# Fire safety through mathematical modelling

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The present state of fire safety design is based largely on the judgement as enshrined in the prescriptive codes. The fundamental laws of physics, chemistry and mathematics are not fully utilized to evolve scientifically-based performance-oriented fire safety design. Performance-based fire safety standards are currently under development to supplement the existing prescriptive standards. The use of performance-based standards provides flexibility in maintaining the accepted level of fire safety, thus reducing the cost of design, construction and maintenance. The present paper discusses a holistic approach on fire safety engineering. Fire models that have been developed at the Central Building Research Institute, Roorkee have been described.

ACCIDENTAL fire – 'unwanted' or 'unfriendly' fire as it is sometimes aptly and popularly referred to – has been a scourge of mankind since time immemorial. While total and complete prevention has remained an unachievable ideal, efforts to minimize losses are continued to be made. These have been increasingly successful as understanding of the phenomenon has grown, prediction of factors responsible for spread of smoke and hot gases has been possible and the protection against fire has been refined and developed.

The understanding of fire science and its application was based largely on the reduced scale physical tests. Fire research is aimed to build up a predictive methodology to be able to forecast the circumstances and conditions under which a fire may grow, and also the impact of fire safety measures on the growing fire. In the last couple of years, a relatively small but consistent effort has been made to determine the basic principles of unwanted fire, to measure the variables involved and to develop coordinated engineering approach to predict the course of fire and the response of fire safety measures. As a result, there is a progressively emerging fire protection engineering technology that can potentially be used to evaluate the fire safety performance of a building, that differs widely from the current prescriptions of the code. Fixing the level of acceptance, one can use these codes to develop an optimum fire safety design. Performance requirements can be specified separately for different parts of the safety system using deterministic approach; however, a holistic approach would include probabilistic theory together with the deterministic modelling.

Efforts have been made at the Central Building Research Institute (CBRI) to evolve mathematical models<sup>1</sup> to analyse the behaviour of fire growth and spread, to evalu-

ate building systems' performance to provide an assessment for the effectiveness of design and material use. Over the past decade, CBRI has developed computer-based models as a predictive tool for estimating the environment when a fire is present. Improvement in the physical basis of these models is the continuous process.

# Fire safety engineering

Fire safety engineering (FSE) is the application of scientific and engineering principles to protect people and the man-made and natural environments from the destructive effects of fire. Safety to life and property is the main concern of the FSE. The level of fire safety is a complex interaction of many phenomena, including fire initiation, fire growth and spread, response of building components (walls, floors, beams, etc.), response of occupants to the presence of fire, and the response of sprinklers/detectors and other fire safety measures to fire. The FSE objectives<sup>2</sup> can be achieved by: (a) minimization of fire occurrence, (b) controlling fire growth and spread rate and (c) provision of safe and accessible fire escape routes.

Ideally, a good fire safety system should include all the three objectives simultaneously. Efforts are to be made to draw maximum benefit for each rupee spent on fire safety. The problem lies with the perception of the fire protection engineer involved. The fire safety decision is guided by his experience and position. There is no universally accepted methodology for the evaluation and analysis of fire safety design.

Figure 1 shows various aspects of the FSE network; it involves two aspects, viz. fire safety and life safety. The attainment of fire safety has traditionally been achieved through control on material flammability and compartmentation. Fire safety can be achieved through preventive and protective means. Preventive measures include good housekeeping and regular maintenance of the occupancy, so that combustibles are not allowed to accumulate at one

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point. Use of non-combustible materials is preferred to reduce the probability of fire occurrence.

Protective measures can be classified into passive and active. Passive fire protection is defined as protection through ignition delays, reduced rate of burning and fire spread. Techniques available for providing passive fire protection include: (a) dividing space into small compartments for fire confinement, (b) fire-resistant structural elements to prevent from collapsing, and (c) use of fire-retardant materials to reduce the rate of burning.

Active fire protection is provided by applying fireextinguishing agents to the burning materials through extinguishers/hydrants/sprinklers or by introducing them into the fire environment through flooding systems. The application of extinguishing agents could be manual or automatic. The most widely used extinguishants are water, carbon dioxide, foam compounds and dry chemical powder.

The provision of safe means of escape helps to maximize the safety to the life of the occupants. For example, it is possible to reduce the level of risk to the occupants of a building by providing enough number of large-width escape routes and means to pressurize them to act as fully protected spaces within the building to allow unescaped occupants to congregate till the fire is extinguished. Other portions of the building may be allowed to perish. On the other hand, if the building is well protected but the escape routes are not in sufficient quantity and capacity or the available escape route may not be fully protected or it is being used for purposes other than the one for which it is provided, it may lead to avoidable deaths.

