3 and EC4 are very similar to BS 5950 Part 8 although some of the terminology differs. EC3 and EC4 Parts 1.2 and BS 5950 Part 8 are only concerned with calculating the fire resistance of steel or composite sections. Three levels of calculation are described in EC3 and 4. Tabular methods, simple calculation models and advanced calculation models. Tabular methods are look up tables for direct design based on parameters such as loading, geometry and reinforcement. They relate to most common designs. Simple calculations are based on principles such as plastic analysis, taking into account reduction in material strength with temperature. These are more accurate than tabular methods. Advanced calculation methods relate to computer analyses and are not used in general design.

Building codes worldwide are moving from prescriptive to performance-based approaches. Performance based codes establish fire safety objectives and leave the means for achieving those objectives to the designer. One of the main advantages of this is that the most recent models and fire research can be used by practicing engineers inevitably leading to innovative and cost effective design. Prescriptive codes are easy to use and building officials can quickly determine if a design follows code requirements. However they are too onerous for many modern designs. This is especially true of modern steel framed buildings. The fire resistance ratings in building codes were not made for these types of structures. By assuming the worst case but realistic natural fire scenario and calculating the heat transfer to the steel, the load carrying capacity of the steel members can be checked at high temperatures and requirements for fire protection, if any, can be judged in a rational manner.

Performance based design has been documented in the literature extensively over the past 10 years [5], [6]. It has been reported report that by 1996 there were 13 countries (Australia, Canada, Finland, France, England, Wales, Japan, The Netherlands, New Zealand, Norway, Poland Spain, Sweden and the USA) and 2 organizations (ISO and CIB) actively developing or using performance based design codes for fire safety. Performance based fire safety engineering design is now implemented and accepted in many countries. The design methodology has key advantages over prescriptive based design. Structural behavior in fire depends upon a number of variables. These include material degradation at elevated temperatures and restraint stiffness of the structure around the fire compartment.

The energy and mass balance equations for the fire compartment can be used to determine the actual thermal exposure and fire duration. This is known as the natural fire method. This method allows the combustion characteristics of the fire load, the ventilation effects and the thermal properties of the compartment enclosure to be considered. It is the most rigorous means of determining fire duration. This is not related in any way to the standard fire resistance test and represents the real fire duration, once flashover has occurred.

III STRUCTURAL FIRE LOAD DESIGN

Consider nonlinear singularly perturbed parabolic system [7],[8]:

$$\frac{\partial\theta}{\partial\tau}+\Pr(V\frac{\partial\theta}{\partial x}+W\frac{\partial\theta}{\partial z})=\nabla\theta+\delta(1-C)^k\exp(\frac{\theta}{1+\beta\theta})-P\theta^4$$

$$\frac{\partial C}{\partial\tau}+\Pr(V\frac{\partial C}{\partial x}+W\frac{\partial C}{\partial z})=L\nabla C+\gamma\delta(1-C)^k\exp(\frac{\theta}{1+\beta\theta})$$

$$\rho\frac{\partial W}{\partial\tau}+\Pr(\rho)(V\frac{\partial W}{\partial x}+W\frac{\partial W}{\partial z})=\frac{4}{3}\Pr(\rho)\nabla W-\frac{\partial p}{\partial z}+(\rho)Fr$$

$$\rho\frac{\partial V}{\partial\tau}+\Pr(\rho)(V\frac{\partial V}{\partial x}+W\frac{\partial V}{\partial z})=\frac{4}{3}\Pr(\rho)\nabla V-\frac{\partial p}{\partial x}$$

$$\frac{\partial\rho}{\partial\tau}+\frac{\partial(\rho V)}{\partial x}+\frac{\partial(\rho W)}{\partial z}=0$$

$$\rho=\frac{\alpha p}{1+\beta\theta}$$ ………………………………………… (1)

The initial conditions are as follows:

$$\tau=0;\theta=\theta_0;\rho(0;x;z)=\rho_0=const.$$
$$C(0;x;z;)=W(0;x;z)=V(0;x;z)=0;$$ ……… (2)

