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Assessment of the software Fire Dynamics Simulator (FDS) for fire simulation in train convoyes

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Introduction

The fires are interesting and dangerous phenomena. They are governed by the laws of thermo- and fluid- dynamics , which give rise to a complex systems. It is still challenging to understand how a fire spread in a given environment in order to guarantee the safety of the present people. Due to its complexity fires have been approached either experimentally or on the basis of previous events. Recently, because of the faster computational resources the numerical approach based on Computational Fluid Dynamics (CFD) constitutes a new methodology. CFD approach allows to study fires in different environment saving both time and money with respect to an experimental analysis. The main drawback of CFD is that it is based on a number of sub-grid models that are needed to perform simulations with the present computational power. Since models are not exact CFD requires a proper validation in order to understand its limit. Since 2000, Fire Dynamics Simulator (FDS) a software developed by National Institute of Standards and Technology (NIST), has been released on an open source license to accurately simulate fires. FDS is based on state-of-the-art models to simulate turbulent flow with chemical reaction. Nowadays FDS assumes a prominent role in fire dynamics simulation. This tool is frequently used by companies to study fire scenarios such as Italferr for fires of trains in tunnels. In this context, the heat release of the fire is usually prescribed on the convoy and the simulation assesses how the soot, carbon monoxide, temperature and other quantities are transported in the tunnel. The main aim of the present thesis project is to employ FDS for simulating a fire scenario which starts inside a fully described train convoy within a tunnel. The present simulation, for the first time, investigates the details on how the fire propagate from a passenger coach to the tunnel providing a comparison with the prescribed heat release usually adopted. Thanks to the collaboration of Ing. Stefano Di Rosa (Italferr), the simulations consider a real tunnel and train geometries.

Contents

Chapter 1

The tools

In this chapter we want to describe the main software used in this thesis.

1.1 FDS

FDS is an acronym that stands for Fire Dynamic Simulator. FDS is a computational fluid dynamics (CFD) model of fire-driven fluid flow. The computer program solves numerically a large eddy simulation form of the Navier-Stokes equation appropriate for low-speed, thermally-driven flow, with an emphasis on smoke and heat transport from fires, to describe the evolution of fire. FDS is free software developed by the National Institute of Standards and Technology (NIST) of the United States Department of Commerce, in cooperation with VTT Technical Research Centre of Finland. The first version of FDS was publicly released in February 2000. To date, about half of the applications of the model have been for design of smoke handling systems and sprinkler/detector activation studies. The other half consist of residential and industrial fire reconstruction. Throughout its development, FDS has been aimed at solving practical fire problems in fire protection engineering, while at the same time providing a tool to study fundamental fire dynamics and combustion. FDS is a Fortran program that reads input parameters from a text file, computes a numerical solution to the governing equations, and writes user-specified output data to files. The geometry that can be modelled with FDS are basically parallelepiped. This is true both for the domain and its relative mesh and for the obstructions. The user put onto the obstructions and on the boundaries of the domain the boundary conditions. Here boundary conditions are meant in a broad sense, in fact the user specifies what kind of surface delimit the obstructions. The principal surfaces allowed by FDS are:

- supply: this type of surface allows the injection of a flux of chemical species.The species could be any mixture,describe in terms of mass fraction of the following gas:
  - AIR
  - CARBON DIOXIDE
  - CARBON MONOXIDE
  - NITROGEN
  - OXYGEN
  - PRODUCTS
  - SOOT
  - WATER VAPOR

  The flux could be specified in terms of velocity components or specific flux.In addition the user could also specify the thermal condition of the flux itself if different from the ambient conditions;

- layered: this type of surface describe the number and the thickness of layer laying on the obstructions. Each layer is made of a single material or a mixture of materials. Each material have their own physical and chemical properties. In FDS there is a library of materials and obviously the user could create add material. The Physical properties are density, specific heat and thermal conductivity. The chemical properties consist in all the parameters relative to the pyrolysis reaction for instance the heat of reaction, the temperature of reaction, the kinetic coefficient, the activation energy, the heat of combustion and so forth.The user could specify the temperature of the objects if different from the ambient temperature;

- burner: this type of surfaces supplies the heat. They are specified by the HRRPUA (heat reaction rate per unit area);

- exhaust: is equal to the supply except for the fact that the flow is dumped instead of injected.

FDS can manage only one reaction in each simulation. The user could chose a reactions from a library or define a new reaction by means of the chemical composition of the fuel and the chemical composition of the products. The chemical composition of the fuel is express by the numbers of the atoms of carbon, hydrogen, oxygen and nitrogen that compound it. The chemical

composition of the products is calculated autonomously by FDS except for the mass fraction of carbon monoxide, soot and hydrogen that if present must be specified. In a similar manner FDS calculate the heat of combustion by the chemical composition of the fuel. Knowing the HRRPUA, specified by the burner surfaces, FDS calculate the quantity of fuel that must be supply for assure the heat released. The pyrolysis reaction that involve the materials produce different gas species among this species there is *fuel*. The *fuel* unleashed could react following the reaction earlier specified. The dimension of the domain and its grid must be specified together with the time of the simulation. The obstacles that are not in the the domain are ignored. The user could also specify ambient condition if different from those default setting.

1.2 Smokeview

Smokeview is the companion software tool designed to visualize numerical calculations generated by fire models such as the Fire Dynamics Simulator (FDS). Smokeview visualizes smoke and other attributes of the fire using traditional scientific methods such as displaying tracer particle flow, 2D or 3D shaded contours of gas flow data such as temperature and flow vectors showing flow direction and magnitude. Smokeview also visualizes fire attributes realistically so that one can experience the fire. This is done by displaying a series of partially transparent planes where the transparencies in each plane (at each grid node) are determined from soot densities computed by FDS. Smokeview also visualizes static data at particular times again using 2D or 3D contours of data such as temperature and flow vectors showing flow direction and magnitude. Shown below there are some smokeview's images.
Smokeview is the only software available for making sense and for visualizing the output of FDS. The quality of the rendering is quite good also with more complex geometry.

1.3 Pyrosim

Pyrosim is a third software developed by Thunderhead Engineering. It function is simple:"to avoid that the user became insane in modelling complex geometry". Pyrosim is in fact a preprocessor. It consist in a solid modelling that allow to construct geometry, put boundary conditions and exploit all FDS functions according with its limits and specifics. A profitable use of Pyrosim implies a proficiency with FDS because only the user that have

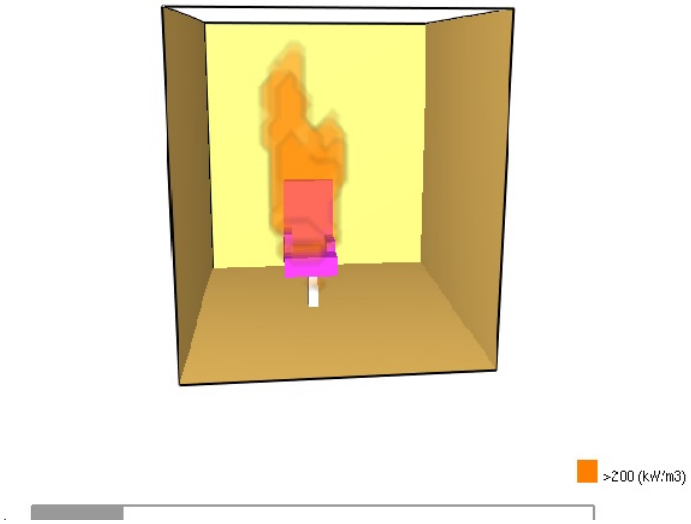


Figure 1.1: example of smokeview

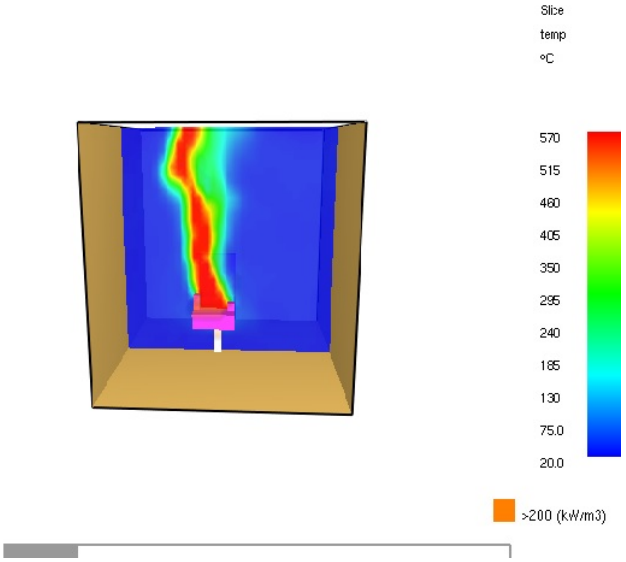
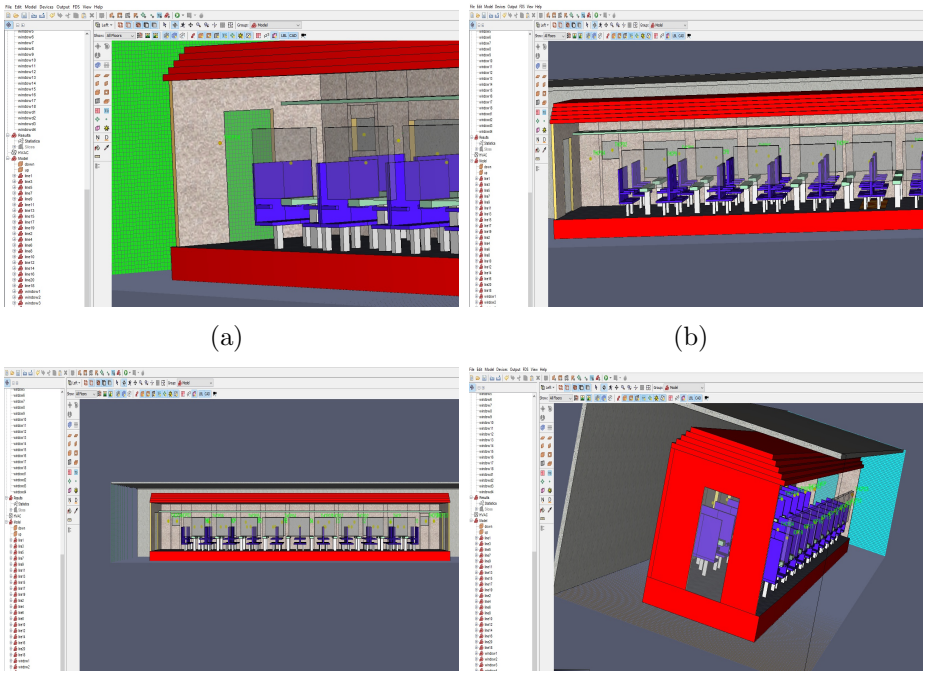


Figure 1.2: example of smokeview's slice

mastered with it first could understand the menu and option of Pyrosim. The following pictures are aimed to present Pyrosim.

Another worthwhile feature of pyrosim is the possibility to load, copy and move the models. In the presence of repeated equal objects the user could



(a) (b)

(c) (d)

Figure 1.3: complex geometries with pyrosim

build only one of these and copy the remainder.

1.4 How to proceed

Here we state how to approach a general problem with this software. Substantially we can split the procedure in four phases:

- gather the data;
- model the problem;
- run the simulation;
- evaluate the results.

The user firstly must procure all the data that he needs. Here for data we mean the geometry of the problem, all the necessary boundary conditions and the type of the materials involved. The geometry is simple the set of the dimension of the problem. These could be gotten easily by a direct measurement of the real system that we want to simulate. Obviously, in this kind

of analysis is not request too much attention to the details, the important thing is to reproduce the geometry at a "macroscopic" level because with the LES we lose the details that are smaller then the grid. About this point FDS does not accept obstruction that are finer than the mesh. This could be a problem if we have to simulate a domain which has got a lot of empty space and only small obstructions in its interior because we are compelled to use a tight grid anyway. We can find a way around using a non-uniform grid which is finer in the neighbourhood of the obstructions and coarser in the rest of the domain. In this manner we have got less cells and therefore we save some runtime without loss of accuracy. The materials which objects are made of, have an impact on both the heat exchange and on the combustion reaction that occur. For the heat exchange the parameters involved are density, conductive coefficient, specific heat and emissivity. This parameter should be all determined accurately because at low temperature the convection is dominant but a high temperature the radiation become relevant. The specific heat and the density together with the geometry are responsible for the thermal inertia. This kind of information could be easily determined from data sheet or table once that the materials under examination are known. The analysis of parameters involved in the combustion reaction is more complicated. The user must asses what kind of material burn and what products are formed. For example the bulk of the metals do not take part to any combustion reaction. At most, if the temperature is very high, the metals could melt but in our analysis this fact can be overlooked. Thus the user must firstly individuate what material are setted on fire and subsequently he must evaluate the heat of reaction unleashed and the products that are formed by the reaction. This part is more complicate because in general is difficult to know the composition of the objects and to know what chemical species are produced. In this phase is also important to asses how much CO (carbon monoxide) and CO_2 (carbon dioxide) are emanated. We evince that this part is the most subtle and the most difficult. Exact reference that describe the reaction involved whit all the chemical parameters needed are not easily found but with the aid of thermochemistry's handbooks a good result can be reached out anyway. In this phase we also have to chose the reaction that take place. We have to remind that FDS lets happened only one reaction therefore we must choose it carefully. The fire is produced by a surface burner thus the user must place it in an appropriate place and set up the correct amount of HHRA. About the boundaries condition we must "cover" all the obstacles with the right material and then we must evaluate the open portion together with the mass flux than eventually leave or enter the domain. Another aspect is the environmental conditions which consist in the air composition its temperature and its pressure. By default this are

at the standard values. Before running the simulation one must set up how many second simulate. This parameters is chosen with a little of experience and good sense. Usually the run phase is in absolutely the longest. It could require also more then one week if we have a cells number in the order of 10^5. Once that the simulation is finished one could evaluate the results, compare they with others obtained by previous simulation or from some similar real case available. The results that we may want could be obtained by mean of the following items:

- slices: these are planes where scalar fields (temperature, pressure etc..) or vectorial fields (velocity) are plotted. We chose where put the planes and what physical quantities assess;
- thermocouple: despite the name this device must be mean in a very large sense because they can evaluate any physical quantities we desire. The difference with the slices is that this item evaluate locally the quantities of interest i.e. only in the point where the device is placed.

At the end of the simulation the outputs are save in a text file so they could be easily elaborate with excel or another analogous software.

Chapter 2

The fire

In this chapter we define the fire and we give describe the dangerous effects that it has on the human being.

2.1 Fire

Fire is the rapid oxidation of a material in the exothermic chemical process of combustion, releasing heat, light, and various reaction products. Fire is hot because conversion of the weak double bond in molecular oxygen, O_2, to the stronger bonds in the combustion products carbon dioxide and water; the bond energies of the fuel play only a minor role here. At a certain point in the combustion reaction, called ignition point, flames are produced. The flame is the visible portion of the fire. Flame consists primarily of carbon dioxide, water vapor, oxygen and nitrogen. Depending on the substances alight, and any impurities outside, the color of the flame and the fire's intensity will be different. Fire in its most common form can result in conflagration, which has the potential to cause physical damage through burning. Fire is an important process that affects ecological system around the globe. The positive effects of fire include stimulating growth and maintaining various ecological systems. The negative effects of fire include hazard to life and property, atmospheric pollution, and water contamination. Fires start when an inflammable or a combustible material, in combination with a sufficient quantity of an oxidizer such as oxygen gas or another oxygen-rich compound (though non-oxygen oxidizers exist), is exposed to a source of heat or ambient temperature above the flash point for the fuel/oxidizer mix, and is able to sustain a rate of rapid oxidation that produces a chain reaction. This is commonly called the fire tetrahedron. Fire cannot exist without all of these elements in place and in the right proportions. For example, an inflammable liquid will start

burning only if the fuel and oxygen are in the right proportions. Some fuel-

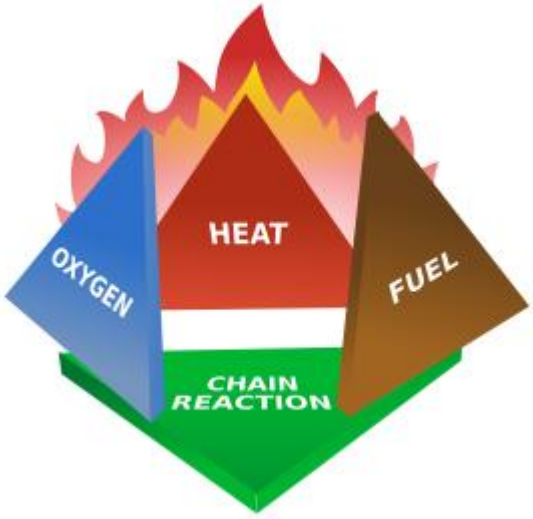


Figure 2.1: The fire tetrahedron

oxygen mixes may require a catalyst, a substance that is not consumed, when added, in any chemical reaction during combustion, but which enables the reactants to combust most readily. Once ignited, a chain reaction must take place whereby fires can sustain their own heat by the further release of heat energy in the process of combustion and may propagate, provided there is a continuous supply of an oxidizer and fuel. If the oxidizer is oxygen from the surrounding air, the presence of a force of gravity, or some similar force caused by acceleration, is necessary to produce convection, which removes combustion products and brings a supply of oxygen to the fire. Without gravity, a fire rapidly surrounds itself with its own combustion products and non-oxidizing gases from the air, which exclude oxygen and extinguish the fire. Because of this, the risk of fire in a spacecraft is small when it is coasting in inertial flight. Of course, this does not apply if oxygen is supplied to the fire by some process other than thermal convection. Fire can be extinguished by removing any one of the elements of the fire tetrahedron. Consider a natural gas flame, such as from a stovetop burner. The fire can be extinguished by any of the following:

- turning off the gas supply, which removes the fuel source;
- covering the flame completely, which smothers the flamen as the combustion both uses available oxidizer (the oxygen in the air) and displaces it from the area around the flame with CO_2;

- application of water, which removes heat from the fire faster than the fire can produce it (similarly, blowing hard on a flame will displace the heat of the currently burning gas from its fuel source, to the same end);
- application of retardant chemical such as Halon to the flame, which retards the chemical reaction itself until the rate of combustion is too slow to maintain the chain reaction.

In contrast, fire is intensified by increasing the overall rate of combustion. Methods to do this include balancing the input of fuel and oxidizer to stoichiometric proportions, increasing fuel and oxidizer input in this balanced mix, increasing the ambient temperature so the fire's own heat is better able to sustain combustion, or providing a catalyst; a non-reactant medium in which the fuel and oxidizer can more readily react.

2.2 flame

A flame is a mixture of reacting gases and solids emitting visible, infrared, and sometimes ultraviolet light, the frequency spectrum of which depends on the chemical composition of the burning material and intermediate reaction products. In many cases, such as the burning of organic matter, for example wood, or the incomplete combustion of gas, incandescent solid particles called soot produce the familiar red-orange glow of "fire". This light has a continuous spectrum. Complete combustion of gas has a dim blue color due to the emission of single-wavelength radiation from various electron transition in the excited molecules formed in the flame. Usually oxygen is involved, but hydrogen burning in chlorine also produces a flame, producing hydrogen chloride (HCl). Other possible combinations producing flames, amongst many, are fluorine and hydrogen, and hydrazine and nitrogen tetroxide. Hydrogen and hydrazine/UHDM flames are similarly pale blue, while burning boron and its compounds, evaluated in the mid-20th century as a high energy fuel for jet and rocket engines, emits intense green flame, leading to its informal nickname of "Green Dragon". The glow of a flame is complex. Black-body radiations is emitted from soot, gas, and fuel particles, though the soot particles are too small to behave like perfect blackbodies. There is also photon emission by de-excited atoms and molecules in the gases. Much of the radiation is emitted in the visible and infrared bands. The color depends on temperature for the black-body radiation, and on chemical makeup for emission spectra. The dominant color in a flame changes with temperature. The common distribution of a flame under normal gravity conditions depends on convection, as soot tends to rise to the top of a general flame, as

in a candle in normal gravity conditions, making it yellow. In micro gravity or zero gravity, such as an environment in outer space, convection no longer occurs, and the flame becomes spherical, with a tendency to become more blue and more efficient (although it may go out if not moved steadily, as the CO_2 from combustion does not disperse as readily in micro gravity, and tends to smother the flame). There are several possible explanations for this difference, of which the most likely is that the temperature is sufficiently evenly distributed that soot is not formed and complete combustion occurs. Experiment by NASA reveal that diffusion flames in micro gravity allow more soot to be completely oxidized after they are produced than diffusion flames on earth, because of a series of mechanisms that behave differently in micro gravity when compared to normal gravity conditions. These discoveries have potential applications in applied science and industry, especially concerning fuel efficiency.