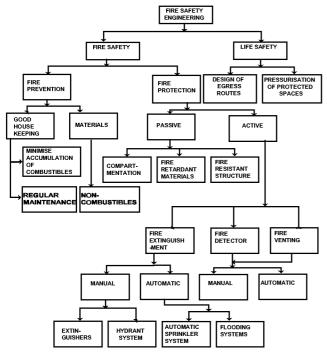
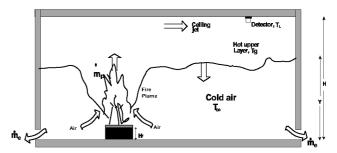


Figure 1. Fire safety engineering network.

In another example, where two fire safety design strategies have been proposed, only passive fire protection systems are considered in the first strategy and in the second strategy, both passive and active systems have been considered. Clearly, in the second strategy the level of passive fire protection may be less than the level pertaining to the first strategy to maintain the same level of fire safety. It is, therefore, essential for a fire protection engineer to have tools to predict the behaviour of individual components of fire safety in case of a fire. The development of the capability to predict the level of fire and life safety requires a set of models to quantify the performance of the building's fire safety system. While much progress has been achieved to develop mathematical models to predict the growth and spread of fire, the response of building components and fire safety measures to fire, efforts are needed to have a comprehensive model which can be used in totality to achieve a satisfactory level of fire and life safety.

## Fire modelling

To predict the behaviour of fire in a compartment, a description of the fire in terms of physical equations must be made. Such a model is an idealization of the compartment fire phenomenon. Consider a fire, which starts at some point below the ceiling and which releases energy and products of combustion. The hot products of combustion reach the ceiling and spread out to form a hot gas layer<sup>3</sup>. On reaching the ceiling, the hot products of combustion turn into a near-ceiling horizontally outward flow. The outward flow of hot gases is checked by the presence of bounding walls of the compartment. A layer of hot gases is soon formed in the upper portion of the compartment. There is a relatively sharp interface between the hot upper layer and the air in the lower part of the compartment. It is assumed that the distribution of temperature and other properties are uniform throughout each layer. Figure 2 is a schematic representation of the fire phenomenon in compartments during early stages of fire. It shows that the room environment is soon turned into a two-layer envi-



**Figure 2.** Schematic representation of fire phenomenon in enclosures.  $T_{\rm L}$ , temperature of heat responsive element of sprinkler/detector, K;  $T_{\infty}$ , ambient temperature, K;  $T_{\rm g}$ , layer temperature, K;  $\dot{m}_{\rm p}$ , plume mass flow rate, kg/s;  $\dot{m}_{\rm e}$ , mass flow rate of air through leakages, kg/s;  $H_{\rm f}$ , height of fire source, m.

ronment after the fire has occurred. The meeting point between hot and cold layers is called interface. The twolayer environment is modelled as a two-zone model.

The room boundaries, though heated, do not contribute much during the growth period. Under certain conditions when the room boundaries begin to influence the fire behaviour, rapid spread of fire takes place. These effects magnify as the size of the fire becomes fully developed, as shown in Figure 3. The transition of fire from the growing stage to a fully developed stage is termed as the 'onset of flashover'. The onset of flashover<sup>4</sup> leads to inclusion of large number of combustibles in the fire. The preflashover fire is of decisive significance with regard to the level of safety required for the rescue of people. The response of detectors and sprinklers belongs to this period of the fire. The post-flashover fire is significant with respect to the fire behaviour of the load-bearing components of the structures, the spread of fire from one compartment to another via partitions and ventilation systems.

Full scale and reduced scale experiments on compartment fires are familiar examples of physical models of fire. Experimental models of an enclosure fire simulate typical conditions that may be experienced in an accidental fire. This class of models has provided valuable information on a number of aspects of fire behaviour. The results obtained through physical modelling are applicable to the conditions experimented upon, and cannot be applied commonly. Unfortunately, materials burn in a way that is determined by their environment and therefore fire tests which classify their behaviour for one environment condition can only be of limited value. What is needed are predictive methods for describing fire growth and smoke spread based on properties of materials which can be used to relate test data to practical scenarios. With such methods, it should be possible to develop cost-effective fire safety designs which allow sufficient time for occupants to escape.

The availability of fast modern computing systems has stimulated rapid development in the theoretical modelling of fire. Mathematical models based upon fundamental principles of conservation of mass, momentum and energy

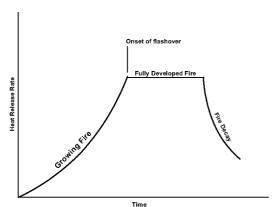


Figure 3. Variation of heat release rate with time in enclosure fire.

are quite general in nature and once validated for their application, these models can predict complete fire environment economically, within a reasonable time frame. Mathematical models can also be used to examine the consequences of adopting alternative fire protection designs. Information on gas temperatures, species concentration, and heat fluxes to boundaries and occupants that can be derived easily by the use of mathematical models, is of great value in establishing engineered fire safety.