The boundary conditions are as follows:

x=0; 1; z=0; 1;

$$\theta=0;\frac{\partial C}{\partial n}=\frac{\partial\rho}{\partial n}=0;V=W=0$$ ……………… (3)

Where:

$\theta=\frac{(T-T_*)E}{RT_*^2}$ - Dimensionless Temperature;

$\beta=\frac{RT_*}{E}<<1$ – Dimensionless parameter;

$\gamma=\frac{c_pRT_*^2}{QE}$ - Dimensionless parameter that characterizes the amount of fuel burned in the compartment before the temperature had reached the referenced point of $T_*=300^oC$. If this parameter is small, then the fire will have a flash-over point, and if it is large – the fire will proceed stationary until the decay stage.

$0<\gamma<1$.

$C=[1-P(t)/P_o]$ - Concentration of the burned fuel in the compartment.

$\delta=(\frac{E}{RT_*^2})(\frac{h^2}{\lambda})Qz(\exp(-\frac{E}{RT_*}))$ - Frank-Kamenetskii's parameter [9].

$P=\frac{e\sigma K_v(\beta T_*)^3h}{\lambda}$ - Thermal radiation dimensionless coefficient [10].

$\sigma=5.67(10^{-8})$ [watt/m^{2}K^4] –Stefan-Boltzman constant

e –emissivity coefficient

K_v= Ah/V – Dimensionless opening factor

$\tau=\frac{a^2}{h}t$ - Dimensionless time

$\varsigma=\frac{x}{h}$ - Dimensionless coordinate

k –Order of the chemical reaction

λ – Thermal conductivity (J/sm°C)

Let's consider now the average distribution of temperature and concentration in space. The equation (1) and (2) are simplified [9]:

$$\frac{d\theta}{d\tau}+\Pr(V\frac{\partial\theta}{\partial x}+W\frac{\partial\theta}{\partial z})=\delta(1-C)^k(\exp\frac{\theta}{1+\beta\theta})-P\theta^4$$ …………… (3)

$$\frac{dC}{d\tau}+\Pr(V\frac{\partial C}{\partial x}+W\frac{\partial C}{\partial z})=\gamma\delta(1-C)^k(\exp\frac{\theta}{1+\beta\theta})$$ …...(4)

Parameter "δ" is calculated based on [9]:

$$\delta_{cr}=12.1(\ln\theta_*)^{0.6}$$ .... (5)

First two equations are describing the heat and mass transfer, the second two – the Navier-Stokes equations – describe the motion of fluid substances, that is substances which can flow. They are one of the most useful sets of equations because they describe the physics of a large number of phenomena of academic and economic interest. They may be used to model weather, ocean currents, water flow in a pipe, flow around an airfoil (wing), etc. As such, these equations in both full and simplified forms are used in the design of aircraft and cars, the study of blood flow, the design of power stations, the analysis of the effects of pollution, etc. The Navier–Stokes equations dictate not position but rather velocity. A solution of the

Navier–Stokes equations is called a velocity field or flow field, which is a description of the velocity of the fluid at a given point in space and time. Once the velocity field is solved for, other quantities of interest (such as heat flow rate) may be found. In case of structural fire design loads these equations can be further simplified based on the following assumptions: 1) Thermal properties such as conductivity, specific heat, density, and other physical parameters for all practical purposes can be assumed constant and the values shell be taken at the maximum temperature. This practice has been used for many years in theory of explosion and combustion [11], and it will allow to obtain the solution of Navier-Stokes equations separately from the energy conservation equations; 2) the pressure in the compartment is assumed to be equal to the atmospheric pressure, because the windows in the compartment are open (the grasses are broken), therefore the derivatives of pressure are zero;3) the Navier-Stokes equations should consider the low-speed, thermally-driven flow with an emphasis on heat transport from fires. This assumption rules out the scenario involving flow speeds approaching the speed of sound, such as in case of explosion and detonation; 4) irradiative heat transfer is included in the model via heat losses thru the open compartment's windows, and it is based on the Stefan-Boltzmann law [10];