It is true that objects at specific temperature do radiate visible light. Objects whose surface is at a temperature above approximately 400 ^{o}C will glow, emitting light at a color that indicates the temperature of that surface.

2.3 Fire's Dynamics

A fire is characterized by four stages:

- Ignition: this first stage begins when heat,oxygen and fuel source combine and have a chemical reaction resulting in fire. This is also know as "ignition" and is usually represented by a very small fire which often (and hopefully) goes out on its own, before the following stages are reached. Recognizing a fire in this stage provides your best change at suppression or escape;

- Growth: the growth stage is where the structures fire load and oxygen are used as fuel for the fire. There are numerous factors affecting the growth including where the fire started, what combustibles are near it, ceiling height and the potential for "thermal layering". It is during this shortest of the four stages when a deadly "flashover" can occur;

- Fully Developed:when the growth stage has reached its max and all combustible material have been ignited, a fire is considered fully developed. This is the hottest phase of a fire and the most dangerous for anybody trapped within;

- Decay: usually the longest stage of a fire, the decay stage is characterized by a significant decrease in oxygen or fuel, putting an end yo the

fire. Two common dangers during this stage are first the existence of a non-flaming combustibles, which can potentially start a new fire if not fully extinguished and second, there is the danger of a backdraft when oxygen is reintroduced to a volatile, confined space.

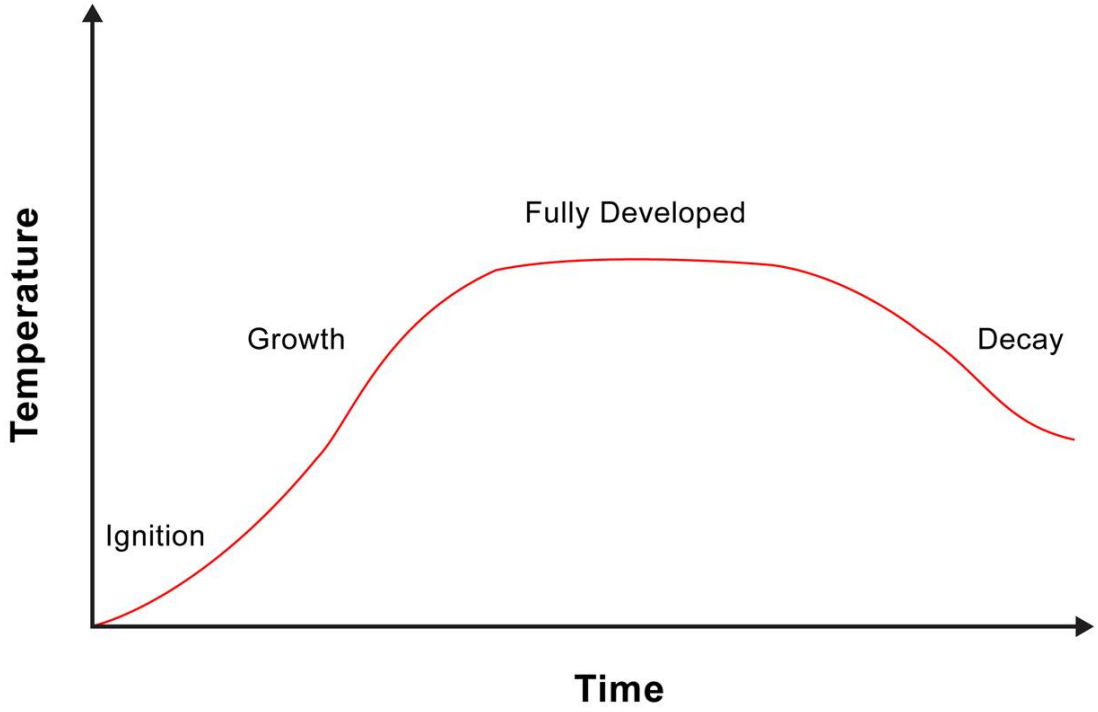


Figure 2.2: The fire's curve

A flashover is the near-simultaneous ignition of most of the directly exposed combustible in an enclosed area. When certain organic materials are heated, they undergo thermal decomposition and release flammable gases. Flashover occurs when the majority of the exposed surfaces in a space are heated to their autoignition temperature and emit flammable gases. Flashover normally occurs at 500^oC for ordinary combustibles. A common example of flashover is ignition of a piece of furniture in a domestic room. The fire involving the initial piece of furniture can produce a layer of hot smoke which spread across the ceiling in the room. The hot buoyant smoke layers growths in depth, as it is bounded by the walls of the room. The radiated heat from this layer heats the surfaces of the directly exposed combustible materials in the room, causing them to give off flammable gases via pyrolysis. When the temperatures of the evolved gases become high enough, these gases will ignite throughout their extent. The flash point is the lowest temperature at

which vapours if a volatile material will ignite, when given an ignition source. Pyrolysis is a thermochemical decomposition of organic material at elevated temperatures that release combustible gases.

2.4 The killing fumes

Most fire deaths are not caused by burns, but by smoke inhalation. Often smoke incapacitates so quickly that people are overcome and can't make it to an otherwise accessible exit. The synthetic materials commonplace today produce especially dangerous substances. As a fire grows inside a closed spaces, it will often consume most of the available oxygen, slowing the burning process. This "incomplete combustion" result in toxic gases. Smoke is made of components that can each be lethal in its own way:

- Particles: unburned, partially burned, and completely burned substances can be so small they penetrate the respiratory system's protective filters, and lodge in the lungs. Some are actively toxic and others are irritating to the eyes and digestive system;
- Vapors: foglike droplets of liquid can poison if inhaled or absorbed trough the skin;
- Toxic gases:
  - Carbon monoxide (CO): it is a toxic, odourless and colourless gas. It is produced by partial combustion and therefore it is present in combustions characterized by oxygen's deficiency. Usually this gas is the most dangerous. It combines with hemoglobin to produce carboxyhemoglobin, which usurps the space in hemoglobin that normally carries oxygen, but is ineffective for delivering oxygen to bodily tissue. Concentrations as low as 667 ppm may cause up to 50% of the body's hemoglobin to convert to carboxyhemoglobin. A level of 50% carboxyhemoglobine may result in seizure, coma, and fatality. The most common symptoms of carbon monoxide poisoning may resemble other types of poisoning and infections, including symptoms such as headache, nausea, vomiting, dizziness,fatigue and feeling of weakness. A more precise evaluation of the effects are reported in the following:
    * 35 ppm (0,0035%) : Headache and dizziness within six to eight hours of constant exposure;
    * 100 ppm (0,01%) : Slight headache in two to three hours;

    * 200 ppm (0,02%) : Slight headache within two to three hours and loss of judgement;
    * 400 ppm (0,04%) : Frontal headache within one to two hours;
    * 800 ppm (0,08%) : Dizziness, nausea, and convulsion within 45 minutes. Insensible within 2 hours;
    * 1600 ppm (0,16%) : Headache, increased heart rate, dizziness, and nausea within 20 minutes. Death in less than 2 hours;
    * 3200 ppm (0,32%) : Headache, dizziness and nausea in five to ten minutes. Death within 30 minutes;
    * 6400 ppm (0,64%) : Headache and dizziness in one minutes. Convulsion, respiratory arrest, and death in less than 20 minutes;
    * 12800 ppm (1,28%): Unconsciousness after 2 or 3 breaths. Death in less the three minutes.

- Carbon dioxide (CO_2): is an asphyxiating gas which can augment the respiratory rate. Air with 3% of CO_2 could double the respiratory rate and therfore the inhalation of the others toxic gases. A 10 % of carbon dioxide may result fatal;
- Hydrogen sulfide(H_2S): it is a colourless gas with the characteristic foul odor of rotten eggs. Hydrogen sulfide is a broad-spectrum poison, meaning that it can poison several different systems in the body, although the nervous system is most affected. The toxicity of H_2S is comparable with that of carbon monoxide. It binds with iron in the mitochondrial cytochrome enzymes, thus preventing cellular respiration. Since hydrogen sulfide occurs naturally in the body, the environment, and the gut, enzymes exist to detoxify it. It is product in all the fire's material that contain sulphur like for instance rubbers.
- Solfur dioxide (SO_2): At standard atmosphere, it is a toxic gas with a pungent, irritating smell. Sulfur dioxide is the product of the burning of sulfur or of burning of materials that contain it.
- Ammonia (NH_3): it is product of the burning of materials that contain nitrogen. It is a irritating gas.
- Hydrogen cyanide (HCN): sometimes called prussic acid, it is a colorless, extremely poisonous and flammable liquid that boils slightly above room temperature, at 25.6 ^oC. It is present only in partial combustion of synthetic resins such as acrylic and polyamide resins.

- Hydrochloric acid (HCl): is a combustion product of material that contain chlorine like the major part of plastic material used today. A concentration of 0,01% is fatal over 30 minuts of exposure. It is easily perceived owing its pungent odor.
- Nitrogen dioxide (NO_2): exposures above 0,07% may result deadly in a short period.
- Phosgene ($COCl_2$): thi colorless gas gained infamy as a chemical weapon during world war I. Phosgene is an insidious poison as the odor may not be noticed and symptoms may be slow to appear. The odor detection threshold for phosgene is 0,4 ppm, four times the threshold limit value. Its high toxicity arises from the action of the phosgene on the proteins in the pulmonary alveoli, the site of gas exchange: their damage disrupt the blood-air barrier, causing suffucation. It is present in the combustion of materials that contain chlorine like plastic material.

In addition to producing smoke, fire can incapacitate or kill by reducing oxygen levels, either by consuming the oxygen, or by displacing it with other gases. Heat is also a respiratory hazard, as superheated gases burn the respiratory tract. When the air is hot enough, one breath can kill. The following table shows the oxygen concentrations effects:

When oxygen levels are at ...	... a person experiences:
21 percent	Normal outside air
17 percent	Impaired judgement and coordination
12 percent	headache, dizziness, nausea, fatigue
9 percent	Unconsciousness
6 percent	Respiratory arrest, cardiac arrest, death

A last parameter that should be mentioned is the visibility. This parameter is obviously important during the evacuation and it is related on the density of the fumes and on the concentration of soot.

2.5 Fire Characteristics and Fire Curves in Tunnels

2.5.1 Fire Characteristics

The tunnel fires are peculiar due to the characteristics of burning fuel and vehicles with high calorific potential in combination with high the confine-

ment of the heat released. These features can lead to remarkably high heat release (HRR) and gas temperature, as well as long fire duration. the highest thermal impact appears normally at the top of the tunnel (ceiling), owing to the direct flame impingement, an becomes smaller at th benches. Smoke and toxic gases emitted from the burning materials can greatly reduce the visibility and subsequently impede both evacuation and fire-fighting. Therefore, sufficient ventilation capacity is one of the most important issues in tunnel fire safety, affecting the HRR, the fire size and the spread, as well as the smoke control. In general, the ventilation systems can be either natural or mechanical (forced). The latter systems contain longitudinal and transverse configurations that involve several components such as fans, ducts and dampers to control the air movement.

2.5.2 Fire Curves

Various time-temperature curves have been proposed. The most popular of them are:

- ISO 834 standard fire curve: this cellulosic curve is widely used in fire testing of structural elements. It applies to materials found in typical buildings and thus is adequate for the estimation of the thermal response of corresponding members such as beams, columns and slabs. It was used for many years for tunnels, but proved inadequate for highly combustible materials.

- ASTM E119 fire curve: this curve is similar to the ISO time-temperature curve involving a continuously increasing furnace temperature (whit decreasing rate), thereby being, again, unsuitable for highly combustible material.

- HC (Hydrocarbon) fire curve: The hydrocarbon curve applies to hazardous materials, for example, fuels and chemicals, including those for petrochemical industries. In opposition to the previous cases, it provides a rapid increase of the air temperature within the first few minutes reaching its maximum value after half an hour.

- HCM (Hydrocarbon modified) or Hc$_i nc$ (Hydrocarbon increased) fire curve: This raised hydrocarbon curve was initially proposed in France, representing a more severe scenario with rapid and complete combustion of the hazardous materials. It is approximately derived from the original HC curve by multiplying the corresponding temperatures by a factor of 1300/1100 . The maximum temperature is 1300 ^{o}C instead of 1100 ^{o}C.

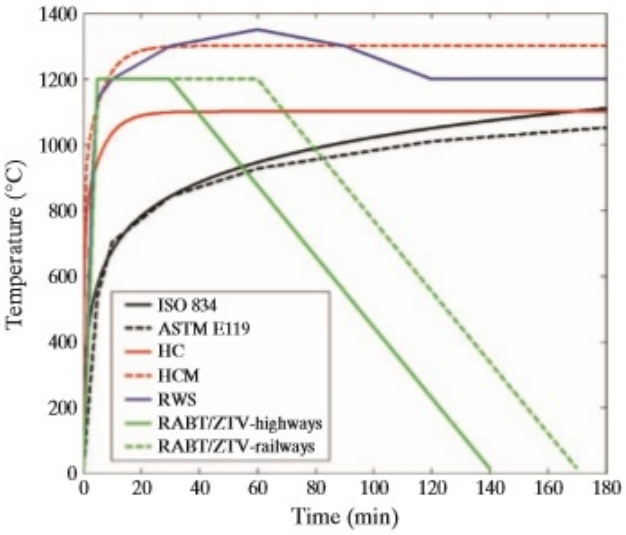


Figure 2.3: Characteristic time-temperature fire curves for tunnels

- RWS (Rijkswaterstaat) fire curve: This curve was developed in the Netherlands exclusively for the design of tunnels, after laboratory testing. It presents a small temperature reduction after 60 minutes of fire exposure, but there is no cooling branch similarly to the previous curves.

- RABT/ZTV fire curves: Under the German regulations, there separate fire curves for highway and railway tunnels. The latter one implies an extension of the plateau for 30 minutes, while both of them provide a linearly descending (cooling) phase of 110 minutes.

2.6 Concrete Behaviour in Fire

Concrete neither burns nor emits any toxic fumes or smoke when exposed to fire, offering a high degree of fire resistance. Additionally, the slow rate of heat transfer (low thermal conductivity) enables concrete to act as an effective fire shield. This excellent performance is due to the main constituents of its mixture, namely cement and aggregates. Both material and structural behaviour of concrete are well described in the literature. However, a brief overview is presented in the following for completeness.

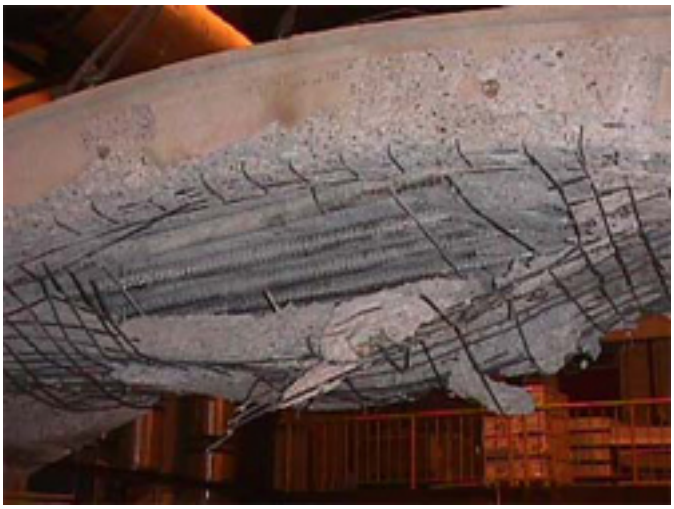


Figure 2.4: Example of severe spalling on reinforced concrete

2.6.1 Material Behaviour

Concerning the material behaviour of concrete at elevated temperatures, an irreversible loss of stiffness and strength takes place, which is referred to as thermal damage (or softening) and thermal decohesion, respectively. As a result, the elastic (Young's) modulus and the compressive and tensile strength can be expressed with respect to the temperature, constituting temperature-dependent variables. Several relations and curves (either prescriptive-codified or experimental) have been proposed not only for concrete, but also for the steel reinforcement. When exposed to high temperature, the chemical composition and physical structure of concrete change considerably. Microstructural analysis of fire damaged concrete has show that both thermal damage and decohension result from the dehydration of concrete on the microlevel, while the cement paste, the type of aggregates and the water content affect the overall response to a large degree.

2.6.2 Structural Behaviour

Concerning the structural behaviour of concrete exposed to high temperatures, it may be characterized by spalling where pieces of concrete fall off the surface of a structural element. Several types of spalling are defined in literature. An instructive approach is to consider the location of its occurrence and its origin. Depending on the first factor, spalling can be divided into three categories, namely, aggregate, corner and surface spalling; while depending on the second factor, it can be divided into two categories, namely,

progressive and explosive spalling. Explosive spaalling is the most violent form of spalling, ehich may be encountered in tunnels because of the special fire characteristics as described in the section Fire Characteristics and Fire Curves.

2.6.3 Explosive Spalling

The main feature of explosive spalling is the burst-out of concrete pieces accompanied by sudden release of energy and loud sounds. Numerous factors affect the explosive spalling of concrete and are summarized in the following list:

- Heating rate;
- Heating profile;
- Section size;
- section shape;
- Moisture content;
- Pore pressure;
- Concrete permeability;
- Concrete age;
- Concrete strength;
- Compressive stress before and during heating;
- Restraint to thermal expansion;
- Aggregate type;
- Aggregate size;
- Cracking;
- Reinforcement;
- Steel;
- Air entrainment.

Two main mechanisms are considered for the explanation of this phenomenon: the hydraulic and the thermal spalling. The first is attributed to the low permeability of concrete, especially in combination with high moisture content, resulting in a pore pressure build-up (tensile stress). The second is caused by the restrained thermal dilatation of the region close to the heated surface by the cooler inner concrete, leading to high compressive stress parallel to it. Additionally, a combination of the above mechanisms has been proposed, whereas the external loading is of great importance in any approach.

Chapter 3

Combustion fundamentals

To understand the formation of the products given off during a combustion reaction, we must first understand the nature of the materials burned, the thermodynamics of the combustion process and some aspects of flame structure.