Fire, although complex, can be described with the help of a set of mathematical equations representing physical and chemical changes occurring during the growth of a fire. The mathematical model, as the set of equations is called, is quite general in nature and can be applied to a variety of scenarios. Such models are helpful in early prediction of occurrence of hazardous conditions and to suggest preventive measures well in advance. Figure 4 gives an account of various types of models commonly used in the area of FSE.

Of the mathematical modelling techniques<sup>5</sup>, the deterministic type is preferable to the stochastic model. It can forecast a specific parameter such as temperature as a function of time and space for any situation under consideration and is thus the mathematical counterpart of a laboratory experiment. The deterministic models can be classified as zone and field models. Mathematically, zone models consist of a set of time-dependent ordinary differential equations, while the field model comprises a set of convection-diffusion partial differential equations in two or three dimensions as dictated by the accuracy or generalization desired. Solution of zone models is straightforward, but the field models are difficult to solve and require good knowledge of advanced numerical methods and correspondingly adequate computing facilities. Zone models could be empirical or semi-empirical depending upon how many empirical formulae have been used in the development of a model. Stochastic or probabilistic models are based upon the probability of occurrence of a par-

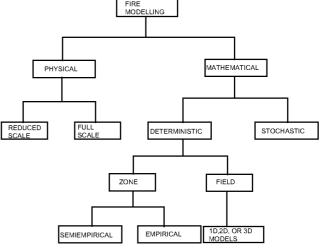


Figure 4. Fire modelling technology.

ticular phenomenon. While deterministic models are quite popular, research has been initiated recently on stochastic modelling. Stochastic models will take some more time to come to be accepted.

Physical models are the experimental models created in a laboratory to study, for example, change in temperature with changing rate of burning, in a compartment with and without doors/windows. Physical models could be full scale/reduced scale models. Fire being destructive, the cost of experimentation is quite high; so reduced scale models are preferred. The disadvantage with reduced scale physical model is that complete similarity between full scale and reduced scale tests cannot be preserved. Alternatively, mathematical models based upon fundamental laws of conservation of mass, momentum and energy are quite general in nature and economical.

Figure 5 shows how one can make use of fire models in evaluating the risk and assessing the response of fire safety systems<sup>6</sup>. Figure 5 explains that once the level of

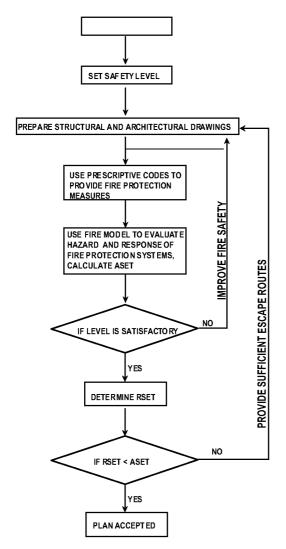


Figure 5. Use of fire models in examining the risk.

fire safety is fixed and structural/architectural drawings are made, one can use prescriptive codes to decide the list of safety measures. The efficacy and sufficiency of the fire protection measures are then determined with the help of fire models. Assuming that the prescribed fire protection measures are sufficient, then we have to determine the values of Available Safe Egress Time (ASET) and Required Safe Egress Time (RSET). The latter is the minimum time required for safe evacuation from a building under fire and the former is the time which is actually available to the users before the fire becomes hazardous. Clearly, for life safety ASET has to be larger than RSET. In case the time of evacuation, and hence RSET is excessively large, one has to provide additional means of fire escape for which architectural drawings have to be modified. The value of ASET may be determined by using, say, CALFIRE model<sup>7</sup> and RSET can be determined using SAFE-R model, discussed later in the article.

# Modelling activities at CBRI

Zone models are comparatively simple, running cost is small, and so they are popular among the fire safety community. Considerable efforts have been made at the CBRI, Roorkee, to bring zonal modelling application as exemplified by the CALFIRE model to assist a designer to perform hazard evaluation studies in compartment fires. The laboratory has developed the following models for use by the community to fulfill the requirements of FSE: (a) CALFIRE: CALculate Fire In Room and Enclosure, (b) NEST: Numerical Estimation of Sprinkler actuation Time, (c) SAFE-R: Safe and Accessible Fire Escape Route.

#### **CALFIRE**

CALFIRE is a semi-empirical, knowledge-based, interactive computer program that has been designed to rapidly give the user a quantified assessment of a given fire scenario<sup>7,8</sup>. Its database contains a set of physical, chemical and thermodynamical properties of a number of materials – both combustible and non-combustible, to make it truly user-friendly. Data entered through a keyboard are stored and simultaneously transferred to other places where they are needed. Checks are made to ensure that calculations are not used beyond their valid range, to prevent the user from misusing the program.