IV SIMPLIFICATION OF MAIN PARABOLIC SYSTEM (1)

Since the average dimensionless temperature and combustion rate are the functions of time only, the energy conservation portion of the main system (1) can be simplified [9]:

$$\frac{d\theta}{d\tau} = \delta(1-C)^k(\exp\frac{\theta}{1+\beta\theta}) - P\theta^4 \quad \ldots\ldots\ldots\ldots (6)$$

$$\frac{dC}{d\tau} = \gamma\delta(1-C)^k(\exp\frac{\theta}{1+\beta\theta}) \quad \ldots\ldots\ldots\ldots\ldots (7)$$

The direct solution of equations (6) and (7) is the "normal" way of solving the problem. The mathematical modeling of the physical and chemical transformations of real materials as they burn is in very early stage of development. A reliable heat transfer model should be based on accurate input data including material properties and boundary conditions. Such calculations have, however, been haunted by the uncertainty of measured values, especially, of the chemical quantities. As it is stated in NIST's report [3] regarding the mathematical modeling of FDS "…Indeed, the mathematical modeling of the physical and chemical transformations of real materials as they burn is still in its infancy", and "… we must learn to live with idealized descriptions of fires and approximate solutions to our idealized equations".) In order to overcome this uncertainty of input values, the mathematical theory of optimal control [12] has been used: this allows us to obtain the solution of differential equations and the dimensionless "uncertain" parameters based on an extra requirement (so-called "payoff functional"), which in our case is the maximum temperature that is known from the fire tests results, or the area between the temperature-time curve and the horizontal line of T=300°C. This allows us also automatically connect the performance based and the prescriptive design methods.

V APPROXIMATE SOLUTION OF THE NAVIER-STOKES EQUATIONS

It has been assumed in our case of computing the structural fire load that the air-gas density and the pressure are constant in the compartment, therefore the motion of fluid equations can be simplified as follows:

$$\frac{\partial W}{\partial \tau} + \Pr(V\frac{\partial W}{\partial x} + W\frac{\partial W}{\partial z}) = \frac{4}{3}\Pr\nabla W + Fr \quad \ldots. (8)$$

$$\frac{\partial V}{\partial \tau} + \Pr(V\frac{\partial V}{\partial x} + W\frac{\partial V}{\partial z}) = \frac{4}{3}\Pr\nabla V \quad \ldots\ldots\ldots\ldots (9)$$

$$\frac{\partial V}{\partial x} + \frac{\partial W}{\partial z} = 0 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (10)$$

W & V – Dimensionless vertical and horizontal components of velocity vector; Pr=L=1.

Differentiating the first with respect to z, the second with respect to x and subtracting the resulting equations will eliminate pressure and any potential force. Defining the stream function ψ through:

$$V = \frac{\partial \psi}{\partial z}; W = -\frac{\partial \psi}{\partial x} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (11)$$

Results in mass continuity being unconditionally satisfied (given the stream function is continuous), and then incompressible Newtonian 2D momentum and mass conservation degrade into one equation:

$$\frac{\partial}{\partial t}(\nabla^2\psi) + \frac{\partial \psi}{\partial z}\frac{\partial}{\partial x}(\nabla^2\psi) - \frac{\partial \psi}{\partial x}\frac{\partial}{\partial z}(\nabla^2\psi) =$$
$$= \nu\nabla^4\psi \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (12)$$

Where ∇^4 is the (2D) biharmonic operator and ν is the kinematics viscosity, $\nu = \frac{\mu}{\rho}$. This single equation together with appropriate boundary conditions describes 2D fluid flow, taking only kinematics viscosity as a parameter. Approximate solution of non-linear equation (12) can be obtained, if the stream function is presented as follows:

$$\psi(\tau, x, z) = \exp(-\alpha\tau)\sin(\pi x)\sin(\pi z) \ldots\ldots\ldots (13)$$

Substituting (13) into (12) and solving for α:

$\alpha = 2\pi^2\nu$ and ν=4/3.