3.1 Combustion stoichiometry

Complete oxidation of simple hydrocarbon fuels forms carbon dioxide (CO_2) from all of the carbon and water (H_2O) from the hydrogen, that is, for a hydrocarbon fuel with general composition C_nH_m,

$$C_nH_m + (n + \frac{m}{4})O_2 \quad \longrightarrow \quad nCO_2 + \frac{m}{2}H_2O \tag{3.1}$$

Even in the idealized case of complete combustion, the accounting of all species present in combustion exhaust involves more than simply measuring the CO_2 and H_2O. Since fuel are burned in air rather than in pure oxygen, the nitrogen in the air may participate in the combustion process to produce nitrogen oxides.Also, many fuels contain elements other than carbon, and these elements may be transformed during combustion. Finally, combustion is not always complete, and the effluent gases contain unburned and partially burned products in addition to CO_2 and H_2O. Air is composed of oxygen, nitrogen and small amounts of carbon dioxide, argon and other trace species. Since the vast majority of the diluent in air is nitrogen, for our purpose it is perfectly reasonable to consider air as a mixture of 20,9% (mole basis) O_2 and 79,1% (mole basis) N_2. Thus for every mole of oxygen required for combustion, 3.78 mol of nitrogen must be introduced as well. Although nitrogen may not significantly alter the oxygen balance, it does have a major

impact on the thermodynamics, chemical kinetics, and formation of pollutants in combustion system. For this reason it is useful to carry the "inert" species along in the combustion calculations. The stoichiometric relation for complete oxidation of a hydrocarbon fuel, C_nH_m, becomes

$$C_nH_m+(n+\frac{m}{4})(O_2+3.78N_2) \quad \longrightarrow \quad nCO_2+\frac{m}{2}H_2O+3.78(n+\frac{m}{4})N_2 \quad (3.2)$$

Thus for every mole of fuel burned, 4,78(n+m/4) mol of air are required and 4,78(n+m/4)+m/4 mol of combustion products are generated. Few combustions are operated precisely at the stoichiometric condition because of the difficulty of achieving such intimate mixing between fuel and air that perfect conversion is attained and therefore they occurs in an excess of oxygen.

3.2 Combustion thermodynamics

Substantial energy is released in a very short time when a fuel is burned, leading to a dramatic temperature increase of the combustion gases. Temperature in excess of 2000 K are common in flames. It is the high temperature that allows rapid oxidation of hydrocarbons and carbon monoxide to carbon dioxide and water but also makes possible the oxidation of N_2 to form nitric oxide. Thermodynamics provides us with good estimates of the flame temperature that are needed not only to assess the combustion process itself but also to calculate the concentrations of many chemical species produced by the reaction itself. In the following we recall most prominent thermodynamics issue that we need.

3.2.1 First Law of Thermodynamics

The first law of thermodynamics states that the change in the total energy of a closed system of fixed mass and identity is equal to the heat transfer to the system from its surrounding minus the work done by the system on its surrounding; that is, for an infinitesimal change of state,

$$dE = \delta Q - \delta W \quad (3.3)$$

The total energy of the system, E, includes the internal energy, U, the kinetic energy, and the potential energy. The energy is a property of the system that is independent of the path taken in going from one state to another. In contrast, the heat transfer, δQ, and the work transfer, δW, for any change in the state of the system depend on the manner in which the state of the system is changed. The change in the system energy is described by a total

differential, dE. Since the work and heat transfer depend on the path followed by the system, the *delta* is used to indicate that these increments are not total differentials. For most system of concern here, the kinetics and potential energy terms can be neglected, so we may express the system energy in terms of the internal energy, that id,

$$dU = \delta Q - \delta W \tag{3.4}$$

integrating over a finite change of state from state 1 to state 2, the first law for a closed system becomes

$$U_2 - U_1 = Q_{12} - W_{12} \tag{3.5}$$

Only rarely in the consideration of combustion processes can we limit ourselves to a fixed mass in a closed system. More generally, the fuel and air enter the combustion zone across certain boundaries. We must therefore use an expression valid for the change in state of a fixed volume in space, called control volume. A control volume may be defined in terms of any volume in space in which one has interest for a particular analysis. We do not give a proof of the follow equation, which could be found in any book of thermodynamics, but only explain the terms that it involves.

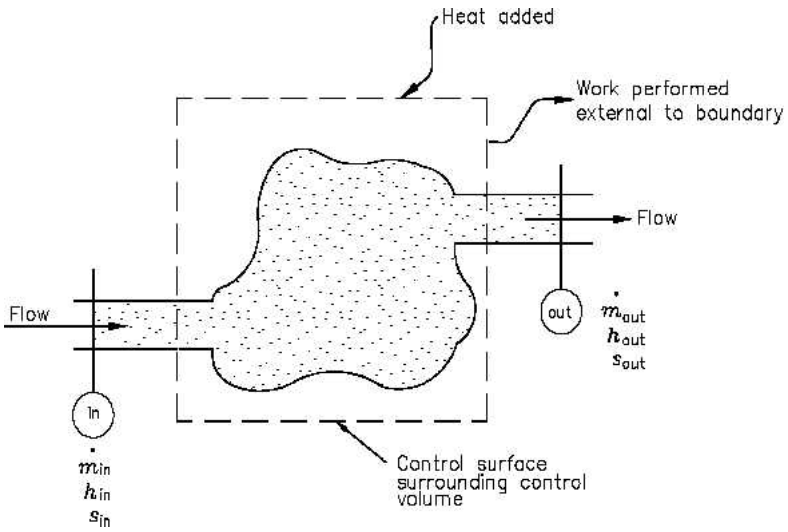


Figure 3.1: a typical sketch of a control volume

$$\frac{dE}{dt} + \sum_{\substack{j=1 \\ outet}}^{n} (e_j + pv_j)\dot{m}_j - \sum_{\substack{i=1 \\ inlet}}^{m} (e_i + pv_i)\dot{m}_i = Q - W_x \tag{3.6}$$

Where in that's equation the terms $\dot{m}$ are the mass flow rates leaving or entering the control volume, Q is the rate of heat transfer to the system, and W_x, is the rate at which is done by the system on its surrounding other than associated with flows across the control volume boundary. As noted above, in the combustion applications of interest here we can generally neglect the kinetic and potential energy contributions to the total energy, giving

$$\frac{dU}{dt} = \sum_{\substack{i=1 \\ inlet}}^{n} (h_i)\dot{m}_i - \sum_{\substack{j=1 \\ outlet}}^{m} (h_j)\dot{m}_j + Q - W_x \tag{3.7}$$

where the mass specific enthalpy, h, is defined as

$$h = u + pv \tag{3.8}$$

It is useful in this kind of equation, when chemical reactions occur, use the molar flow rate and the and molar specific enthalpy. We indicate this quantities with $\dot{\bar{m}}$ and $\bar{h}$ respectively. Let us apply the foregoing to analyze the chemical reaction

$$aA + bB \quad \longrightarrow \quad cC + dD \tag{3.9}$$

occurring at steady state and constant pressure in the isothermal conditions where the feed and effluent flows are at their stoichiometric values. Applying the steady-state form of the first principle of the thermodynamics with molar mass flow rate and molar enthalpy, without any work except that due to flows across the boundary, we get

$$c\dot{\bar{m}}h_C(T_1) + d\dot{\bar{m}}h_D(T_1) - a\dot{\bar{m}}h_A(T_1) - b\dot{\bar{m}}h_B(T_1) = Q \tag{3.10}$$

Dividing through $\dot{\bar{m}}$, and indicating with the symbol $\Delta h_r(\mathrm{T}_1)$, that is

$$\Delta\ h_r(T_1) = \frac{Q}{f} = ch_C(T_1) + dh_D(T_1) - ah_A(T_1) - bh_B(T_1) \tag{3.11}$$

We see that the enthalpy of reaction is just the difference between the molar specific enthalpies of the products and reactants taking into account the stoichiometry of the reaction. To define the enthalpy of a species requires a reference state at which the enthalpy is taken to be zero. That reference state is arbitrary as long as a consistent reference state is used throughout the calculations. Generally, the reference temperature and pressure are taken to be T_0= 298 K and p_0 = 1 atm, respectively.The enthalpy of a compound relative to the reference states of its constituent elements is the enthalpy of the reaction of these elemental species that form 1 mole of the compound.

When evaluates for reactants and products at the same temperature, T, this quantity is called the *enthalpy of formation*. By definition, the enthalpies of formation of the elemental reference compounds are zero. The enthalpy of a compound at any temperature may be written as the sum of enthalpy of formation at the reference temperature and a sensible enthalpy term associated with the temperature change from the reference temperature to the desired temperature. Thus the enthalpy of species i at temperature T relative to the reference state is

$$h_1^o(T) = h_i(T) - h_i(T_0) + \Delta\ h_{fi}^o(T_0) \tag{3.12}$$

where the superscript ^{o} stands for at standard conditions. The sensible enthalpy term may be evaluated as an integral over temperature of the specific heat at constant pressure, $c_p = \frac{\partial h}{\partial T}|_p$, that is,

$$h_i(T) - h_i(T_0) \quad = \quad \int_{T_0}^{T} c_{p,i}(T^{'})\, dT^{'} \tag{3.13}$$

The specific heat generally varies with temperature. If the range of temperature variation is large, as is commonly the case in combustion applications, one must account for the dependence of $c_{p,i}$ on temperature. For our purpose, it is suffice to approximate the specific heat as a linear function of temperature, $c_{p,i} \approx a_i + b_i T$. This approximate form allows calculation of the sensible enthalpy over the range of temperatures commonly encountered in combustion calculations(i.e., 300 to 3000 K) within about 10%. The first law of thermodynamics for a chemically reacting open system may now be written as

$$\frac{dU}{dt} = \sum_{\substack{i=1 \\ inlet}}^{n} ((h_i(T) - h_i(T_0) + \Delta h_{fi}^o)\dot{m}_i - \sum_{\substack{j=1 \\ outlet}}^{m} ((h_j(T) - h_j(T_0) + \Delta h_{fj}^o \dot{m}_j + Q - W_x \tag{3.14}$$

If the chemical composition and thermodynamic properties of the fuel are known the foregoing equation allows us to calculate temperature change, heat transfer or work performed in any combustion systems.

3.2.2 Adiabatic flame temperature

Combustion reactions generally occur very fast, on the order of 1 ms and little heat or work transfer takes place on the time scale of combustion. For this reasons the maximum temperature achieved in the combustion process is

often near that for adiabatic combustion. This so-called *adiabatic flame temperature* may readily be calculates by applying the first law of thermodynamics to an adiabatic combustor. Here we report adiabatic flame temperature of some common gases/material.

Fuel	Oxidizer	$T_{ad}(^oC)$
Acetylene(C_2H_2)	Air	2500
Acetylene(C_2H_2)	Oxygen	3480
Butane(C_4H_10)	Air	1970
Cyanogen(C_2N_2)	Oxygen	4525
Dicyanoacetylene(C_4N_2)	Oxygen	4990
Ethane (C_2H_6)	Air	1955
Ethanol (C_2H_5OH)	Air	2082
Gasoline	Air	2138
Hydrogen (H_2)	Air	2254
Hydrogen (H_2)	Oxygen	3200
Methane (CH_4)	Air	1963
Methane (CH_4)	Oxygen	5004
Methanol (CH_4O)	Air	1949
Natural gas	Air	1960
Pentane (C_5H_12)	Air	1977
Propane (C_3H_8)	Air	1980
Propane (C_3H_8)	Oxygen	1980
Toluene (C_7H_8)	Air	2071
Wood	Air	2093
Light fuel oil	Air	2104
Medium fuel oil	Air	2101
Heavy fuel oil	Air	2102
Bituminous Coal	Air	2172
Anthracite	Air	2180
Zirconium	Oxygen	4005

The fact that adiabatic flame temperature is higher with only oxygen than in air is due to the fact that alone oxygen take part in the reaction and therefore the others inert components are heated up only. Thus with pure oxygen there are not inert mass to heat up and the temperature result obviously higher.

3.2.3 Chemical Equilibrium

We have, so far, assumed that the fuel reacts completely, forming only CO_2,H_2O, and other fully oxidized products. For fuel-lean combustion with

product temperatures below about 1250 K, the stable species, CO_2,H_2O,O_2 and N_2 are the usual products and this is a good assumption. Element balances are sufficient to determine the composition of the combustion products under these conditions. Most combustion system, however, reach temperatures much higher than 1250 K. We have seen that adiabatic flame temperature can reach 2300 K for stoichiometric combustion. At such high temperature, species that are stable at ambient temperatures can dissociate by reaction such as

$$CO_2 \overleftrightarrow{} CO + 0.5O_2$$

$$H_2O \overleftrightarrow{} H_2 + 0.5O_2$$

so carbon monoxide, hydrogen, and other reduced species may be present even though sufficient oxygen is available for complete combustion. In fact, these species are oxidized rapidly, but they are continually replenished by dissociation and other reactions that occur in the hot gases. The concentrations of these species are determined by the balance between those reactions that lead to their formation and those that consume them, Chemical equilibrium provides a reasonable first approximation to the composition of the combustion products at high temperature since the equilibrium state is that which would be achieved given a time sufficiently long for the chemical reactions to proceed. The conditions for thermodynamics equilibrium are derived from the second law of thermodynamics. These condition may be concisely stated in terms of the *Gibbs free energy*, G = H-TS. For a closed system at a constant temperature and pressure, the Gibbs free energy is a minimum at thermodynamics equilibrium. Thus, for any change *away* from equilibrium state at constant T and p, dg $>$ 0. The Gibbs free energy is a function of the temperature, pressure and composition i.e., G= G(T,p,n_1,n_2,...). Thus we may write

$$dG = \frac{\partial G}{\partial T}|_{p,n_j} dT + \frac{\partial G}{\partial p}|_{T,n_j} dp + \frac{\partial G}{\partial n_1}|_{T,p,n_j} dn_1 + \frac{\partial G}{\partial T}|_{p,n_2} dn_2 + ... \qquad (3.15)$$

The partial derivative of the Gibbs free energy with respect to the number of moles of a species, i, is the chemical potential

$$\mu_i = \frac{\partial G}{\partial n_i}|_{T,p,n_j} \qquad (3.16)$$

Recalling the definition of G, we may write

$$dG = dU + pdV - TdS + Vdp - SdT + \sum_{i=1}^{n} \mu_i dn_i \qquad (3.17)$$

Using the first law of thermodynamics, it can be shown that

$$dU + pdV - TdS = 0 \tag{3.18}$$

Hence

$$dG = Vdp - SdT + \sum_{i=1}^{n} \mu_i dn_i \tag{3.19}$$

The partial molar Gibbs free energy may be written

$$\mu_i = \frac{\partial}{\partial n_i}(H - TS)_{T,p,n_{j\neq i}} = h_i - Ts_i \tag{3.20}$$

where s_i is the partial molar entropy of species i. For the purpose of examining most combustion equilibria, we may focus on ideal gases and simple condensed phases since the pressure of combustion are generally near atmospheric. The enthalpy of an ideal gas is independent of pressure. The entropy is

$$s_i(T,p) = s_i^o(T_0) + \int_{T_0}^{T} \frac{c_{p,i}(T')}{T'}\, dT' + Rln\frac{p_i}{p_O} \tag{3.21}$$

where $s_i^o(T_0)$ is the entropy at the reference state. Since the partial pressure is usually expressed in units of atmospheres, the partial pressure term of (3.21) is commonly expressed as lnp_i.

$$\mu_i = \mu_i^o(T) + RTlnp_i \tag{3.22}$$

where $\mu_i^o(T)$, the standard chemical potential of species i, is the chemical potential of i at the reference pressure, $p_o = 1$ atm. For a pure condensed phase at modest pressure, the entropy depends only on temperature,

$$s(T) = s^o(T_0) + \int_{T_0}^{T} \frac{c_p(T')}{T'}\, dT' \tag{3.23}$$

Since the enthalpy is also independent of pressure, the partial molar Gibbs free energy is a function only of the temperature, that is,

$$\mu_i = \mu_i^o(T) \tag{3.24}$$

The condition for thermodynamic equilibrium may now be written as

$$(dG)_{T,p} = \sum_{i=1}^{n} \mu_i dn_i \geq 0 \tag{3.25}$$

for any change away from the equilibrium state. Consider a chemical reaction

$$\sum_{j=1}^{m} \nu_j A_j = 0 \tag{3.26}$$

We may express the progress of the reaction in terms of the number of moles of a product species generated divided by the stoichiometric coefficient, the extent of reaction,

$$d\zeta = \frac{dn_j}{\nu_j} \tag{3.27}$$

The condition of chemical equilibrium at constant T and p is then

$$\sum_{j=1}^{m} \nu_j \mu_j = 0 \tag{3.28}$$

This condition must be satisfied at equilibrium for any dζ , regardless of sign. Using (3.22) we obtain

$$\sum_{j=1}^{m} \nu_j \mu_j^o + \sum_{j,gas} RTlnp_j^{\nu_j} = 0 \tag{3.29}$$

at equilibrium. This expression now defines the equilibrium composition of the gas. separating the pressure-dependent terms from the temperature-dependent terms yields a relation between the partial pressure of the gaseous species and temperature, that is,

$$\prod_{j,gasonly} p_j^{v_j} = exp(-\sum_{j=1} m\nu_j \frac{\mu_j^o}{RT}) \equiv K_p(T) \tag{3.30}$$

The function K_p(T) is the equilibrium constant in terms of partial pressures. Note that the quantities of the pure condensed phases do not enter explicitly into this relation. It is often convenient to work in terms of mole fraction or concentrations instead of partial pressures. The partial pressure is, according to Dalton's law,

$$p_i = y_i p \tag{3.31}$$

where y_i is the mole fraction of species i, calculated considering gas-phase species only. Substituting into the expression for K_p yields

$$\prod_{j,gasonly} (y_j p)^{\nu_j} = K_p(T) \tag{3.32}$$

Similarly, using the ideal gas relation, $p_i = c_i RT$, the equilibrium constant in terms of concentrations is found to be The composition of a system at equilibrium is determined by solving a set of the equilibrium relation subject to element conservation constraints. When reactions involving condensed-phase species are considered, equilibria involving the condensed-phase species do not explicitly indicate the amounts of each of those species present.

3.3 Flame Propagation And Structure

We now turn our attention from combustion thermochemistry to the physical processes that govern the way fuels burn. One of the striking features of most combustion is the existence of a flame, a luminous region in the gas that is associates with the major heat release. Some flames, such as that of a candle, are relatively steady, whereas others fluctuate wildly due to turbulent motions of the gas. The flame is a reaction front created by diffusion of energy or free radicals from the hot burned gases into the cooler unreacted gas or by the mixing of fuel and air. A flame that is stabilized at a fixed location is actually propagating into a flow of fuel and/or air. In this case the propagation velocity must match the gas velocity for the flame itself to remain fixed in space.

3.3.1 Laminar Diffusion Flames

When fuel and air enter a combustion system separately, they must mix on a molecular level before reaction can take place. The extent of reaction is strongly influenced by the extent to which that mixing has occured prior to combustion. this mixing may be achieved solely by molecular diffusion, as in a candle flame, or may be enhanced by turbulence. We shall again begin our discussion with the laminar flame because of simplicity it affords. In a laminar diffusion flame fuel and air enter in separate streams, diffuse together, and react in a narrow region. While a single value of the equivalence ratio could be used to characterize a premixed flame, the equivalence ratio in the diffusion flame varies locally from zero for pure air to infinity for pure fuel. Combustion in a confined flow may be characterized by an overall equivalence ratio based on the flow rates of fuel and air, but that value may differ dramatically from the value in the flame region. A hydrocarbon diffusion flame may have two distinct zones:

- the primary reaction zone, which is generally blue;
- a region of yellow luminosity.

Most of the combustion reactions take place in the primary reaction zone where the characteristic blue emission results from the production of electronically excited molecules that spontaneously emit light, so-calle chemiluminescence. Small particles composed primarily of carbon, know as *soot*, are formed in extremely fuel-rich, hot regions of the flame and emit the brighter yellow radiation. The soot particles generally burn as they pass through the primary reaction zone, but may escape unburned if the flame is disturbed. If the combustion reactions were infinitely fast, the combustion would take place entirely on a surface where the local equivalence ratio is equal to 1. This "thin flame sheet" approximation is the basis of an early model developed bu Burke and Schumann (1928). Assuming that the fuel and oxygen cannot coexist at any point greatly simplifies the calculations by replacing the chemical kinetics with stoichiometry or, at worst, chemical equilibrium calculations. The simplified calculations yield remarkably good results for adiabatic laminar diffusion flames larger than several millimeters in size since the reaction times at the adiabatic flame temperature near stoichiometric combustion are short compared to typical diffusion times. Only when heat is transferred from the flame at a high rate, as when the flame impinges on a cold surface, or when the scale of the is very small, as in the combustion of a small droplet, does the reaction time approach the diffusion time.