CALFIRE contains a set of calculation algorithms to determine fire size, flame length, room temperature and the depth of hot gas layer in naturally ventilated, forced ventilated and closed rooms. Further options have been provided for the determination of vent size for effective smoke venting and response time of sprinkler/detector for fire control. CALFIRE is relevant for fires in domestic, commercial and small industrial buildings.

CALFIRE has been developed for a model scenario as depicted in Figure 2. The temperature of a hot gas layer has been calculated by assuming that the addition of heat to a fixed volume of an ideal gas in a compartment does not cause pressure to rise inside the compartment. Permitting leakage of air through openings at the floor level compensates for any increase in the pressure of the contained gases. The amount of air leaking through the openings may be calculated by considering the overall energy balance in the compartment and is given as follows:

$$\dot{m}_{\rm e} = \frac{(1 - \lambda_{\rm c})\dot{Q}}{C_{\rm p}T_{\infty}},\tag{1}$$

where  $\dot{m}_{\rm e}$  is the mass flow rate of air through leakages in kg/s,  $\dot{Q}$  is heat release rate in kW,  $C_{\rm p}$  is heat capacity of air in kJ/kg-K,  $T_{\infty}$  is ambient temperature in K and  $\lambda_{\rm c}$  is the heat loss fraction through boundaries. The value of  $\lambda_{\rm c}$  varies between 0.6 and 0.9.  $(1-\lambda_{\rm c})\dot{Q}$  is thus the net amount of heat added to the volume. The final form of CALFIRE equations  $^7$  is as follows:

$$\frac{\mathrm{d}T_{\mathrm{g}}}{\mathrm{d}t} = -T_{\mathrm{g}}[\dot{m}_{\mathrm{p}}(T_{\mathrm{g}} - T_{\infty}) - \dot{m}_{\mathrm{e}}T_{\infty}]/A_{\mathrm{F}}\rho_{\infty}T_{\infty}(H - Y),$$
(2)

$$\frac{\mathrm{d}Y}{\mathrm{d}t} = -(\dot{m}_{\mathrm{p}} + \dot{m}_{\mathrm{e}})/\rho_{\infty}A_{\mathrm{F}},\tag{3}$$

where  $T_{\rm g}$  is the layer temperature in K,  $A_{\rm F}$  is compartment floor area in sq m,  $\rho_{\infty}$  is ambient air density in kg/m³, H is ceiling height in m, Y is height of interface in m, t is time in seconds and  $\dot{m}_{\rm p}$  is the plume mass flow rate at the interface level Y. Interface level is the height below which cold lower layer exists and above which upper hot gas layer exists. The following expression has been used for determining  $\dot{m}_{\rm p}$  (ref. 9).

$$\dot{m}_{\rm p} = 0.21 \rho_{\infty} \left[ \frac{(1 - \lambda_{\rm r}) \mathbf{g}}{C_{\rm p} \rho_{\infty} T_{\infty}} \right]^{1/3} \dot{Q}^{1/3} (Y - H_{\rm f})^{5/3},$$
 (4)

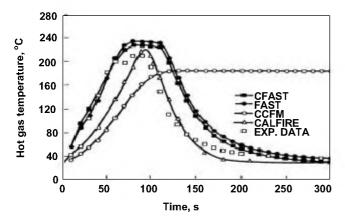


Figure 6. Variation in upper layer temperature with time.

where **g** is acceleration due to gravity in m/s<sup>2</sup> and  $H_f$  is height of fire source in m.  $\lambda_r$  is the radiative heat loss fraction,  $(1 - \lambda_r) \dot{Q}$  is the net amount of heat convected upwards through the plume. Following Cooper<sup>10</sup>  $\lambda_r = 0.35$  has been used for typical hazardous flaming fires. Thus  $(Y - H_f)$  is the clear height to which plume gases have to travel before entering the upper layer. Model equations (1)–(4) have been solved numerically with the help of the fourth-order Runge–Kutta method to determine the temperature and depth of hot gases at any instant of time t. The depth of the hot gas layer is the distance between ceiling and the interface (H - Y), as shown in Figure 2.

The validity of CALFIRE model equations (1)–(4) has been determined by comparing its predictions with Chow's<sup>11</sup> experimental data. Chow has carried out experiments in a closed chamber – 4 m length, 2.9 m width and 2.83 m height – to determine the rise in the hot layer temperature and its thickness. Gasoline was burned to create the experimental fire. The heat release rate was obtained by the product of the mass loss rate of gasoline with its heat of combustion (43.7 MJ/kg). The experimentally measured temperature and layer thickness have been compared with the values predicted by three other zone models, namely CFAST<sup>12</sup>, FAST<sup>13</sup>, and CCFM.VENT<sup>14</sup>, used quite frequently all over the world.