Finally, the stream function is:

$$\psi = \{\exp[-\frac{4}{3}(1+b^2)\pi^2]\tau\}(\sin \pi x)(\sin \pi z) \,. \quad (14)$$

Where: b=L/h>1; L – compartment's horizontal dimension; h – height of the compartment; x=x1/bh; z=z1/h – dimensionless coordinates. Dimensionless vertical and horizontal components of velocity vector are as follows:

$$V = -W =$$
$$= \pi\{\exp[-\frac{4}{3}(1+b^2)\pi^2]\tau\}(\sin \pi x)(\sin \pi z) \quad ...\ (15)$$

Velocities "V" and "W" are presenting the convection process in the air-gas flow. Now substitute (15) in first two equations of system (1) and assume conservatively that the gradient of dimensionless temperature can be substituted by the difference between the temperature inside and outside of the compartment. In this case the equations are as follows:

$$\frac{\partial \theta}{\partial \tau} + \Pr(\pi\{\exp[-\frac{4}{3}(1+b^2)\pi^2]\tau\}(\theta - \theta_0)) =$$
$$= \delta(1-C)^k \exp(\frac{\theta}{1+\beta\theta}) - P\theta^4 \text{..............}(16)$$

$$\frac{\partial C}{\partial \tau} + \Pr(\pi\{\exp[-\frac{4}{3}(1+b^2)\pi^2]\tau\}(C - C_0)) =$$
$$= \gamma\delta(1-C)^k \exp(\frac{\theta}{1+\beta\theta}) \text{..........................}(17)$$

Solutions of equations (16) and (17) are similar to equations (6) and (7).

VI EXAMPLES

Example #1: Data: $T_*=600^0$ K; δ=20; K_v=0.05; β=0.1; P=0.157; 0< τ<0.2;

882^0K< T_{max}< 1092^0K; Fast Fire.

Result: 0.05<γ< 0.175

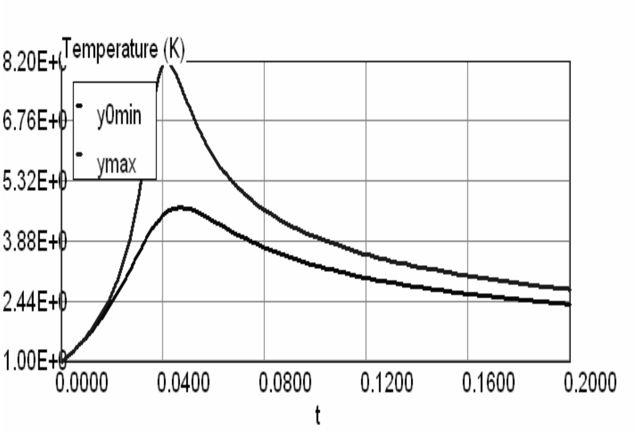

Fig. 1 Dimensionless temperature-time curves

The final approximation of the dimensionless temperature – time curve (see Fig.1) is as follows:

$$\theta = 0.09 + 193.8\tau - 2951.8\tau^2 + 16740\tau^3 - 32750\tau^4$$
…………………………………………………… (18)

Example #2: Data: : Data: T_*=600 K; δ=20; K_v=0.05; β=0.1; P=0.157; 0< τ<0.2;

807^0K< T_{max}< 882^0K; Medium Fire.

Result: 0.175<γ< 0.275

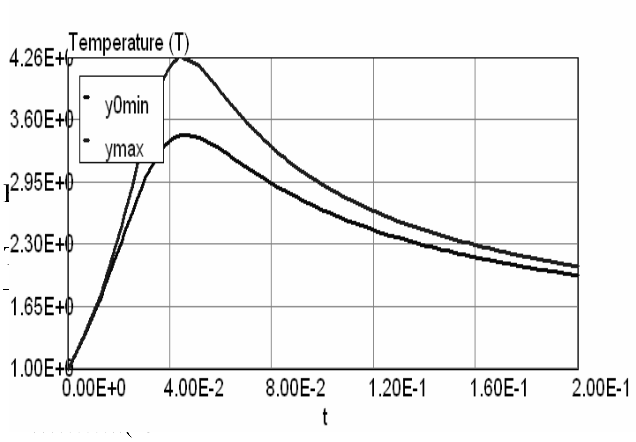

Fig. 2 Dimensionless temperature-time curves

The final approximation of the dimensionless temperature – time curve (see Fig. 2) is as follows:

$$\theta = 0.26 + 175.3\tau - 2767\tau^2 + 16080\tau^3 - 32090\tau^4$$
……………………………………………………….(19)