3.3.2 Turbulent Diffusion Flames

The small-scale structures of the turbulent flow fields in premixed and diffusion flames are similar. Many of the features of the flow in diffusion flames are made apparent by the distribution of composition in the flame. Large-scale eddies persist for long times in turbulent flows. The development of a turbulent flow is controlled by such structure. Entrainment of one fluid stream into another takes place when fluid is engulfed between large coherent vortices. Fuel and air are introduces separately into turbulent diffusion flames. Since the reactants must be mixed on a molecular scale to burn, this entrainment and the subsequent mixing control the combustion rate. As in the laminar diffusion flame, the gas composition in the flame is distributed continuously from pure fuel to pure air. The structure of a turbulent diffusion flame that results when a fuel jet is released into air, for some distance, the central core of the jet contains unreacted fuel. Combustion takes place at the interface between the fuel and air flows. The flame front is distorted by the turbulent motion but is, as in the laminar diffusion flame, relatively thin. Whether combustion will be complete depends on both the combustion kinetics and the mixing processes in the flame. Simple jet flames are used in relatively few combustion system because they are easily extinguished. A

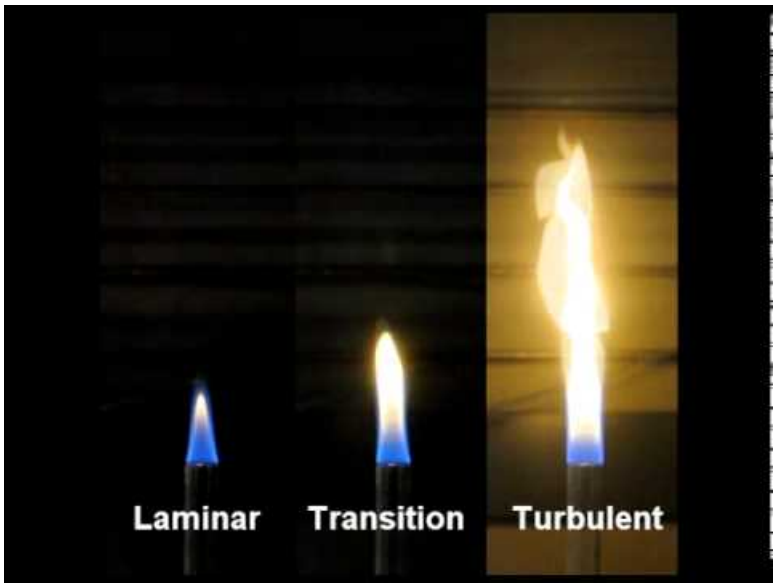
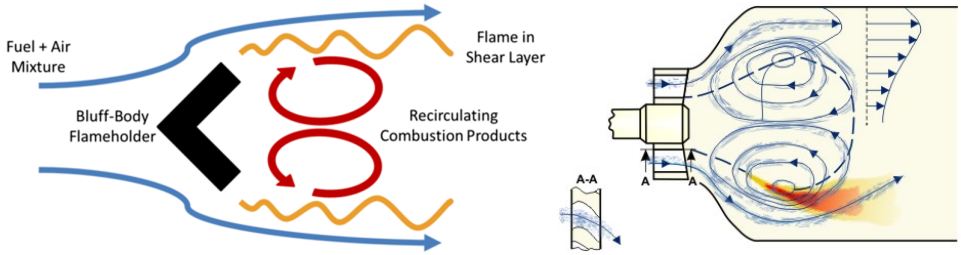


Figure 3.2: laminar, transition and turbulent flame



(a) (b)

Figure 3.3: Flow recirculation: (a) bluff body; (b) swirl vanes

continuous ignition source must be supplied to achieve stable combustion. This is commonly accomplished by inducing flow recirculation, either with a bluff body or with swirling flow, as illustrated in fig.3.3. The low-pressure region in the near wake of the bluff body or in the center of the swirling flow causes a reverse flow bringing hot combustion products into the vicinity of the incoming fuel and air. Generally, only a small fraction of the combustion takes place within the recirculation zone. The remaining fuel burns as it mixes with air and hot products downstream of the recirculation zone. The flame in this downstream region may be a clearly defined jet that entrains gases from its surroundings. The extent of mixing in the flame can be characterized in terms of a *segregation* factor. For detailed theoretical developments we refer to Pompei and Heywood, 1972.

3.3.3 Carbon Monoxide

Carbon monoxide is an intermediate species in the oxidation of hydrocarbon fuels to CO_2 and H_2O. In fuel-rich regions of a flame, the CO levels are necessarily high since there is insufficient oxygen for complete combustion. Only if sufficient air is mixed with such gases at sufficiently high temperature can the CO be oxidized. For CO dangerous, the study of its reaction deserve some attention. The predominant reaction leading to carbon monoxide oxidation in hydrocarbon combustion is

$$CO + OH \quad \overleftrightarrow{} \quad CO_2 + H \tag{3.33}$$

Where $k_d = 4.4T^1.5e^372/T$ $m^3mol^-1s^-1$ is the rate constant of the direct reaction and k_i=k_d/K_c is the rate constant of the reverse reaction. The rate equation describing the total change in the CO level must include the reverse reactions:

$$R_{CO} = -k_d[CO][OH] + k_i[CO_2][H] \tag{3.34}$$

Thus, to describe the CO oxidation kinetics, we must know the concentrations of OH and H. This approach is only theoretical. In fact the dependence of CO production with the fuel air ratio and the temperature is difficult and it is not still understood.

3.4 How FDS Works

The default reaction equation in FDS, known as "simple chemistry" is defined as follows:

$$\nu_0(\nu_{O_2,0}O_2 + \nu_{N_2,0}N_2 + \nu_{H_2O,0}H_2O + \nu_{CO_{2,0}}CO_2) + \nu_1 C_m H_n O_a N_b \longrightarrow \nu_2(\nu_{CO_2,2} + \nu_{H_2O,2}H_2O + \nu N_2, 2N_2 + \nu_{CO,2}CO + \nu_{S,2}Soot) \tag{3.35}$$

Formula (3.35) describe clearly what FDS do. It is made up of three terms:

- the term multiplied by ν_0 is the ambient atmosphere which has its own value that user may change;
- the term multiplied by ν_1 is the fuel and the user have to set the coefficients a, b, n and m;
- the term multiplied by ν_2 is the products of the combustion. Carbon monoxide and soot are zero by default but the user could specify their mass fraction values.

FDS use the “mixed is burnt” assumption with an infinite combustion rate. Thus the heat released is calculated simply by the fuel’s chemical formula. We must recall that FDS allow only one reaction in each simulation and therefore it can distinguish the different nature of the material burnt. In this manner a lot of analytical complexity is saved.

Chapter 4

Fluid dynamics

This chapter is devoted to describe briefly the equations of fluid dynamics that are used in this thesis. We recall that a fluid is a substance that continually deforms (flows) under an applied shear stress. Fluid are subset of the phases of matter and include liquids, gases, plasma, and to some extent, plastic solids. In this thesis our fluid is the mixture of air and the gas gave off by the combustion.

4.1 Navier-Stokes equations

The Navier-stokes equations (N.S.E. for short) are the foundation of all the fluid mechanics. These equations describe perfectly all kind of phenomenon that involved any fluid. They may be used to model, amongst others, the weather, ocean currents, water flow in a pipe and air flow around a wing. Somewhat surprisingly, given their wide range of practical uses, it has not yet been proven that in three dimensions solutions always exist, or that if they do exist, then they are smooth, i.e. they do no contain any mathematical singularity. These balance equation arise from applying Newton's second law to fluid motion together with the constitutive relations between stress and shear. The constitutive relation identifies what sort of fluid is treated.

4.1.1 Differential form of continuity equation

The continuity equation states that the mass is conserved i.e. no matter is created nor destroyed. In tensor notation the differential form of continuity equation is:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \tag{4.1}$$

or in vector notation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{u} = 0 \tag{4.2}$$

where ρ is the density of the fluid and $\vec{u}$ is the velocity vectorial field. The derivation of continuity equation may be found in any text of fluid dynamics.

4.1.2 Differential form of momentum balance equation

Every force acting on a body belongs to one of the two following categories:

- mass forces: these forces acting directly on the volume of the body by means of long distance interactions. Examples of these forces are the gravity and electromagnetic forces. With $\vec{f}$ we indicate the body forces per unit of mass;

- surface forces: these are contact force that effecting the body through its surface. Example of these forces are the pressure and the stress.

The differential form of momentum balance equation is derived from the integral momentum balance equation. Such derivation is found in any book of fluid dynamics. Here we report only the equation. In tensor notation:

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = \rho f_i + \frac{\partial \sigma_{ij}}{\partial x_j} \tag{4.3}$$

where σ_{ij} is the stress tensor. Recalling the definition of substantial or material derivative [1] and the continuity equation we can rewrite (4.3) as:

$$\rho \frac{du_i}{dt} = \rho f_i + \frac{\partial \sigma_{ij}}{\partial x_j} \tag{4.4}$$

and in vector notation using the fact that the material derivative of the velocity is the acceleration $\vec{a}$:

$$\rho \vec{a} = \rho \vec{f} + \nabla \cdot \sigma \tag{4.5}$$

We recall furthermore that σ is a symmetric tensor and it could be proved by the angular momentum balance equation. It is worthwhile to point out that no mention to the kind of fluid is been made and therefore all said until now is valid for every fluid.

[1] the substantial derivative is defined as $\frac{d\bullet}{dt} = \frac{\partial \bullet}{\partial t} + \vec{u} \cdot \nabla \bullet$

4.1.3 The strain

Generally any tensor A could be resolved into a symmetric component and an antisymmetric component. In matrix notation:

$$A = \frac{1}{2}A + \frac{1}{2}A^T \tag{4.6}$$

or in tensor notation:

$$A_{ij} = \frac{1}{2}A_{ij} + \frac{1}{2}A_{ji} \tag{4.7}$$

Applying this relations to the velocity gradient, we get:

$$\nabla\vec{u} = \frac{1}{2}\nabla\vec{u} + \frac{1}{2}\nabla\vec{u}^T = E + \Omega \tag{4.8}$$

and

$$\frac{\partial u_i}{\partial x_j} = \frac{1}{2}(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}) + \frac{1}{2}(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}) = e_{ij} + \Omega_{ij} \tag{4.9}$$

E is the strain instead Ω is a rigid motion component.

4.1.4 Constitutive relations

From a mathematical point of view we have introduced 4 scalar equation i.e. the continuity equation (1 scalar) and the momentum balance equation (1 vectorial equation equal to 3 scalar equations) with 10 scalar unknowns namely the vector velocity field $\vec{u}$ (3 scalar unknowns) the density ρ (1 scalar unknown) and the stress tensor components (6 scalar unknowns, it should be remembered that T is a symmetric tensor). We have therefore to close the problem, i.e. even the equations with the unknowns, and we make this through the constitutive relations which depending on the nature of the fluid, link stress and strain together. The constitutive relations must obey to Noll's axioms:

- determinism's principle: the tension in a continuum is determined only by its past and present not by its future;
- local effect's principle: the tension in a point P of a body is affected only by the motion in a suffice little neighbourhood of the point P itself. This mean that the motion in a part of the body does not affect the stress in other parts;
- independence of the reference system: the constitutive relations must be resulted invariable for change of the reference system and thus for change of the observer.

We can satisfy this axiom with the following assumption:

- the determinism's principle is satisfied if we assume that the stress tensor σ depends only on the current body's state of motion;
- the local effect's principle is satisfied if we assume that the stress tensor σ in a point P depends only on the velocity gradient and on the thermodynamic variables in the point P;
- the independence of the reference system is fulfilled if we assume that the stress tensor σ depends only on the symmetric component E of the gradient velocity vector and does not depend on the antisymmetric component Ω.

In addition we observe experimentally that for a fluid at rest the stress tensor is spherical (otherwise said hydrostatic) namely at rest the tensor σ is:

$$\begin{aligned} \sigma_{ij} &= -p\delta_{ij} \\ \sigma &= -pI \end{aligned} \tag{4.10}$$

p is the hydrostatic pressure that for a compressible it can be identified with the thermodynamics pressure. Furthermore a fluid is said Stokesian if he satisfies the following hypothesis:

- the stress tensor σ is a continuity function of the strain tensor E and of the local thermodynamic state;
- at rest the stress tensor is like in eq. 4.10 (σ=-pI);
- the stress tensor is isotropic, namely he has not got preferential directions and thus the constitutive relation does not depend on the orientation;
- the stress tensor is homogeneous, namely it does not depend explicitly on the position $\vec{x}$ but through the strain tensor E and the thermodynamic variables which depend on $\vec{x}$.

If in addition it is requires that σ is a linear function of E we get the Newtonian fluid a subclass of the Stokesian fluid. Air and water amongst others commonly important fluid are Newtonian. For this class the constitutive relation is:

$$\begin{aligned} \sigma_{ij} &= (-p + \lambda e_{kk})\delta_{ij} + 2\mu e_{ij} \\ \sigma &= (-p + \lambda \nabla \cdot \vec{u})I + 2\mu E \end{aligned} \tag{4.11}$$

where p is the thermodynamic pressure and λ,μ are coefficients of viscosity that usually depend on temperature. If valid, the Stoke's Hypothesis yield:

$$\lambda = -\frac{2}{3}\mu \tag{4.12}$$

4.1.5 Navier-Stokes equations

Finally, substituting eq. 4.11 in eq. 4.4 and assuming $\lambda = \text{cost}$ $\mu = \text{cost}$ we get:

$$\rho\frac{du_i}{dt} = \rho f_i - \frac{\partial p}{\partial x_i} + (\lambda+\mu)\frac{\partial}{\partial x_i}(\frac{\partial u_k}{\partial x_k}) + \mu\frac{\partial^2 u_i}{\partial x_j \partial x_j} \tag{4.13}$$

and in vector form:

$$\rho\vec{a} = \rho\vec{f} - \nabla p + (\lambda+\mu)\nabla(\nabla\cdot\vec{u}) + \mu\nabla^2\vec{u} \tag{4.14}$$

and these are the famous Navier-Stokes equation for Newtonian fluids.

4.2 Reactive Navier-Stokes equations

When we treat the combustion, we have got chemical reaction, and therefore the foregoing equation must be modified taking into consideration the fact that some chemical species are transformed in other species. We treat mixtures of gases which are composed by N gases with a total mass M and occupy a volume V. Every component in the mixture has got a molecular weight W_i, a mass M_i and a number of moles n_i. It is known that when mixtures are treating the quantity of each component must be specified. This is done by mean of one of the following parameters:

- mass fraction: $Y_\alpha = \frac{M_\alpha}{M}$ it is the ratio between the mass of the component α and the total mass of the mixture;
- molar fraction: $X_\alpha = \frac{n_\alpha}{n}$ it is the ratio between the number of moles of the component α and the total number of moles of the mixture;
- partial density: $\rho_\alpha = \frac{M_\alpha}{V}$ is the ratio between the mass of the component α and the total volume of the mixture;
- partial concentration: $C_\alpha = \frac{n_\alpha}{V}$ is the ratio between the number of moles of the component α and the total volume of the mixture.

These parameters are easy relate each other trough the molecular weight of the species and the sum of a parameters extent to each component is equal to 1 i.e. for instance $\sum_{\alpha=1}^{N} X_\alpha = 1$. In addition in any point of the field there is a velocity $\vec{u}_\alpha$ for each component. The weigthed avarage of these velocity with the mass fraction defines the significative mean velocity:

$$\vec{u} = \sum_{\alpha=1}^{N} Y_\alpha \vec{u_\alpha} \tag{4.15}$$

Furthermore the difference between the velocity of the single component and the mean significative velocity is named diffusion velocity $\vec{v}_\alpha$, and we have:

$$\begin{aligned} \vec{v}_\alpha &= \vec{u}_\alpha - \vec{u} \\ \sum_{\alpha=1}^{N} Y_\alpha \vec{v_\alpha} &= 0 \end{aligned} \tag{4.16}$$

We now rewrite the balance equation taking the variation of the concentration of the species into account. The continuity equation for a specie $_\alpha$ becomes:

$$\frac{\partial \rho Y_\alpha}{\partial t} + \nabla \cdot (\rho Y_\alpha \vec{u}_\alpha) = \dot{\omega}_\alpha \tag{4.17}$$

where $\dot{\omega}_\alpha$ is the production rate of the specie α (mass per unit of volume and time) due to chemical reactions. Expressing the velocity of the single specie α according to eq. 4.16 we get:

$$\frac{\partial \rho Y_\alpha}{\partial t} + \nabla \cdot (\rho Y_\alpha \vec{u}) = \dot{\omega}_\alpha - \nabla \cdot (\rho Y_\alpha \vec{v}_\alpha) \tag{4.18}$$

taking into account that $\sum_{\alpha=1}^{N} \dot{\omega}_\alpha = 0$ and summing for all species yields:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{u} = 0 \tag{4.19}$$

where is equal to eq. 4.2 except for the definition of $\vec{u}$. In a similar manner the momentum balance equation for the species α is:

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) = \nabla \cdot \sigma + \sum_{\alpha=1}^{N} \rho Y_\alpha \vec{f_\alpha} \tag{4.20}$$

in which $\otimes$ in the diadic product.[2] Similarly the equation of the internal energy U is:

$$\frac{\partial \rho U}{\partial t} + \nabla \cdot (\rho \vec{u} U) = \sigma : \nabla \vec{u} - \nabla \cdot \vec{q} + \sum_{\alpha=1}^{N} \rho Y_\alpha \vec{f_\alpha} \cdot \vec{v}_\alpha \tag{4.21}$$

[2]the diadic product of the vectors $\vec{a}$ and $\vec{b}$ is a tensor C such that $C_{ij}=a_i b_j$

where $\vec{q}$ is the heat flux vector and : is the double dot product.[3] We have to close the equations because the density ρ for each species is not defined by the continuum mechanics. We easy solve the problem assuming that all the species involved are ideal gases. Therefore recalling the Dalton's law of partial pressure[4] we have got that:

$$\begin{aligned} p_\alpha &= \rho Y_\alpha \frac{R}{W_\alpha} T \\ p &= \rho R T \sum_{\alpha=1}^{N} \frac{Y_\alpha}{W_\alpha} \end{aligned} \tag{4.22}$$

The internal energy U of the single species could be expressed:

$$U_\alpha = h_\alpha - \frac{p_\alpha}{\rho Y_\alpha} \tag{4.23}$$

therefore the total internal energy will be:

$$U = \sum_{\alpha=1}^{N} Y_\alpha h_\alpha - \frac{p}{\rho} \tag{4.24}$$

We have to model the diffusion terms:

- for the mass diffusion we use Fick's law and for each species we have got:
$$\rho Y_\alpha \vec{v}_\alpha = -D \nabla Y_\alpha \tag{4.25}$$
- for the diffusion of the linear momentum assuming a Newtonian fluid we get:
$$\sigma = -(p + \frac{2}{3}\mu \nabla \cdot \vec{u}) I + \mu[\nabla \vec{u} + (\nabla \vec{u})^T] \tag{4.26}$$
- diffusion energy: it is models via Fourier's law and the enthalpy flow:
$$\vec{q} = -k \nabla T + \rho \sum_{\alpha=1}^{N} h_\alpha Y_\alpha \vec{v}_\alpha \tag{4.27}$$

[3] given two tensor a_{ij} and b_{ij} the double dot product is a scalar which is defined as $a_{ij} b_{ji}$ i.e. it is the trace of the product of the tensors a and b.

[4] Dalton's law states that in a mixture of non-reacting gases, total pressure exerted is equal to the sum of the partial pressure of the individual gases.