Figure 6 shows the variation in upper layer temperature with time. The figure shows that predictions made by CCFM.VENT follow similar trend during the fire growth period only. Predictions made by CALFIRE are in good agreement with the experiment. This shows the validity of our model.

Figure 7 shows the variation in layer thickness with time. It is clear from Figure 7 that the layer descends to the fire level in just about 10 s and remains at this level for the remaining period. CFAST, FAST and CCFM.VENT predict that the layer descends much below the fire level. Maximum descendance is predicted by the FAST model. After reaching the lowest level in about 70 s, remaining at this level for about 40 s, the layer shrinks and ascends almost to the fire level in another 40-s period.

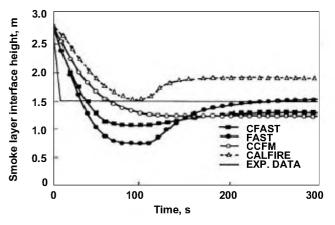


Figure 7. Variation in layer thickness with time.

CALFIRE predicted that the layer reaches the fire level after 90 s – the time corresponding to the maximum layer temperature; remains at this level for a very short time, say 20 s; and then shrinks further to settle slightly above the fire level. The shrinkage occurs due to lowering of the layer temperature.

### **NEST**

An automatic sprinkler system constitutes an effective tool of fire safety in a building. It not only performs the role of fire detection, but can simultaneously and automatically carry out the equally important job of fire limitation and extinction. Each role of the sprinkler is performed separately and one is related to the other insofar as early detection makes extinction easy. Sprinkler, being a constant operating temperature device, activates only when its heat responsive element, a glass bulb or a fusible metal link, achieves a specific operating temperature. The operating time of a sprinkler will, however, depend upon the rate at which heat from the hot gas layer is absorbed by it.

NEST has been developed to determine the operating time of sprinkler/detector fitted in enclosures<sup>15</sup>. The following equations have been solved in conjunction with CALFIRE equations (1)–(4) to determine the time of operation of the sprinkler/detector.

$$\frac{\mathrm{d}(\Delta T_{\mathrm{L}})}{\mathrm{d}t} = \frac{\Delta T_{\mathrm{c}} - \Delta T_{\mathrm{L}}}{\tau},\tag{5}$$

$$\tau = \frac{mC_{\rm L}}{hA},\tag{6}$$

where  $\tau$  is time constant in seconds, m is mass of sprinkler/detector link in kg,  $C_{\rm L}$  is heat capacity of sprinkler link in kJ/kg-K, h is surface heat transfer coefficient of link in kW/m<sup>2</sup>-K and A is link surface area in m<sup>2</sup>.  $\Delta T_{\rm c}$  and  $\Delta T_{\rm L}$  are the excess temperatures of the ceiling-jet and the heat responsive element of the sprinkler/detector, above prevailing ambient temperature  $T_{\infty}$ . Hot layer temperature,  $T_{\rm g}$  is calculated by using CALFIRE equations (1)–(4),  $\Delta T_{\rm c}$  is calculated with the help of following equation  $^{16}$ ,

$$\frac{\Delta T_{\rm c} - \Delta T_{\rm g}}{T_{\rm c}} = 0.0184 \, \frac{(\dot{Q}/r)^{2/3}}{H} \,, \tag{7}$$

where r is radial distance of sprinkler/detector location in m.  $\tau$  is not really a constant, it varies with the inverse of the square root of velocity due to the presence of h in eq. (6). It is the quantity  $\sqrt{u_c}$  which is constant, where  $u_c$  is ceiling-jet velocity. The product of the time constant and the square root of gas velocity is called the response time index (RTI). Thus

$$\tau = \frac{RTI}{\sqrt{u_c}}.$$
 (8)

Equation (5) together with eq. (8) gives

$$\frac{\mathrm{d}(\Delta T_{\mathrm{L}})}{\mathrm{d}t} = \frac{u_{\mathrm{c}}^{1/2}(\Delta T_{\mathrm{c}} - \Delta T_{\mathrm{L}})}{\mathrm{RTI}}.$$
 (9)

 $u_c$  is calculated with the help of the following equation <sup>17</sup>.

$$u_{\rm c} = 0.196 \frac{\dot{Q}^{1/3} H^{1/2}}{r^{5/3}}, \text{ for } r/H > 0.15.$$
 (10)

The validity of NEST model equations (5)–(10) has been determined with the help of Evans<sup>18</sup> model. The calculations have been performed for the same input data as those used by Evans<sup>18</sup>, to have a fair comparison of the predictions by two models under similar conditions.