Example #3: Data: T_*=600 K; δ=20; K_v=0.05; β=0.1; P=0.157; 0< τ<0.2;

711^0K< T_{max}< 798^0K; Slow Fire.

Result: 0.275<γ< 1.0

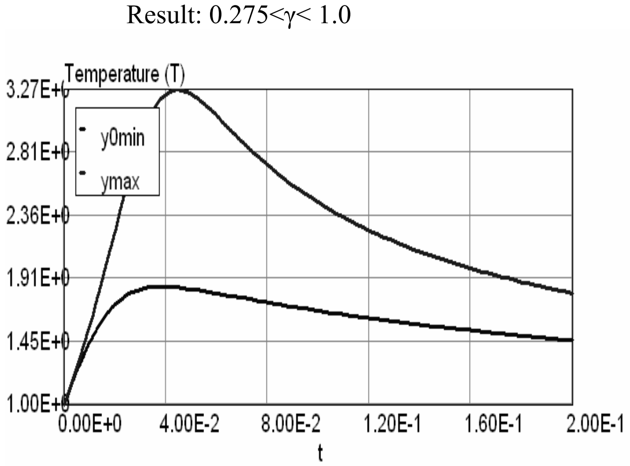

Fig. 3 Dimensionless temperature-time curves

The final approximation of the dimensionless temperature – time curve (see Fig.3) is as follows:

$$\theta = 0.67 + 119.4\tau - 1904\tau^2 + 11150\tau^3 - 22450\tau^4$$
.
……………………………………………………..…(20)

REFERENCES

1. Becker, W.H.K., "Report on the Work of ISO/TC 92/SC 4 `Fire Safety Engineering", *Intl. Fire Safety Engineering Conf.*, Commonwealth Scientific and Industrial Organization, Sydney, Australia (1992).
2. Statutory Instrument SI 1985, No. 1965. *Her Majesty's Stationery Office*, London, 1985.
3. NIST Special Publication 1018-5 "Fire Dynamics Simulator (Version 5)" Technical Reference Guide,2008 Volume 1: Mathematical Model
4. "CEN TC 250/SC1, Draft for Eurocode 1: Part 2.7"-April European Committee for Standardization, 1993
5. Babrauskas, Dr. V.," Performance-Based Fire Safety Engineering Design: The Role of Fire Models and Fire Tests", Interflam 99, Edinburgh, Scotland, June 1999.
6. Society of Fire Protection Engineers," The SFPE Engineering Guide to Performance-Based Fire Protection Analysis and Design", December, 1998.
7. Razdolsky, L., "Explosion in a High-Rise Building", METROPOLIS&BEYOND Proceedings of the 2005 Structures Congress and the 2005 Forensic Engineering Symposium New York, NY, 2005
8. Razdolsky, L., Petrov, A., Shtessel, E., "Critical conditions of local ignition in a large medium with convective heat transfer" Physics of combustions and explosions, National Academy of Science, 1977
9. Frank-Kamenestkii, D.A., "Diffusion and Heat Transfer in Chemical Kinetics". Plenum Press, New York, 1969
10. John H. Lienhard IV and John H. Lienhard V, "Heat transfer textbook", 3rd Edition. Phlogiston Press, Cambridge, MA, USA, 2008
11. Zeldovich, Ya.B. G.I. Barenblatt, V.B. Librovich and G.M. Makhviladze, "The mathematical theory of combustion and explosions". Consultants Bureau, New York, 1985
12. Lawrence C. Evans, L.,C.," An Introduction to Mathematical Optimal Control Theory", Version 0.2 Department of Mathematics University of California, Berkeley, CA, 1983