Equations from 4.18 to 4.27 constitute what is called fully-compressible formulation. In reality this formulation is substituted with the Low-Mach system which stems from the previous by means an asymptotic expansion. The low-Mach system is simpler and faster than the fully-compressible and it is an apt model for the bulk of real cases which in fact occur at low speed. The Low-Mach system neglects elastic acoustic propagation of sound and it is instead characterized by an instantaneous elliptic propagation, typical of the incompressible Navier-Stokes equation. The exact formulation used by FDS can be found in its technical reference.

4.3 Turbulence

It is known that the motion of a fluid could be laminar motion or turbulent. Both are solutions of N.S.E. but the turbulent motion is more complex than the laminar motion. Two remarkable peculiarities of the turbulence are the capacity of mixing two or more different fluids (for instance during a combustion process) or two or more parts of the same fluid at a different temperature (for instance during a heat transfer process) and the capacity of dissipating kinetic energy. Actually these two properties are presented also in the laminar motion but in a turbulent motion are magnified due to the chaotic transport of the particles. If the N.S.E. are solved for a suffice high Reynold number[5] with assigned initial condition (i.c.) it is got an instantaneous field of motion that could be extremely different is the i.c. are slightly varied. Therefore the turbulence has got a strong dependence on the i.c. which is typical of chaos. Because it is not possible to fix in an exact manner the i.c. the correct way to confront the problem is via statistic methods. Thus, for the experimental study of a phenomenon, one must realise more experiments that reproduce the phenomenon itself. These experiments are nominally identical but differ for the i.c. with could not be exactly the same. Each experiment will give different instantaneous fields of motion and with these one must perform an ensemble average that will give the mean motion. The ensemble average is a temporal mean which allow us to write a general scalar or vectorial quantity as the sum of a mean part plus a deviation from the mean. This idea bring to the development of the Reynolds Average Navier-Stokes equation (RANS for short) which carry Reynold stress and the relative closure problem. For a detailed treatise we refer to book specific book on turbulence such as that

[5]The number of Reynold is a dimensionless number which is the ratio between inertial forces to viscous forces. It is analytically defined as $\mathrm{Re} = \frac{\rho u L}{\mu}$ where ρ is the density of the fluid(kg/m^3), u is the velocity of the fluid (m/s), L is a characteristic linear dimension (m) and μ is the dynamic viscosity of the fluid (Pa·s)

in the bibliography.

4.3.1 Turbulence scale and Direct Numerical Simulation

The method apparently simpler for the numerical simulation of turbulent flows seems to be that of discretize the N.S.E. This technique is called direct numerical simulation (DNS for short). Because the N.S.E. embed the thorough physics of turbulent flows, for a proper discrete evolution it is necessary to capture all the physical processes that occur in the turbulence. This imply a very heavy computational cost but on the other side a detailed and accurate reproduction of the flow thus the simulation acquire a value comparable to that of an experiment. To asses the computational cost of a DNS we refer to the phenomenological theory of Richardson and to the formal theory K41 of kolmogorov. In a turbulent flow the introduction of kinetic energy occurs on spatial scales that have a dimension comparable to the size of the body which spawns the turbulence. We call this dimension integral scale and we indicate it with L. The biggest vortical structures, which has therefore a dimension in the order of L, are unstable and falling apart they create smaller structure originating the phenomenon of energy cascade. In this phenomenon the energy introduced at scale L is transferred to smaller and smaller structures by mean of an inertial process in which the kinetic energy is not dissipated. The energy cascade is interrupted at Kolmogorov scale η which is much smaller than the integral scale L. At kolmogorov scale the vortical structures are so small that can spawn dissipative process which convert kinetic energy into heat. In flows characterized by an high Reynolds number there is a broad separation between the integral scale L and the dissipative scale η. This is the heaviest problem that occur in DNS because the computational domain will have a dimension similar to that of the integral scale while the dimension of the grid will be comparable with the dissipative scale. In fact if we use a grid having dimensions bigger than η, the dissipative process could not occur at the proper spatial scale, and thus the entire physics of the turbulence will be altered getting erroneous results. The number of points in each direction must be proportional to the ratio of integral scale to Kolmogorov scale namely

$$N_x = \frac{L_x}{\Delta x} \propto \frac{L}{\eta} \tag{4.28}$$

An estimate of this ratio can be obtained by means of the dimensional analysis. We know that the kinetic energy dissipation, in high Reynolds flows, is proportional to the representative dimension of the big scale (u^3 and L^-1)

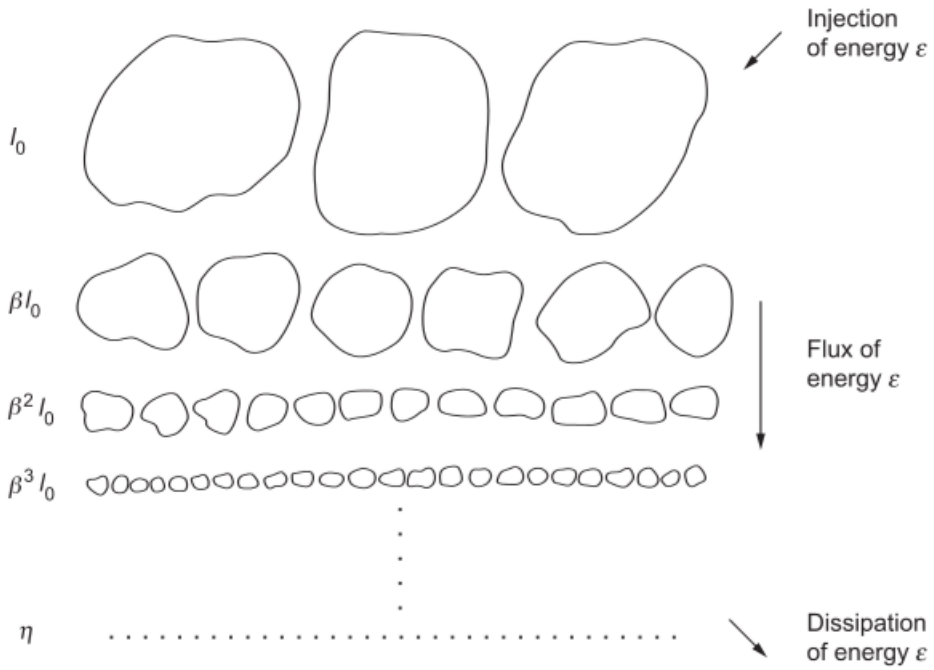


Figure 4.1: The energy cascade

namely, $\epsilon \propto \frac{u^3}{L}$, while the Kolmogorov scale depends only on the dissipation ϵ and on the viscosity ν[6] namely $\eta = (\frac{\nu^3}{\epsilon})^{\frac{1}{4}}$. Therefore we can have an evaluation of the number of points in each direction:

$$N_x = \frac{L_x}{\Delta x} \propto \frac{L}{\eta} = \frac{L}{(\frac{\nu^3}{\epsilon})^{\frac{1}{4}}} \propto \Big(\frac{L^4 u^3}{L\nu^3}\Big)^{\frac{1}{4}} = Re^{\frac{3}{4}} \tag{4.29}$$

This estimate must clearly be extended to the three dimensions, therefore:

$$N \propto N_x^3 \propto Re^{\frac{9}{4}} \tag{4.30}$$

It is apparently that the number of points increase very rapidly with the Reynolds number. We must also to assess the time required for the simulation namely we have to consider the temporal discretization. For do this, the temporal increment should be able to resolve the characteristic kolmogorov time: $= \tau_\eta = \frac{\eta}{u_\eta} = (\frac{\nu}{\epsilon})^{\frac{1}{2}}$. The big scale time is $T = \frac{L}{u}$, therefore the number

[6] ν is the cinematic viscosity which is the ratio of the dynamics viscosity to the density $\nu = \frac{\mu}{\rho}$

of temporal steps will be proportional to the ratio of T τ_η:

$$N_t \propto \frac{T}{\tau_\eta} = Re^{\frac{1}{2}} \tag{4.31}$$

The total time of a simulation will be proportional to the product of N and N_t namely we get:

$$T_{tot} \propto N \cdot N_t \propto Re^{\frac{11}{4}} \cong Re^3 \tag{4.32}$$

To really understand how demanding a DNS is, let's take a cylindrical duct with a turbulent flow of water in its interior. We know that, for a flow of water ($\nu = 10^-6 m^2/s$) in a pipe of diameter D = 1cm = 10^-2m with a mean speed of u = 0.5 m/s, Reynolds results $\mathrm{Re}_D, 1 = 5300$.[7]Using a proper number of points N = 2,5 $\cdot 10^6$ it is needed a computation's time of 1 hour $\mathrm{T}_{tot,1}$ = 1h on a 8 cpus IBM power5. For an industrial application we should have a pipe with a duct D = 1m, a mean speed u=1 m/s for which we get a $\mathrm{Re}_D, 2 = 5{,}3 \cdot 10^6$. Thus:

$$\frac{T_{tot,2}}{T_{tot1}} = \left(\frac{Re_{D,2}}{Re_{D,1}}\right)^3 = 10^9 \tag{4.33}$$

Therefore we need one billion of hours i.e. one-hundred-thousand years. We conclude that a DNS is not applicable to industrial applications because the computational cost is too high. On the other side the quality of the results obtained via a DNS are comparable to an experimental. The DNS gives the actual local motion field which is experimentally difficult to obtain due to the presence of probes which alter the field itself.

4.3.2 Reynolds Averaged Navier-Stokes

We have seen that DNS are not of practical use and in addition engineering flows request, at first approximation, the steady average velocity field. This considerations bring us to evaluate the mean and not the instantaneous velocity. Furthermore the mean field is smoother than the instantaneous field and therefore in a numerical simulation the dimensions of the grid result constrained by the gradients of the mean motion. In addition the mean motion could reacquire the symmetries due to the geometry. Indicating with a bar $\bar{\cdot}$ the average quantities and with a $\cdot'$ the fluctuating quantities, the RANS for an incompressible flow, are:

- continuity equation:

$$\frac{\partial \overline{u_j}}{\partial x_j} = 0 \tag{4.34}$$

[7]In a duct flows characterized by a Re>2400 are fully turbulent.

- momentum balance equation:

$$\frac{\partial \overline{u_i}}{\partial t} + \overline{u_j}\frac{\partial \overline{u_i}}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} + \frac{1}{\rho}\frac{\partial (2\mu \overline{e_{ij}})}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} \tag{4.35}$$

- average strain tensor:

$$\overline{e_{ij}} = \frac{1}{2}\Big(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\Big) \tag{4.36}$$

- Reynolds stress:

$$\tau_{ij} = -\overline{u_i' u'_j} \tag{4.37}$$

In this equation the Reynolds stress tensor is unknown and therefore recalling that this tensor is symmetric, we have 6 scalar unknowns. We have thus to model the tensor τ_{ij} as a function of the mean velocity field through appropriate hypothesis. A first hypothesis was advanced by Boussinesq with the concept of turbulent viscosity. Diffusion and transport are more efficient in a turbulent flow than in a laminar flow because in the latter these properties depend only on the molecular properties of the fluid (ν) while in the former these are accelerated by the vortical structure. Boussinesq, therefore exploited a formal analogy with the molecular stress i.e.:

$$\tau_{ij} = -\overline{u_i' u'_j} = -\frac{2}{3}K\delta_{ij} + 2\nu_T \overline{e_{ij}} \tag{4.38}$$

in which $\mathrm{K} = \frac{\overline{u_i' u_j'}}{2}$ is the turbulent kinetic energy and $\nu_T = \nu_T(x,t)$ is the turbulent viscosity[8] that is function of time and space. Thus, while ν derive from molecular properties and depend on the type of fluid and its thermodynamics state, ν_T depend only on the state of motion and does not depend on the type of fluid. We have moved the problem from that of modelling τ_{ij} (6 scalar unknowns) to that of modelling ν_T (1 scalar unknown). For to this, a lot of model exist. Such as example we could take the K-ϵ model which is one of the largest used. Exploiting the dimensional analysis, this model lets:

$$\nu_T = C_\mu \frac{K^2}{\epsilon} \tag{4.39}$$

The kinetic turbulent energy K gives us an evaluation of the turbulent fluctuation in the flow field, while the dissipation of energy ϵ indicates us how much energy is wasted and converted into heat per unit of time. The coefficient C_μ is the first calibration constant and it varies according to the flow

[8] The turbulent viscosity has got the same unit of the cinematic viscosity i.e. m^2/s

considered. Eq. 4.39 gives the turbulent viscosity provided that we know K and ϵ. We must therefore model these two quantities by means of other two scalar equations. For the kinetic turbulent energy the equation is:

$$\frac{\partial K}{\partial t} + \overline{u_j}\frac{\partial K}{\partial x_j} = \frac{\partial(-\overline{u_j'p} - \overline{u_i'u_i'u_j'} + 2\nu\overline{u_i'e_{ij}'})}{\partial x_j} - \overline{u_i'u_j'}\overline{e_{ij}} - \epsilon \tag{4.40}$$

in which at left hand side, the first term between round parenthesis is the spatial flux of energy, the second term is the production and the third is the dissipation of kinetic turbulent energy. The spatial flux of energy is totally unknown because it depends only on fluctuation quantities e it is modelled trough a gradient diffusion (as the same token of molecular diffusion):

$$\frac{\partial(-\overline{u_j'p} - \overline{u_i'u_i'u_j'} + 2\nu\overline{u_i'e_{ij}'})}{\partial x_j} = \frac{C_\mu}{\sigma_k}\frac{\partial K}{\partial x_j} \tag{4.41}$$

where σ_k is the second calibration coefficient of the K-ϵ model. The production term is known because we have already model the Reynolds stress:

$$\Pi = -\overline{u_i'u_j'}\overline{e_{ij}} = C_\mu\frac{K^2}{\epsilon}\overline{e_{ij}e_{ij}} \tag{4.42}$$

We may rewrite equation 4.40 as:

$$\frac{\partial K}{\partial t} + \overline{u_j}\frac{\partial K}{\partial x_j} = \frac{\partial\left(\frac{C_\mu}{\sigma_k}\frac{\partial K}{\partial n_j}\right)}{\partial x_j} + \Pi - \epsilon \tag{4.43}$$

The dissipation energy ϵ is model trough a similar transport-diffusion/production-dissipation equation:

$$\frac{\partial \epsilon}{\partial t} + \overline{u_j}\frac{\partial \epsilon}{\partial x_j} = \frac{\partial\left(\frac{C_\mu}{\sigma_\epsilon}\frac{\partial \epsilon}{\partial n_j}\right)}{\partial x_j} + C_{\epsilon 1}\frac{\epsilon}{K}\Pi - C_{\epsilon 2}\frac{\epsilon^2}{K} \tag{4.44}$$

in which appear other three calibration constants namely $\sigma_\epsilon, C_{\epsilon 1}, C_{\epsilon 2}$ for a total of five calibration constants. Some reference values for these constants for isotropic and homogeneous flows are:

- $C_\mu = 0{,}09$;
- $C_{\epsilon 1} = 1{,}44$;
- $C_{\epsilon 2} = 1{,}92$;
- $\sigma_k = 1$;

- $\sigma_\epsilon = 1{,}3$.

This brief dissertation has highlighted that RANS models terms which are of extreme relevance for N.S.E.. This technique is antithetic to DNS and results more suitable for real application because the computational cost is affordable. The results of a RANS analysis should be combined with experimental data for sake of accuracy.

4.3.3 Large Eddy Simulation

We have seen that DNS describes thoroughly instance for instance all the physical process of the turbulence which, as known, are not steady and are chaotic. On the other side the RANS is a technique that resolves directly the average equations through a model that influence heavily the dynamics and in addition this model is characterized by calibration coefficients which depend on the flow in exam. Another problem with the RANS is the impossibility to describe unsteady phenomena which could result interesting in some application (for instance meteorology). This drawbacks have urged the development of another class of models: the Large Eddy Simulation (LES for short). LES is a technique more advance than RANS because is based on similarity and universality hypothesis which underlying kolmogorov's theory K41. From k41 it is known that the big scales depend on the flow's geometry while the small scales are universal and irrespective of the geometry. The base idea of the LES is that to simulate the big scale which depend on the treated flow and to use the model for evaluating the effect of small scales on the big scales. The hope is that to obtain a universal model (taking advantage from the universality of small scales) which can simulate unsteady processes typical of turbulence. LES are carried out in four conceptual steps:

- 1. define the G_Δ operator which is a filtering operator. It separates small scales velocity from big scales velocity;
- 2. applying the filtering operator to N.S.E. obtaining the filter equations;
- 3. modelling unknown Sub-Grid-Stress which are terms analogue to Reynolds stress;
- 4. solving numerically the equations obtained.

Starting from first point, we define a filter velocity $\widetilde{u_i}$ through the filtering operator G_Δ:

$$\widetilde{u_j}(x,t) = G[u_j] = \int_V u_j(x-r,t)G_\Delta(r,x)dr \tag{4.45}$$

in which Δ is the characteristic amplitude of the considered filter namely the characteristic length below that the filter cut off the fluctuation, while x and r are respectively the point where we want to calculate the filtered quantity and the distance from such point. Once that the filter has been defined properly, the velocity u_i is resolved as:

$$u_i = \widetilde{u_i} + u_i' \tag{4.46}$$

where u'$_i$ is the sub-grid velocity. For instance, two type of filters are:

- Box: $G_\Delta(r) = \frac{1}{\Delta} H(\frac{\Delta}{2} - |r|)$ with H Heaviside function[9]
- Gauss: $G_\Delta(r) = \sqrt{\frac{6}{\pi\Delta}} e^{-6(\frac{r}{\Delta})}$.

The successive step is that to apply the filtering operator to N.S.E. assuming that it is uniform namely G(x,r) = G(r) which implies that commutates with the derivative operator. Similarly at what done for RANS we get:

- continuity equation:

$$\begin{aligned} G[\frac{\partial u_j}{\partial x_j}] = \frac{\partial G[u_j]}{\partial x_j} = 0 \\ \frac{\partial \widetilde{u_j}}{\partial x_j} = 0 \end{aligned} \tag{4.47}$$

- momentum balance equation:

$$\frac{\partial \widetilde{u_i}}{\partial t} + \frac{\partial \widetilde{u_i u_j}}{\partial t} = -\frac{1}{\rho}\frac{\partial \widetilde{p}}{\partial x_i} + \frac{1}{\rho}\frac{\partial (2\mu \widetilde{e_{ij}})}{\partial x_j}$$

  and adding on both sides:

$$\frac{\partial (\widetilde{u_i}\widetilde{u_j})}{\partial x_j}$$

  we get:

$$\frac{\partial \widetilde{u_i}}{\partial t} + \frac{\partial (\widetilde{u_i}\widetilde{u_j})}{\partial x_j} = -\frac{1}{\rho}\frac{\partial \widetilde{p}}{\partial x_i} + \frac{1}{\rho}\frac{\partial (2\mu \widetilde{e_{ij}})}{\partial x_j} - \frac{\partial \tau_{ij}^r}{\partial x_j} \tag{4.48}$$

  where τ_{ij}^r is sub-grid or residual stress tensor which is defined as :

$$\tau_{ij}^r = \widetilde{u_i u_j} - \widetilde{u_i}\widetilde{u_j} \tag{4.49}$$

[9]The Heaviside function is defined as H(x) = $\begin{cases} 0 & \text{if x}< 0 \\ 1 & \text{if x}\geq 0 \end{cases}$

The system of equations 4.47 and 4.48 is formally equal to that of RANS but in reality is deeply different because the velocity field $\widetilde{u}_i$ and that of the pressure $\widetilde{p}$ are always three-dimensional, unsteady and chaotic namely they are similar at those obtained trough DNS. The differences amongst these three models lay in the additional stress namely:

- DNS: there is not an additional stress tensor. The stress tensor in this equation is due to the actual viscous molecular diffusion ;
- LES: there exists a residual stress tensor τ^r which taking only into account the effect of small scale,
- RANS: there is the Reynolds stress tensor that must models the effect of both small and big scale on the average field.