To determine the actuation times of three types of sprinklers, having RTI values of 25, 100, and 400 m $^{1/2}$  s $^{1/2}$ , it is assumed that these sprinklers are fixed beneath the ceiling at a distance of 2.44 m away from the fire axis. Compartments of height equal to 3.66 m and floor area ranging from 23.8 sq m to 1522 sq m have been used. It is further assumed that  $\lambda_{\rm r}=0$  and  $\lambda_{\rm c}=0.8$ . The sprinkler rating has been selected as  $74^{\circ}{\rm C}$ . The heat release rate as a function of time is given by,

$$\dot{Q} = 0.00293t^2. \tag{11}$$

Figure 8 shows the variations of the sprinkler operating time of three sprinklers with compartment sizes, as predicted by the NEST model and Evans model<sup>18</sup>.

It is evident from Figure 8 that the difference between the NEST values and the Evans values is very small. The comparison showed that the NEST model can be used for calculating the sprinkler's actuation time in compartments of low ceiling height.

# SAFE-R

Incidents in which people are seriously injured or killed due to stampede are not restricted to emergencies such as fire or to conditions of crowd violence or even simple

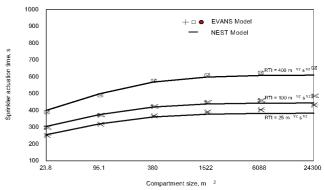


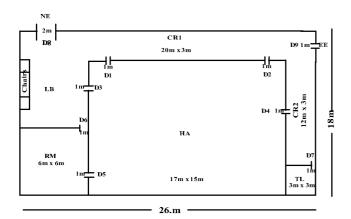
Figure 8. Comparison between NEST and Evans model predictions.

exuberance of some members of a crowd. Such events can occur, and have occurred at sports events, religious gatherings, music concerts, cinema hall and similar assemblies. Serious injury and even death can occur during entry, occupancy and evacuation of a building. It can happen under conditions that might, in every other respect, appear to be normal even to people in close proximity to those hurt in the incident.

There are a number of reasons for which emergency evacuation becomes necessary. Apart from fire and smoke threats, others may include earthquake, toxic gas leak, power failure, bomb threat, and civil defence emergency. The foregoing reasons are of direct concern to building managers, designers and architects, safety officials, and insurance companies. It is the responsibility of all concerned to provide safe and accessible fire escape routes to the people.

While there are various components of the egress problem within the buildings, we are primarily concerned with modelling the adequacy of the facility to handle the evacuation process. Our concern is to develop a model which is capable of determining the following: (a) The overall time to exit a building; (b) potential bottlenecks; (c) effects of blocking and time delays on the exit routes; and (d) adequacy of the number of exits, their capacity, physical configuration and sizing.

Several variable factors involved in an emergency situation that make it difficult to predict with confidence the safety rating of a building, are numerous locations at which a fire may originate and variation in the ways that fire develops and its combustion products can move. However, even more unpredictable are the decisions that occupants may make with regard to movement during an emergency. The SAFE-R model developed at CBRI, provides a methodology for estimating the necessary Time of Evacuation (TOE). A network description of the building together with a simulation of occupants' movements is used to evaluate alternative egress and rescue routes. An algorithm has been developed using path-set method to



**Figure 9.** Plan of a single-storey building (HA, Hall; RM, Room; TL, Toilet; CR, Corridor; LB, Lobby; NE, Normal exit; EE, Emergency exit; D, Door).

identify the various routes that are available for people's movement. Flow equations have been developed to determine TOE through each route. Details of the algorithm are under publication.

Figure 9 shows a single-storey building, which could be a control room in an industry, a conference room, a court room, a bank or similar mercantile building, a cinema hall or similar entertainment hall, or even a religious congregation. It is assumed that 95 people have assembled in the building. Three people are present in the Manager's room and two are using the toilet. The remaining ninety persons are present in the hall. In the lobby, chairs are provided for waiting people. There is a main entrance/exit and one emergency exit. Sizes of various locations within the building are shown in Figure 9.

Figure 10 shows a network representation of the building. The network comprises a number of nodes and arcs. Nodes represent the source; room, hall, corridor, etc. where people can congregate. The path joining two nodes is represented by an arc. Dynamic capacity (DC) and the traversal time (TT) of an arc are represented by a and b, respectively. DC is defined as the number of persons moving through an arc per unit time. TT is the time to traverse the passage represented by an arc. Node capacity represents the maximum capacity of a node. The values inside triangle represent the number of persons present at the node before the evacuation process is initiated.

Having defined the network, available routes are identified and total TT of each route has been calculated. Maximal flow capacity through a route is calculated on the basis of the DC through an arc on the route. Calculations have been performed to determine the TOE as well as the maximum ASET. It is prudent for safe evacuation that TOE < ASET.

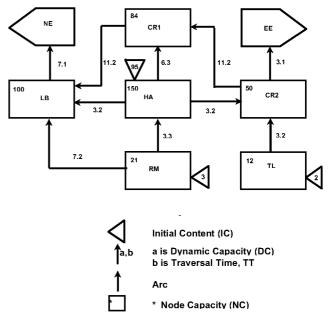
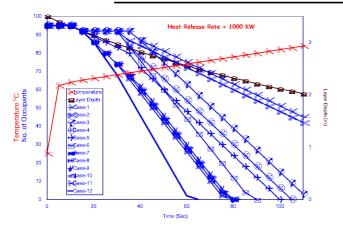


Figure 10. Network representation of the building.

Case	Door closed	Evacuation time (s) (TOE)	Available safe egress time (s) (ASET)	Desirable/ undesirable
Case-1	D1, D3, D4 and D9	185	110	Undesirable
Case-2	D2, D3, D4 and D9	180	110	Undesirable
Case-3	D2, D3 and D9	115	110	Undesirable
Case-4	D3, D4 and D9	105	110	Desirable
Case-5	D1, D3 and D9	100	110	Desirable
Case-6	D3 and D9	90	110	Desirable
Case-7	D1, D4 and D9	80	110	Desirable
Case-8	D2, D4 and D9	80	110	Desirable
Case-9	D1, D2 and D9	80	110	Desirable
Case-10	D4 and D9	80	110	Desirable
Case-11	D9	80	110	Desirable
Case-12	Nil	65	110	Desirable

Table 1. Comparison of evacuation time and safe egress time for a building in different cases



**Figure 11.** Comparison between evacuation time and different cases of door opening (Table 1).

Figure 11 shows the results of our computation. The variation of temperature and depth of the hot gas layer, assuming a heat release rate of 1000 kW has been calculated with the help of CALFIRE. The value of ASET has been calculated on the basis of criterion 1, discussed later as 110 s. TOE has been calculated using SAFE-R for various options of door open. Table 1 gives a comparison of two times, i.e. time of evacuation under different cases of doors closed and the time available for safe evacuation. It is clear from Figure 11 and Table 1 that in all the cases, except cases 1 to 3, the evacuation will be completed well within the ASET.

#### Conclusions

Unwanted fires pose major risk to the safety of life and property in a built environment. India suffers a colossal loss of over Rs 5000 million per annum on account of property alone. In addition to this, several thousand lives are also lost due to fires. Combined with the introduction of advanced systems of fire detection and suppression, there is a need to develop predictive tools for estimating the environment and for measuring the performance of the fire safety systems. CBRI has been carrying out experimental and modelling research programmes to improve the knowledge on the fire growth and spread. Over the

past decade, CBRI has developed a series of computerbased fire models as a predictive tool for estimating the environment which results in a building.

In the present paper, an attempt has been made to introduce a mechanism to allow researchers, fire protection engineers, and others an access to the understanding of the behaviour of fires in buildings. The validity of CALFIRE and NEST models has shown that these models can be used to predict the onset of hazardous conditions in a building under fire. The criteria for deciding whether or not the hazardous conditions are prevailing, are the upper layer thickness and its temperature. These two criteria are referred to as human tenability limits. Evacuation of occupants to a safer place must be completed well before the onset of untenable conditions. It is reported that the threshold of human tenability to heat fluxes falls in the range of 1.2 to 2.5 kw/m<sup>2</sup>. The former corresponds to radiation from a black body at 108°C and the latter corresponds to 183°C. A method has been proposed for calculating the time of onset of hazardous conditions in a building under fire. Two criteria have been considered for determining the time when untenable conditions are developed in a compartment. They are: Criterion 1 – Upper layer interface reaches to head, say, 2.0 m level from ground or its temperature reaches 108°C, whichever happens first; Criterion 2 - Upper layer interface reaches to floor/fire level or its temperature reaches to 183°C, whichever happens first.

Criterion 1 must be considered as an indication for the onset of hazardous conditions, because if the layer interface was to drop below, say, 2.0 m level, it would be impractical to expect safe evacuation of the occupants, due to poor visibility above the layer interface. The duration between criterion 1 and criterion 2 is that period when although untenable conditions exist, it is not fatal until criterion 2 arrives. Rescue operation has to be initiated during this period for those who possibly could not leave the building. Also, the firemen have to enter the building in an already vicious, obscure and heated environment for rescuing people and for the purpose of firefighting. The fatal conditions may occur at the onset of

criterion 2. The time corresponding to criterion 2 has been designated as T-HELP (Time for Human Escape and Life Potential)<sup>20</sup>. T-HELP may be defined as follows:

$$T-HELP = t_{inc} - t_{det}.$$
 (12)

Here time  $t_{\text{inc}}$  refers to the time of incapacitation and  $t_{\text{det}}$  refers to the time of fire detection. The time of incapacitation may be taken as the time when criterion 2 is met.  $t_{\text{inc}}$  and  $t_{\text{det}}$  can be determined with the help of CALFIRE and NEST, respectively.