About LES we have to point out that the amplitude of the filtering Δ must belong to the inertial range. In fact only in this manner we should construct a model which does not depend on the simulated flow because the smaller scales have got an universal dynamics. This property allows to decrease the spatial resolution in comparison with a DNS, in fact the grid step of a LES will be equal or minor than Δ which is certainly major then η. To solve Les, similarly a what we have done with the RANS, we must model the tensor τ^r. We take as example the Smagorinsky's model which use the concept of eddy viscosity. At first we observe that the trace of the tensor τ^r is:

$$\tau_{ii} = \widetilde{u_i u_i} - \widetilde{u}_i \widetilde{u}_i = 2K^r \tag{4.50}$$

in which K^r is the residual kinetics energy. In a similar manner a what done for RANS we write:

$$\tau^r_{ij} = \frac{2}{3} K^r \delta_{ij} - 2\nu^r \widetilde{e_{ij}} \tag{4.51}$$

where $\nu^r = \nu^r(x,t)$ is the residual or sub-grid, cinematic viscosity. We can rewrite the equation 4.47 and 4.48 as:

$$\begin{aligned} \frac{\partial \widetilde{u}_j}{\partial x_j} &= 0 \\ \frac{\partial \widetilde{u}_i}{\partial t} + \frac{\partial (\widetilde{u}_i \widetilde{u}_j)}{\partial x_j} &= -\frac{\partial \widetilde{p^{mr}}}{\partial x_i} + \frac{\partial [2(\mu + \mu^r)\widetilde{e_{ij}}]}{\partial x_j} \end{aligned} \tag{4.52}$$

where

$$\widetilde{p^{mr}} = \frac{2}{3} K^r + \frac{\widetilde{p}}{\rho}$$

For solving this system of equations we must model ν^r which depends on quantities that characterize the level of turbulence on the cell of amplitude

Δ. By means of dimensional analysis we must find quantities that multiplied among them they are homogeneous to a speed for a length i.e. m^2/s (the measure of ν). Smagorinsky proposed the filtering strain rate:

$$\widetilde{S} = \sqrt{2\widetilde{e_{ij}}\widetilde{e_{ji}}} \tag{4.53}$$

to measure the amplitude of velocity gradients around the filtering cell. Because $\widetilde{S}$ is dimensional homogeneous to speed to length we have to multiply it for a characteristic length of the grid. Therefore we get :

$$\nu^r = (C_s\Delta)\widetilde{S} \tag{4.54}$$

Given the value of C_s, which is a calibration constant similar to those for K-ϵ model, we have closed the problem and we can theoretically solve LES equations. The values of C_s that could be found in literature vary from 0,06 to 0,2, although Lilly trough consideration of homogeneity and isotropy obtained the value 0,17.

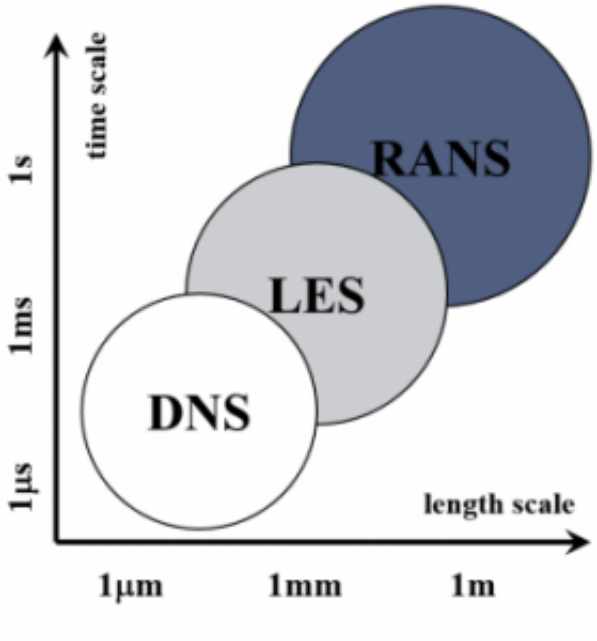


Figure 4.2: A sketch of the scale resolution of the various models

Chapter 5

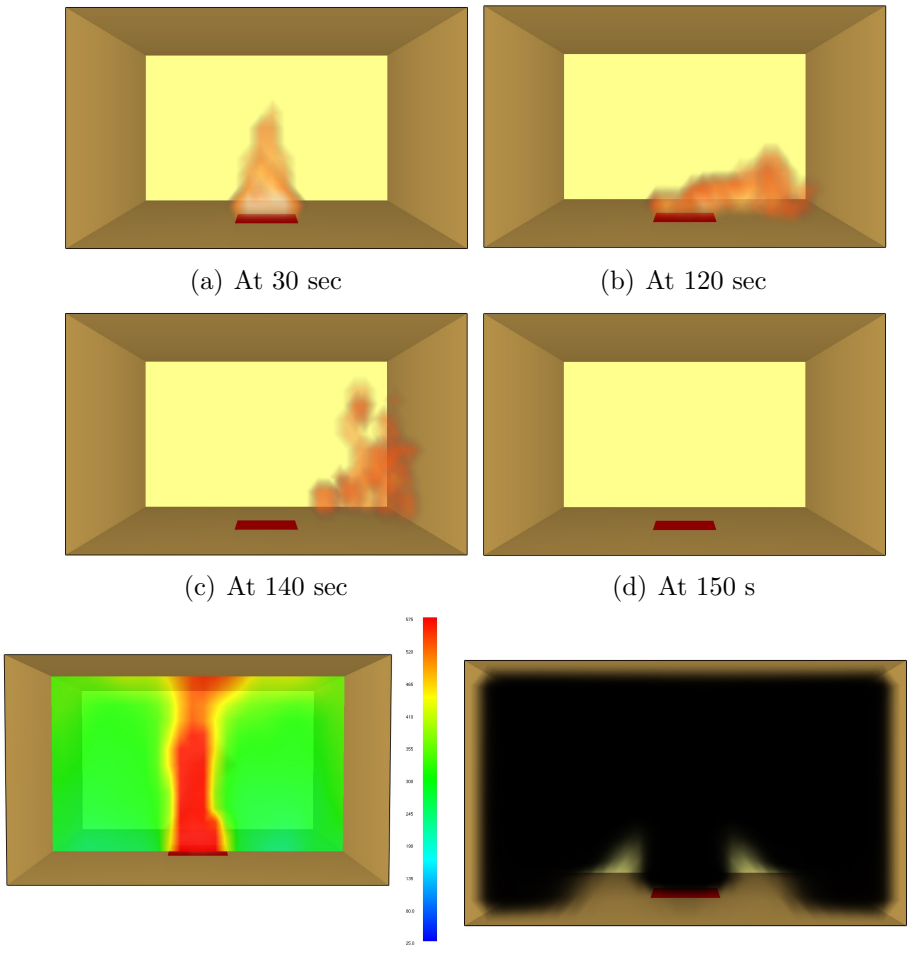
Train coach simulations

Our initial purpose was that to simulate a fire in a coach. Due to the fact that i have no previous experience with FDS or fire simulations in general, i started from scratch. At the beginning i had started with extremely simple models to figure out how FDS works, its potentiality and its limits. Step by step, i had added more complexity and new features to the models and i become acquainted with the dynamics of fire and with the software. Our final result has been the simulation of five coaches within a 1 km long tunnel. This chapter is devoted to the description of this step by step process.

5.1 Preliminary simulations

The first case was very trivial, but he pointed me out some interesting facts anyway. I simulated a 5×5×3m closed space with the boundary adiabatic. A surface of 1 m^2 that provide an HRR of 1 MW was posed in the middle and the reaction that supply the heat was taken from the library of FDS (POLYURETHANE-GM37). Generally we can define our reaction with a lot of chemical parameters setting among which the more interesting for us are the products of the reaction (CO for instance has a prominent role). From this simple simulation we can observe:

- Due to the fact that the system is isolated and in particular there are not openings after finishing the oxygen the combustion stops;
- Analysing the results on pressure it is apparent that it reaches values too excessive (10^7 Pa). This fact depend always on the closed environment which results at constant volume;
- We can define only one reaction;



(a) At 30 sec (b) At 120 sec

(c) At 140 sec (d) At 150 s

(e) Temperature slice (f) The soot

Figure 5.1: Some pictures of the result of the simplest simulation

- The value of HRR in proximity of the fire is ensured by the proper amount of "fuel" until the oxygen is finished.

5.2 Some Test of Material's Combustion

Next step was that of trying to burn some objects. FDS allows two different approaches to simulate pyrolysis one called "direct" and another called "indirect" . Before concerning with these two approaches we must describe in a proper manner what pyrolysis is.

5.2.1 Pyrolysis

Pyrolysis can be defined as a chemical decomposition of a material into one or more other substance due to heat alone and all solid combustibles must undergo pyrolysis in order to generate gaseous fuel vapours for flaming combustion. The energy required to convert a solid material into a vapour through pyrolysis will be referred to as heat of vaporization ΔH_v. The pyrolysis process can follow different paths, depending on the characteristics of solid materials. For example cellulosic materials decompose directly to gaseous vapours whilst thermoplastics (such as polypropylene) follow a two step process (first of all a liquid is formed and then the liquid turns into a gaseous fuel). Despite its physical and chemical complexity, in FDS the pyrolysis process is simply modelled using an Arrhenius equation approach.

5.2.2 Pyrolysis Direct and Indirect Approach

The "direct method" consist in assigning a specific HRRPUA (heat release rate per unit area) to each material that characterizes the fire scenario and therefore since the production rate of gaseous fuel per unit area is controlled by the combustion process, the mass flow rate of gaseous fuel is independent of thermal feedback to the surface. The inception of the pyrolysis process is controlled by a parameter called ignition temperature: when the material achieves this temperature the gaseous fuel release begins. On the contrary, the second approach, which will be referred to as the "indirect method", is based on the heat of vaporization and it accounts for thermal feedback to the solid surface. In this case the code allows the user to model the material either as a thermoplastic or a charring fuel.

5.2.3 The Seat

One of the first not trivial thing that we tried to burn was a seat. This is constituted of a pedestal make of steel and of a backrest, armrest made of a double layer in which the outermost is a thin fabric and the innermost is foam. Our purpose here, was that to answer to the following question:

- which approach use? The direct or the indirect.
- what should be the source of heat?
- if the combustion occurs, will it carry on after we will remove the heat source?

A first drawback of the direct approach is that we lose the possibility to set multilayer obstruction with different chemical properties. On the other hand carrying out simulations which compare the direct and indirect method it turns out that these methods give different results but the latter allows the fire to propagate and therefore as reported in [1-2] (Andreini, Da Soghe, Facchini, Giusti) this is the method to adopt. FDS allow to model the ignition as a surface whose geometry and HHRPUA are setted by the user or as some particles which have a given position and a given temperature setted by the user. Although, with the parameters setted properly, once the combustion takes place these two cases give the same outcome, it is better to chose the former approach because it result more stable than the latter and above all in literature are available HRR data. About the last point, FDS permits to customize the HRRPUA attributed to the burner surface as linear piecewise functions and therefore we can simulate a real source of heat that least a finite time. What has emerged is that after the combustion occur, if we quench the heat source the fact that the fire will carry on or not, depends on the boundary condition. What we can state is that if there are the proper condition of air, the proper quantity of material and if it has adequate thermal properties to foster an high temperature, the fire will be maintained. A valuable feature of FDS is that it allows the obstructions to burn away namely FDS calculates how material is burnt and it makes disappear it. In the following we describe the main characteristics of the simulations:

- Environment: we take a box with inert boundary on all sides except for the ceiling where we put an open boundary condition, which allows to maintain realistic value of pressure, to supply fresh air with oxygen that fuel the combustion and to exhaust the reaction products. The air is at standard condition and concentrations;

- Geometry: the geometry of the seat is:

Part	Length (mm)	width (mm)	height(mm)
pedestal	10	10	35
seat	60	60	10
backrest	10	60	80

- Time: we simulate 600 sec i.e. 10 minutes;

- Material: the seat has got a pedestal made of steel and the upholstery made of fabric and foam;

- Thermal properties: this properties has been taken from FDS and NIST's database

Material	Density (kg/m^3)	Specific heat (kj/(kg·K))	Conductivity (W/(m·K))	Emissivity
Fabric	100	1	0,1	0,9
Foam	40	1	0,05	0,9
Steel	7850	0,46	45,8	0,95

- pyrolysis model: this properties has been taken from FDS and NIST's database in which the heat of reaction is what we have called heat of vaporization before. The vaporization is a physical reaction that adsorb heat from the ambient around.

Material	Heat of combustion (kJ/kg)	Heat of reaction (kJ/kg)	byproducts
Fabric	$1{,}5 \cdot 10^4$	1000	100% reaction fuel
Foam	$3 \cdot 10^4$	800	100% reaction fuel

- the chemical reaction is taken from FDS' library and characterized by the composition express in terms of C,H,O,N atoms which constitute the material, the heat release per unit mass oxygen and the byproduct CO, soot and a fraction of H:

Name	C	H	O	N	Heat per mass oxygen (kJ/kg)	CO (Y_{CO})	Soot Y_s	frac.H
Polyurethane	6,3	7,1	2,1	1	$1{,}31 \cdot 10^4$	0	0,1	0,1

In the following images we report the results of the same seat but with different ignition source:

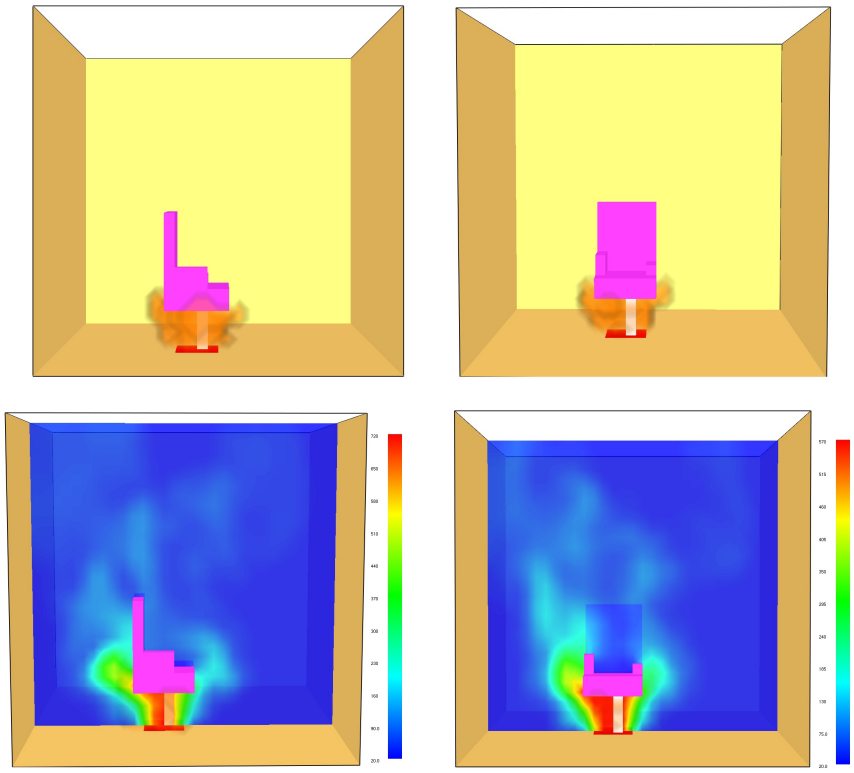


Figure 5.2: Case 1at 5 seconds

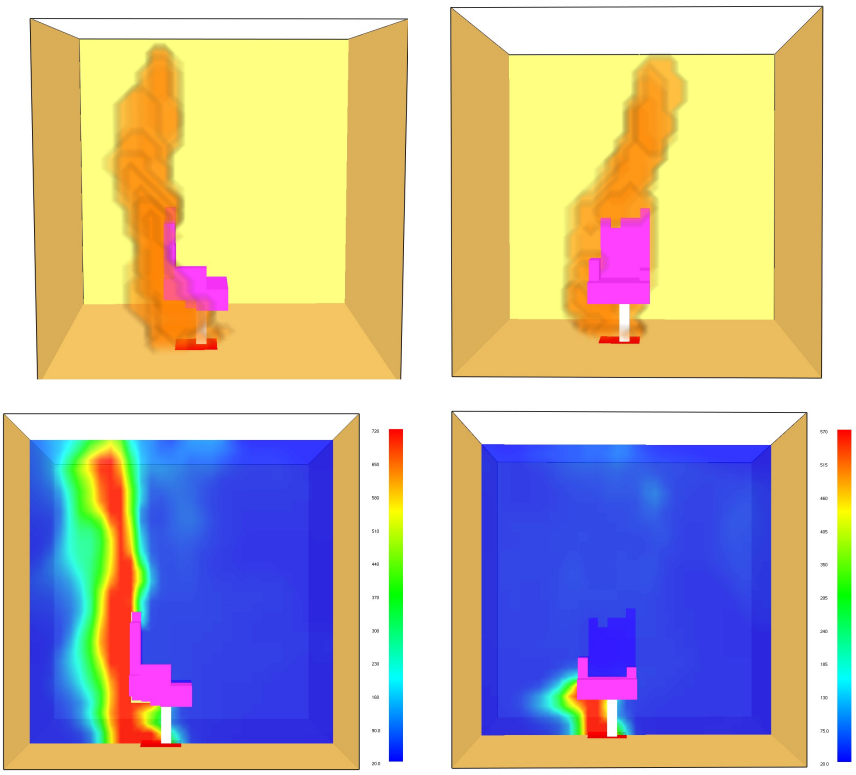


Figure 5.3: Case 1 at 120 seconds

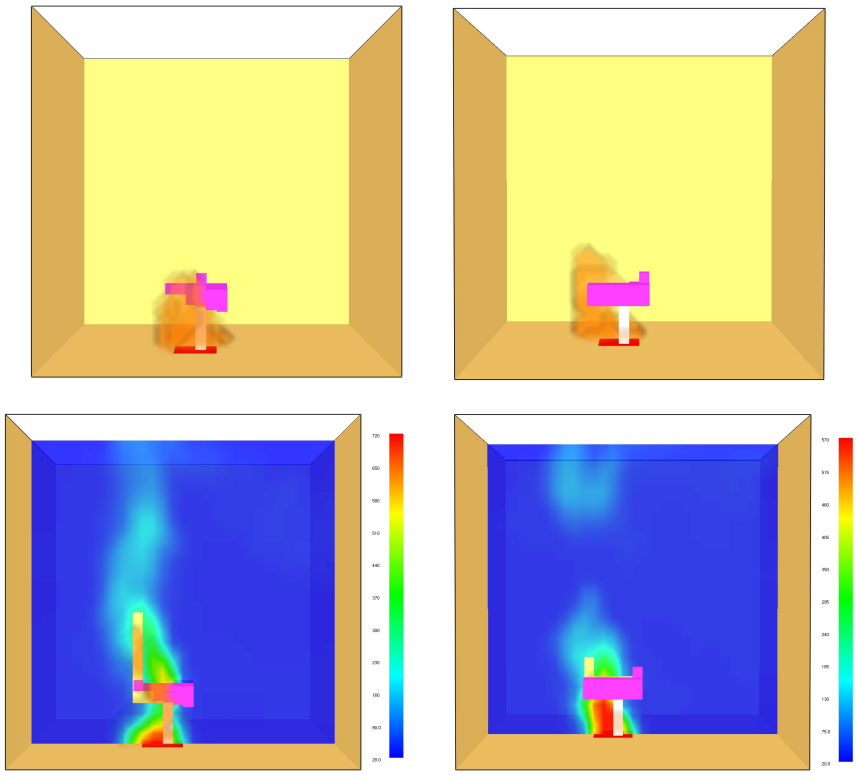


Figure 5.4: Case 1 at 400 seconds

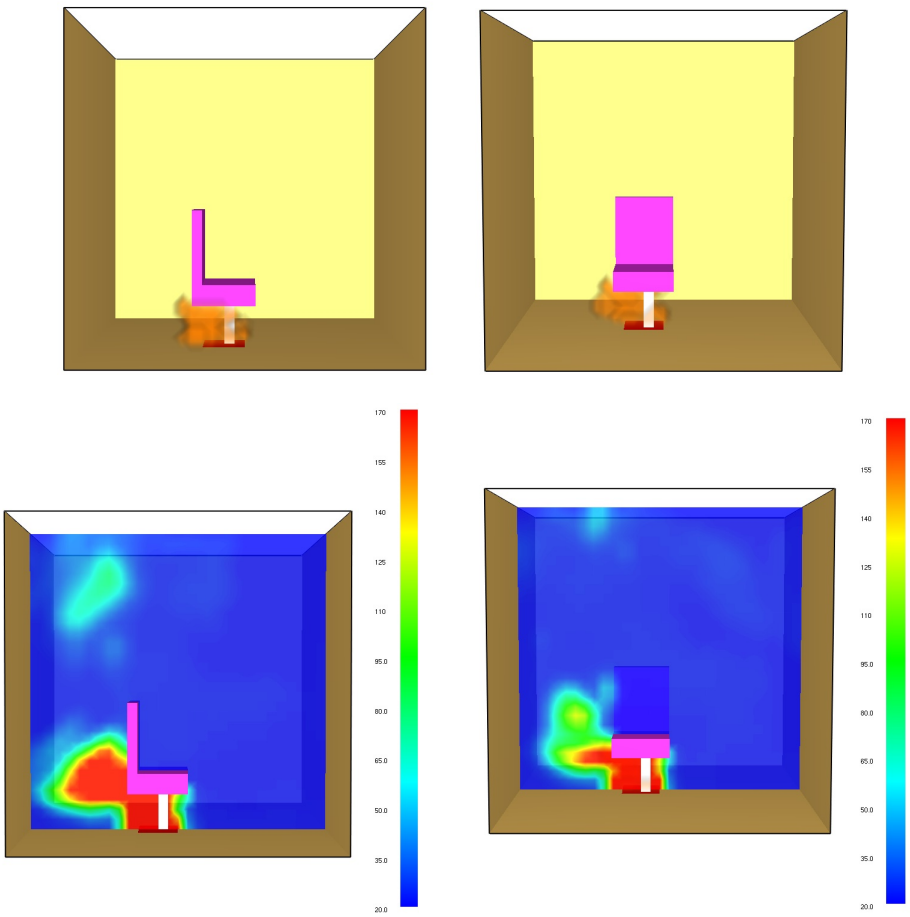


Figure 5.5: Case 2 at 60 seconds

1. constant value of HRRPUA = 1000 W/m^2 on an area of 0.16 m ^{2} underneath the seat.