- 1. Cox, G., Fire Saf. J., 1994, 23, 123-132.
- Shield, T. J., Silcock, G. W. H., Building and Fire, Longman Scientific & Technical, 1987.
- 3. Cooper, L. Y. and Stroup, D. W., Fire Saf. J., 1985, 9, 20-46.
- Thomas, P. H., Bullen, M. L., Quintiere, J. G. and Mc Caffery, B. J., Comb. Flame, 1980, 38, 159–171.
- Gupta, A. K., Ph D thesis, Dept of Chemical Engineering, University of Roorkee, Roorkee, 1990.
- Barham, R., Fire Engineering and Emergency Planning, E & FN SPON, London, 1996.
- 7. Gupta, A. K., Fire Technol., 1994, 30, 304-325.
- 8. Gupta, A. K. and Kumar, R., J. Indian Build. Cong., 1996, 3, 166-175.
- Zukoski, E. E., Kubota, T. and Cetegen, B., Fire Saf. J., 1980/81, 3, 107–121.

- 10. Cooper, L. Y., Fire Mater., 1982, 6, 135-144.
- 11. Chow, W. K., J. App. Fire Sci., 1992-93, 2, 307-332.
- Peacock, R. D., Forney, G. P., Reneke, P., Portier, R. and Jones, W. W., Technical Note 1299, National Institute of Standards and Technology, US Dept of Commerce, Maryland, 1993.
- 13. Jones, W. W. and Peacock, R., Technical Note 1262, National Institute of Standards and Technology, Gaitherburg, Maryland, 1989.
- Cooper, L. Y. and Forney, G. P., Technical Note NISTIR 4342, National Institute of Standards and Technology, Gaitherburg, Maryland, 1990.
- Gupta, A. K., Proceedings ASIAFLAM' 95, Hong Kong, 15 16 March 1995, pp. 219–230.
- Gupta, A. K., Proceedings of the XIV National Conference on I.C. Engines and Combustion, Tata McGraw-Hill Publishing Co. Ltd., New Delhi, 1995, 365–371.
- 17. Alpert, R. L., Fire Technol., 1972, 8, 181-195.
- 18. Evans, D. D., Fire Saf. J., 1985, 9, 147-155.
- Gupta, A. K., Kumar, R., Yadav, P. K. and Naveen, M., Proceedings International Seminar on Thermal and Fire Explosion Hazards in Process Industries, IICT, Hyderabad, 10–11 December 1998.
- 20. Gupta, A. K., J. Appl. Fire Sci., 1997, 7, 195-205.

ACKNOWLEDGEMENT. We thank the Director, CBRI, Roorkee for his kind support and encouragement for the work on fire modelling.

Received 26 November 1999; revised accepted 8 October 2000

# Cyclooxygenase-2 — An attractive target for fruitful drug design

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Cyclooxygenase, an enzyme involved in the conversion of C-20 acids to prostaglandins, exists in two isoforms. A third isoform has been recently encountered. COX-1 is constitutively expressed and has a gastroprotective function. COX-2, induced at the site of injury, is responsible for the expression of pro-inflammatory prostaglandins. Despite overall similarities, COX-1 and COX-2 show subtle differences in amino acid composition at the active sites. COX-2 has valine at positions 89 and 523, while COX-1 has isoleucine, resulting in larger space availability in the former. Further, the presence of valine at position 434 in COX-2 as against isoleucine in COX-1 allows a gate mechanism to operate in favour of the former. Molecular modelling studies explain the preferential COX-2 inhibitory activity of some nonsteroidal anti-inflammatory agents like celecoxib (3), rofecoxib (4), nimesulide (5), meloxicam (6), nabumetone (10) and etodolac (13) in terms of binding, destabilizing and intermolecular energies. A few modified meloxicam derivatives like 19 and 20 are likely to have superior COX-2 selectivity.

THE revolution in biology over the past two decades has resulted in radically new approaches and opportunities for drug discovery. There has been an incredibly rapid increase in the rate of determination of three-dimensional structures of biomolecules. Many of these macromolecules are important drug targets and it is now possible to use the knowledge of the three-dimensional structures as a good basis for drug design. We propose to illustrate this in the case of cyclooxygenase-2, an enzyme responsible for inflammation<sup>1</sup>. This area has attracted immense attention in the last few years and a large number of original

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