2. constant value of HRRPUA = 1000 W/m^2 from 0 to 60 seconds on an area of 0.16 m ^{2} underneath the seat.

3. in this case we supply the heat via particles at 1000^{o}C in proximity of the seat.

We highlight that the mesh of these simulations are constituted by 27000 cells and they require from 30 minutes to 1 hour to be carried out.

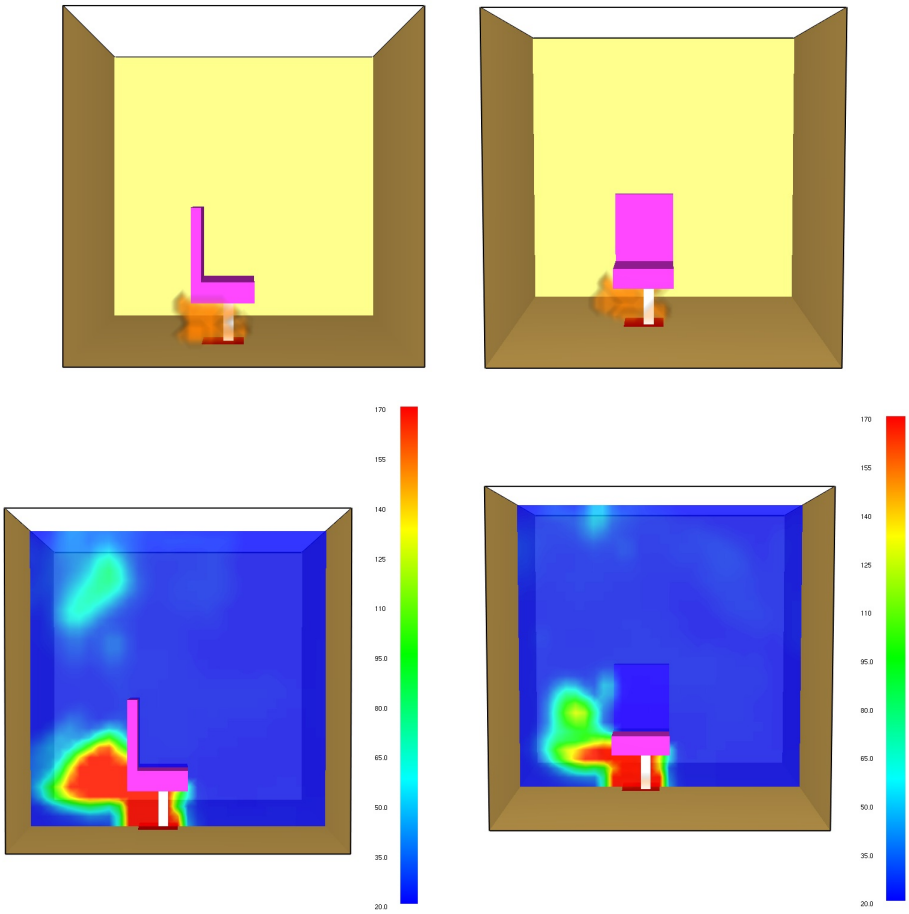


Figure 5.6: Case 2 at 60 seconds

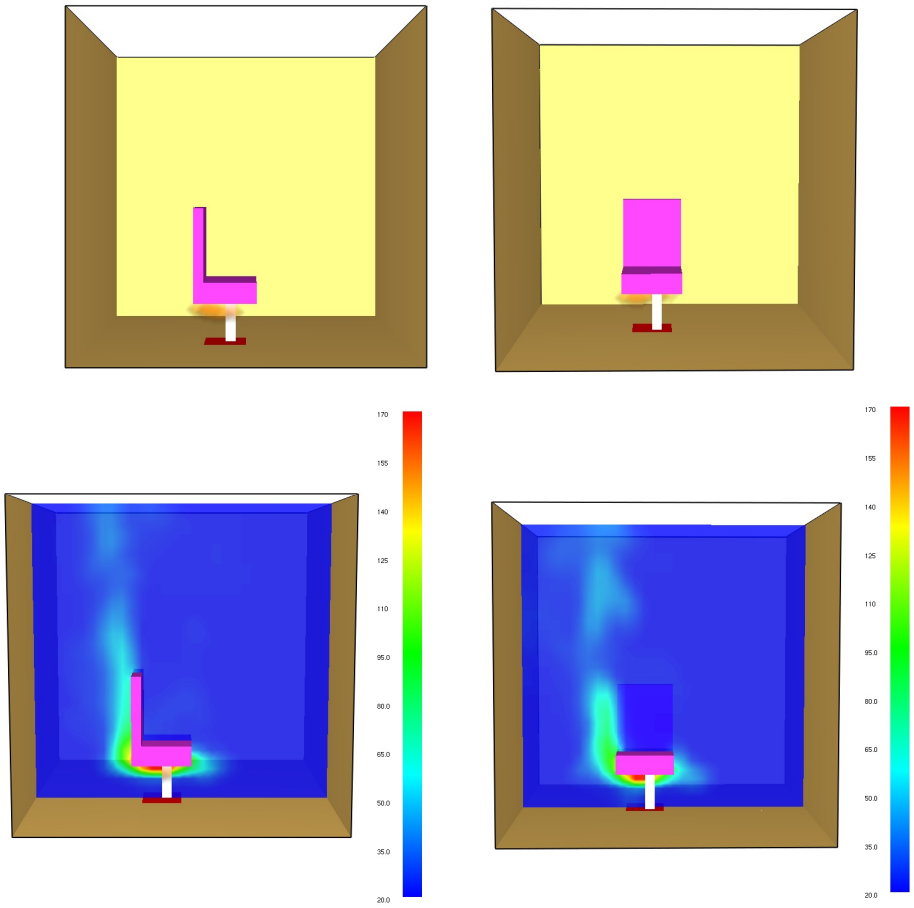


Figure 5.7: Case 2 at 300 seconds

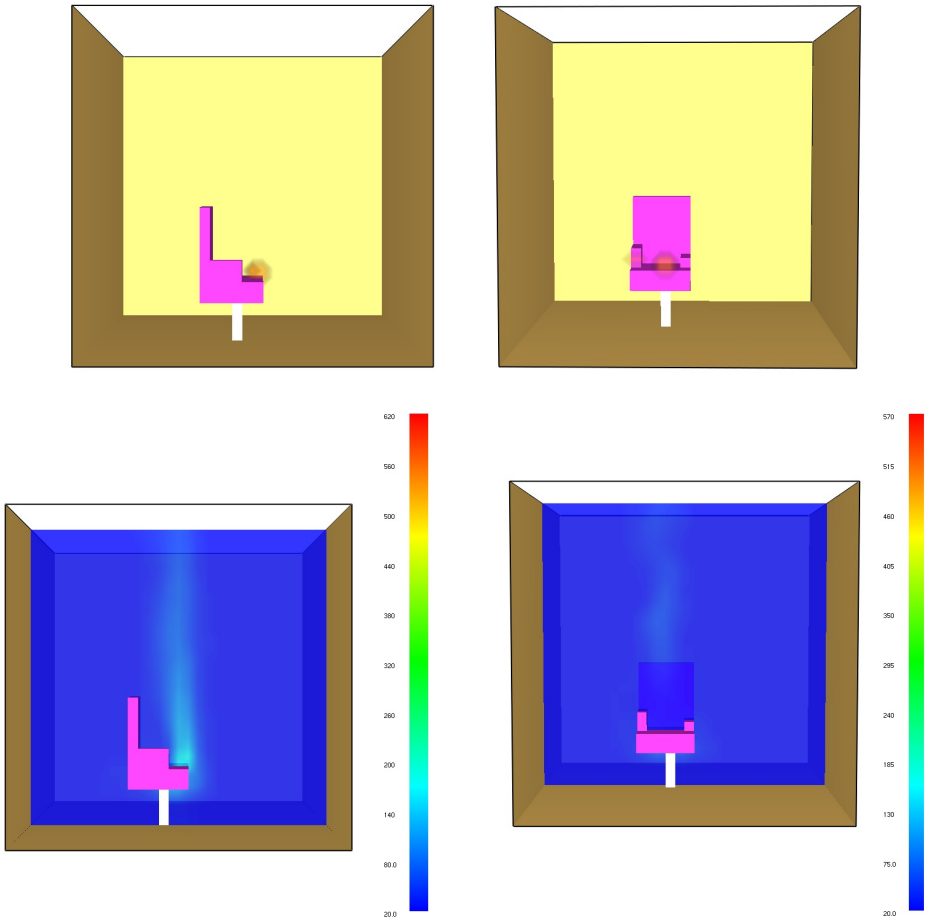


Figure 5.8: Case 3 at 5 seconds

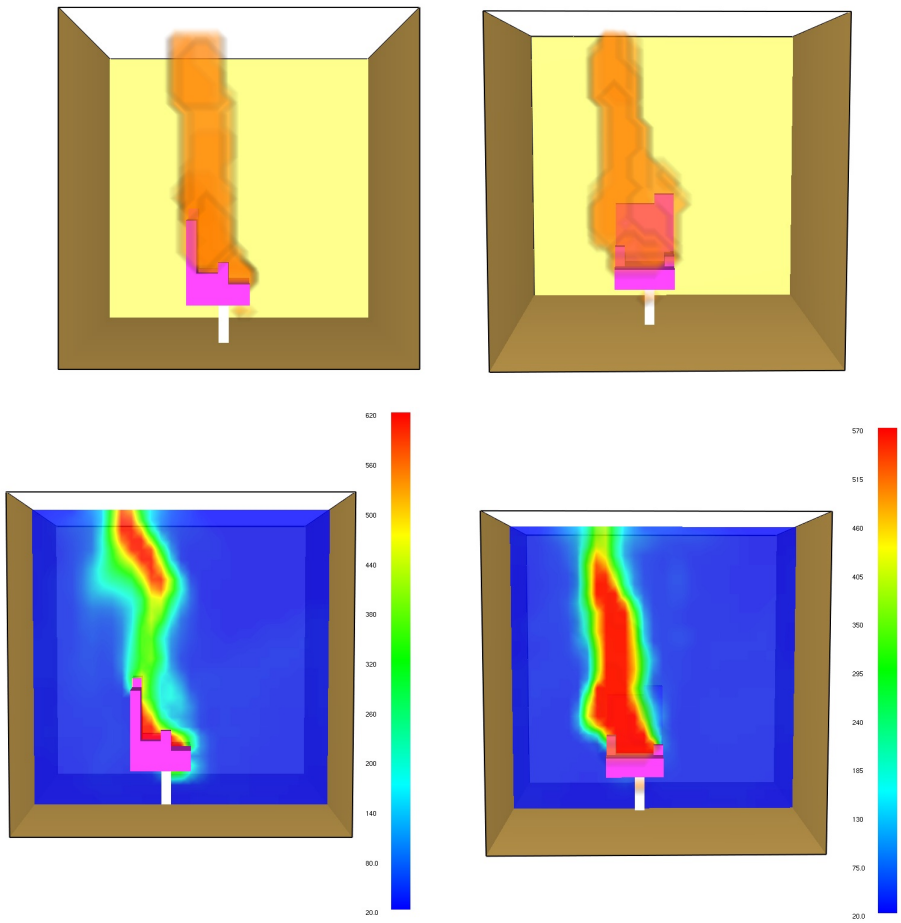


Figure 5.9: Case 3 at 120 seconds

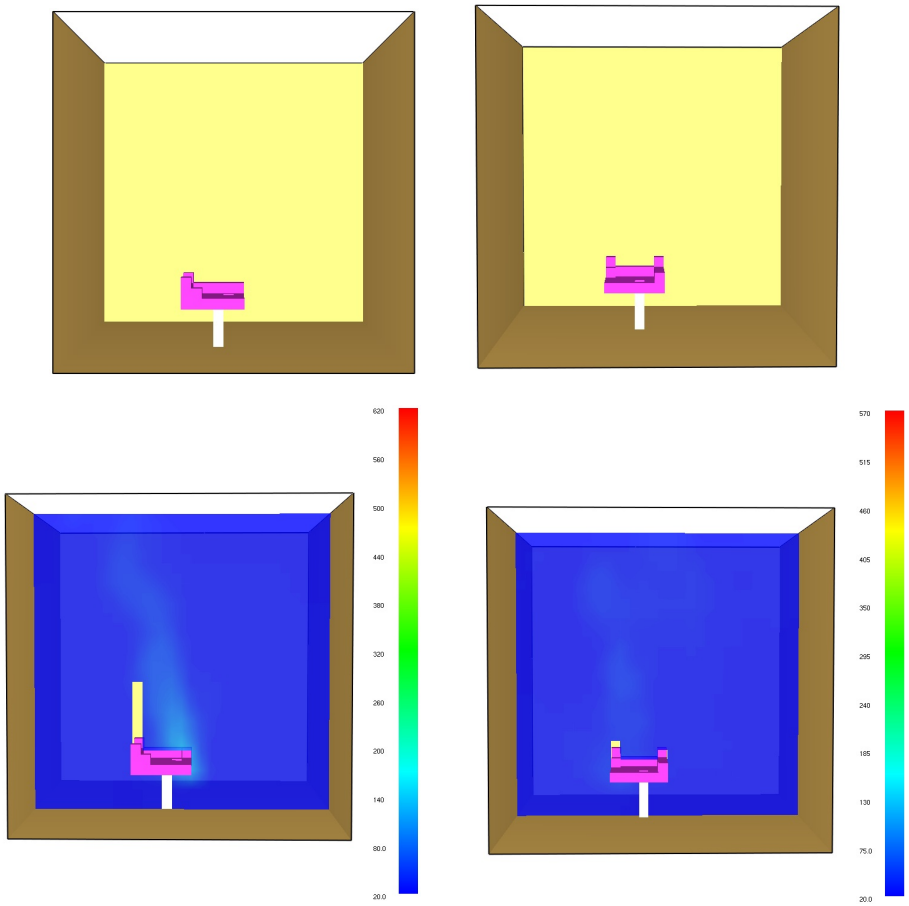


Figure 5.10: Case 3 at 250 seconds

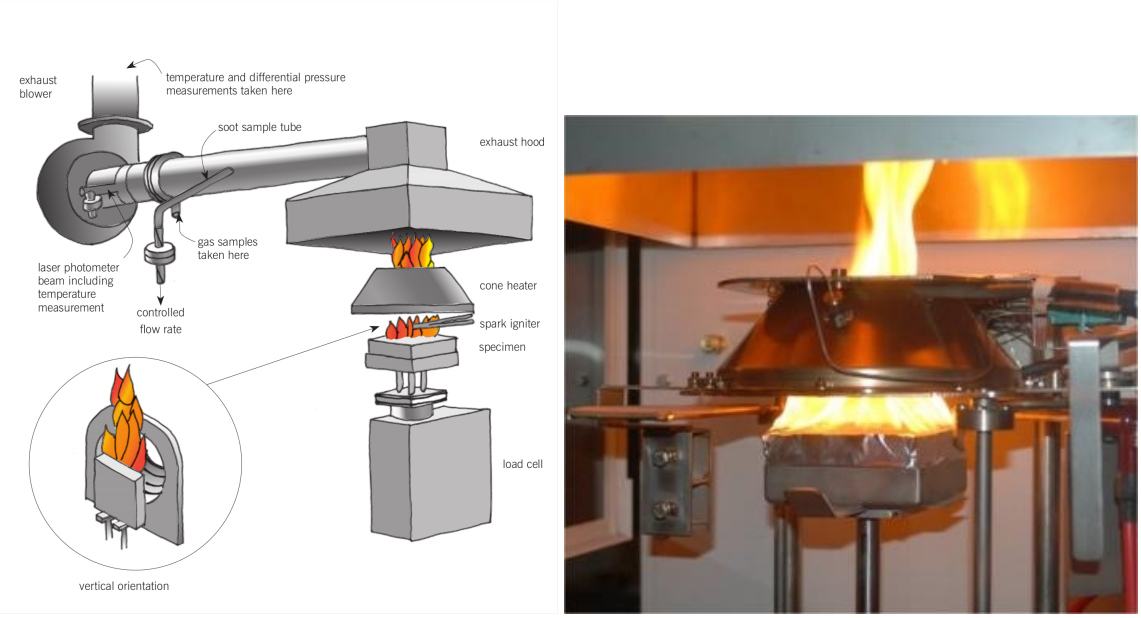


Figure 5.11: A sketch and a picture of a cone calorimeter

5.3 Cone Calorimeter

It is opportune to point out that, for modelling these fire scenarios properly, we have to know the thermal and chemical properties of the materials involved. For doing this, there is a specific instrument : "the cone calorimeter". A cone calorimeter is a modern device used to study the fire behaviour of small samples of various materials in condensed phase. It gathers data regarding the ignition time, mass loss, combustion products, heat release rate and other parameters associated with its burning properties. Device usually allows the fuel sample to be exposed to different heat fluxes over its surface. The principle for the measurement of the heat release rate is based on the Huggett's principle that the gross heat of combustion of any organic material is directly related to the amount of oxygen required for combustion. The cone calorimeter is the most significant bench scale instrument in the fire field of fire testing. Its name comes from the conical shape of the radiant heater that produces a nearly uniform heat flux over the surface of the sample under study.

5.3.1 The Data

We report the cone calorimeter data obtained in [1-2] (Andreini, Da Soghe, Facchini, Giusti) pertinent to a real train carriage.

Parameter	Seat	Floor	Curtain	Headrest	Wall	Ceiling
Heat of combustion (kJ/kg)	23633	18480	15510	13093	14640	20950
Heat of vaporization (kJ/kg)	6478	5000	10782	4348	5572	11463
Density (Kg/m^3)	95	1650	290	339	1652	867
Ignition temp. (^{o})	352	419	436	398	427	462
Heat capacity (kJ/(kgK))	0,345	1,92	8,33	8,32	1,26	1,24
Mass loss rate peak (g/s)	0,21	0,18	0,23	0,28	0,33	0,21
HRP	3,65	3,77	1,44	3,01	2,63	1,83

About this table, we know that the value relative to the seat and the headrest are due to cover plus foam. The floor and wall are made of some rubber and plastic material. We use these data as a reference for our simulations.

5.4 Some Likely Carriage Geometry

The next step described here, is that to simulate some plausible geometry.

5.4.1 The interior

This simulation involves the interior of a carriage in which the geometry is only plausible and is not aimed to reproduce some real model. The main characteristics are:

- the coach is 20 meters long, 3,2 meters large and 2,6 meters hight. The seat are allowed to burn and has the same characteristics of that in sec. 5.2.3., there are 20 rows with four seats each one. Each row has got a glass $0,8\text{m}\times1,4\text{m}$. We added two trunks made of PVC in the upper portion which have got the following properties:

Geometry:

Length (m)	width (m)	height(mm)
20	1,2	10

Thermal properties:

Density (kg/m^3)	Specific heat (kJ/(kg·K))	Conductivity (W/(m·K))	Emissivity
1380	1,4	0,187	0,95

Pyrolysis properties:

Heat of combustion (kJ/kg)	Heat of reaction (kJ/kg)	byproducts
$1{,}5\cdot10^4$	$4\cdot10^3$	100% reaction fuel

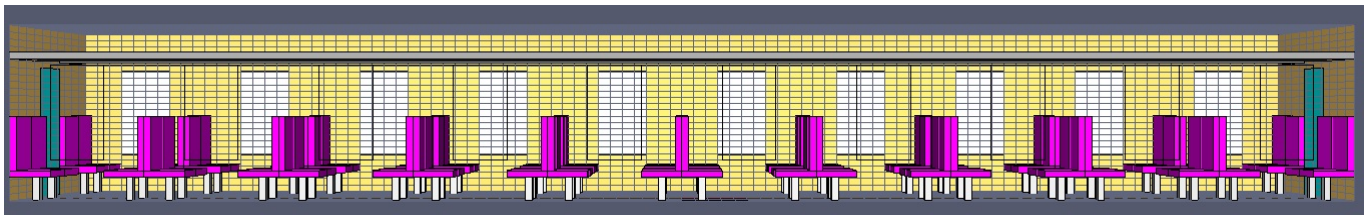
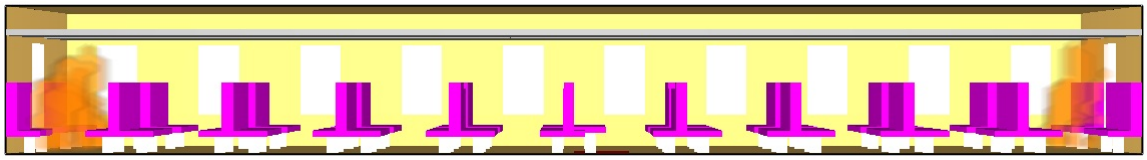


Figure 5.12: The model on PyroSim

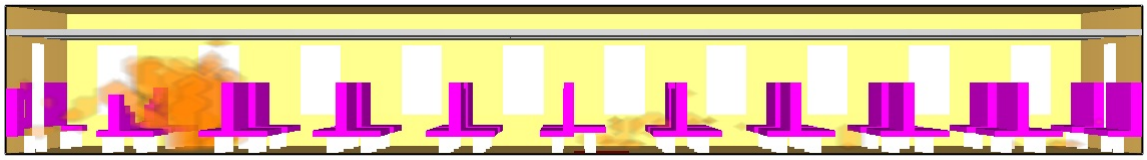
- On the extremity there are two doors modelled as open boundary conditions. The heat source is a 1 m^2 with a constant HRRPUA of 1000 W/m^2 positioned about in the middle and near the wall;
- the time of the simulation is 600 seconds, the number of mesh's nodes is 50000 and it is carried out in about 7 hours.

(a) At 5 seconds

(b) At 40 seconds

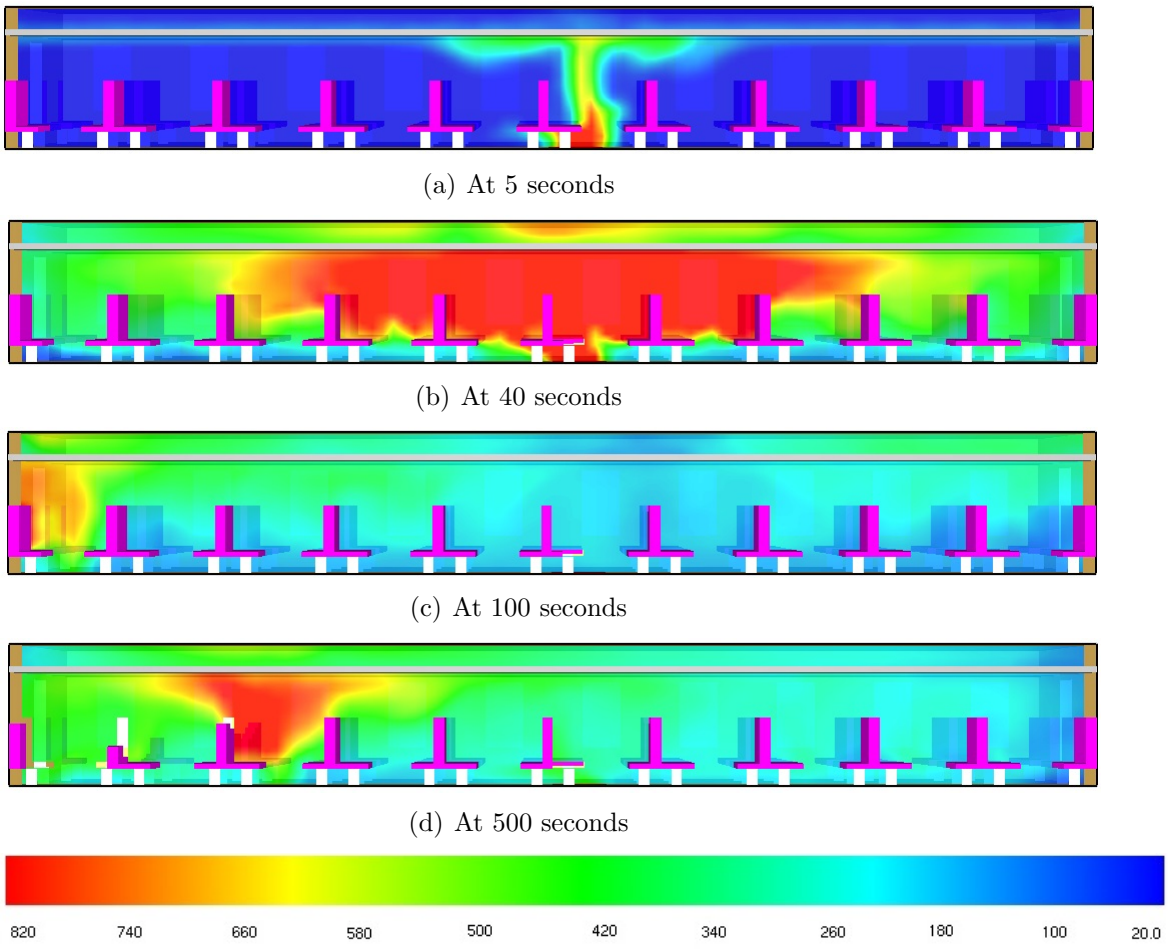


(c) At 100 seconds



(d) At 500 seconds

Figure 5.13: The fire dynamics



(a) At 5 seconds

(b) At 40 seconds

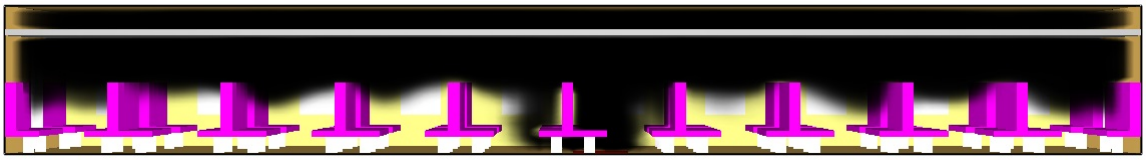
(c) At 100 seconds

(d) At 500 seconds

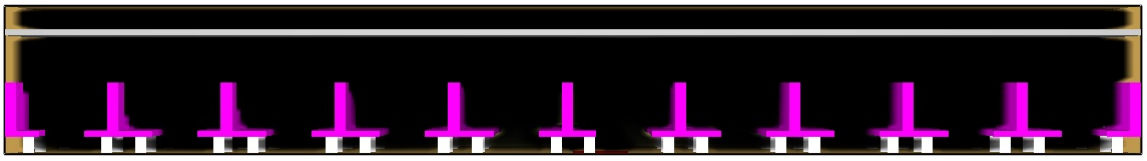
Figure 5.14: The temperature

The prominent result of this simulation is the fact that the fire moves towards the openings. Already at 70 seconds the flame has moved in proximity of the openings and it remain here until 400 seconds, when the amount of the material to burn decrease. The fire, thus come back to the middle where there is more material unburned. About the number of points of the mesh we have to point out that FDS does not allow to burn thin obstructions namely, the cells have to be of the same size of these obstructions. This point, especially on simulation with more object having different dimensions, must be bear in mind because it could result very demanding from the computational time point of view.

(a) At 5 seconds



(b) At 15 seconds



(c) At 30 seconds

Figure 5.15: The soot

Chapter 6

Train Convoy Simulations

In this chapter we treat our initial and principal object the: "Frecciarossa ETR1000".

6.1 The geometrical characteristics

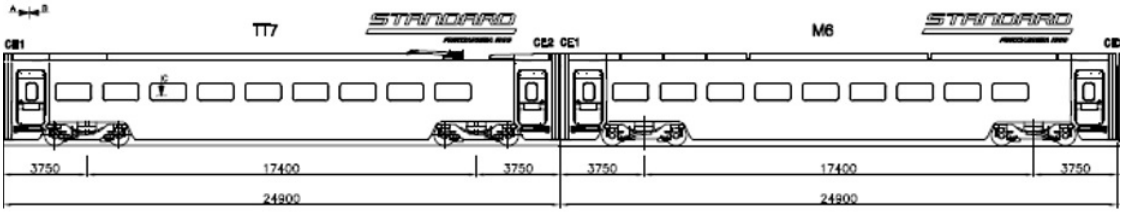
Thanks to Italferr, wich have given us all the needed information and design, we could model a fire spread in an Frecciarossa ETR1000. The geometry of the carriage is reported in figures 6.1.

6.2 Model with One Carriage

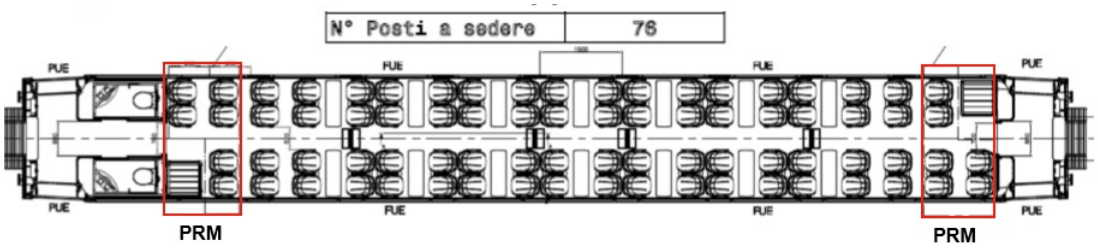
We started out reproducing only one carriage. We simulated the whole coach within a simple tunnel and in addition we modelled the thermal rupture of the glass. This is done through a thermocouple in proximity of the glass which, when reach a setted temperature it actives an hole in the exact position of the glass. In this first simulation we allow only the seat to burn. The pyrolysis properties of the seat are taken in conformity with [1-2]. The thermal properties of the concrete which constitutes the tunnel are:

Density (kg/m^3)	Specific heat (kJ/(kg·K))	Conductivity (W/(m·K))	Emissivity
2280	1,04	1,8	0,9

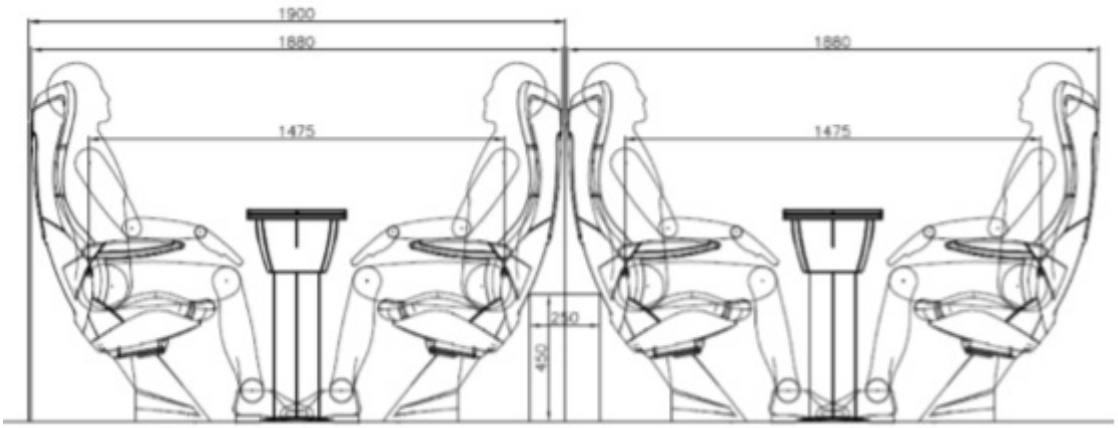
- The boundary condition about the tunnel's extremities are one open and the other supplies 31 m^3/s of air. The HRRPUA is equal to 500 W/m^2 on an area of 1 m^2 placed about in the middle;



(a) The outside



(b) The inside



(c) The seats

Figure 6.1: The carriage's dimensions

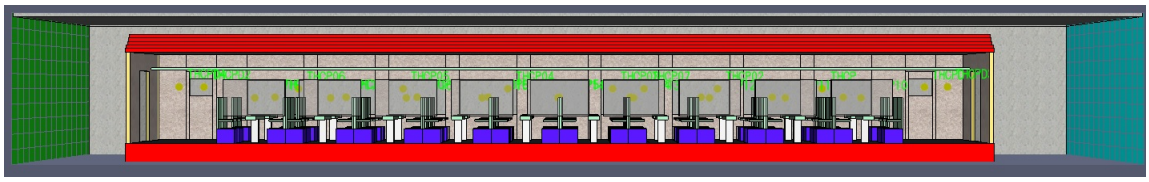
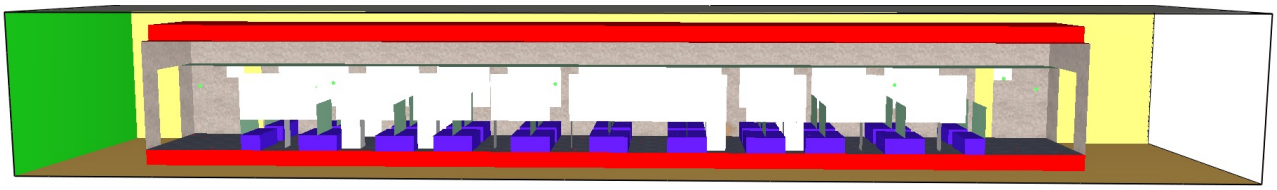
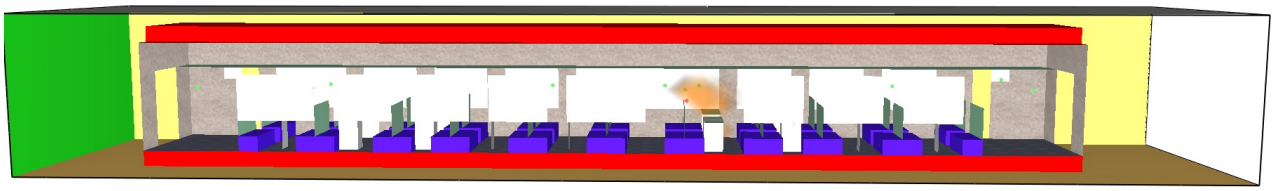


Figure 6.2: Pyrosym's model



(a) At 5 seconds



(b) At 900 seconds the winsows is exploded

(c) At 1200 seconds

Figure 6.3: Fire spreads

- The time simulated are 1200 second (20 minutes), the grid is made of 9000 cells and therefore in a couple of hours the simulation is carried out.

From this simple simulation we conclude that:

- If only the seat could burn, the flame's spread is inherently limited. In addition the HRRPUA resulted too low;

- Due to the inflow of air the soot attain to move uphill only when its concentration is elevated.

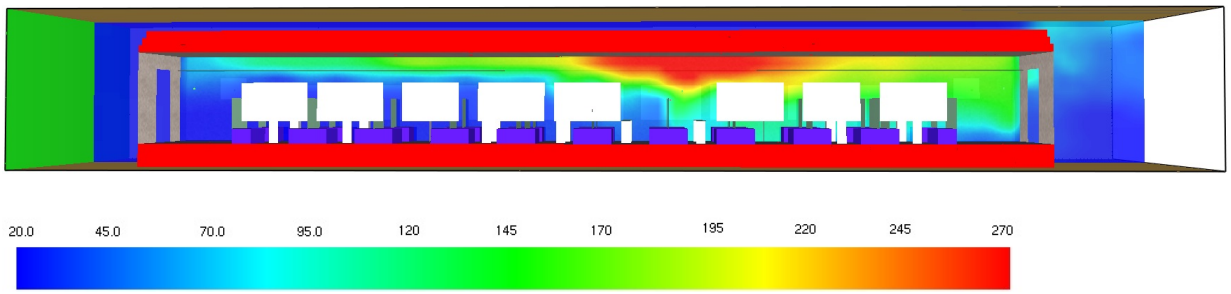
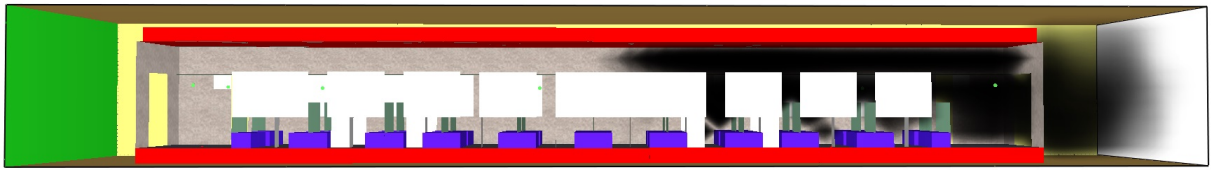
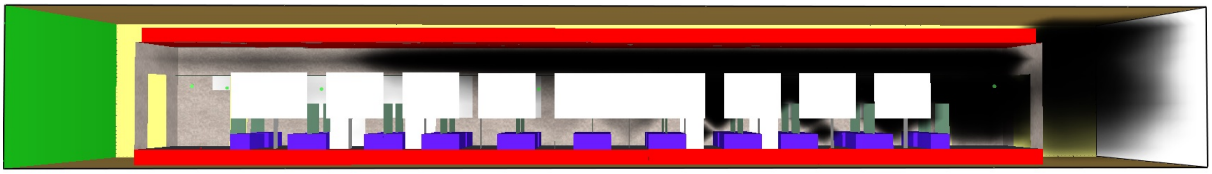


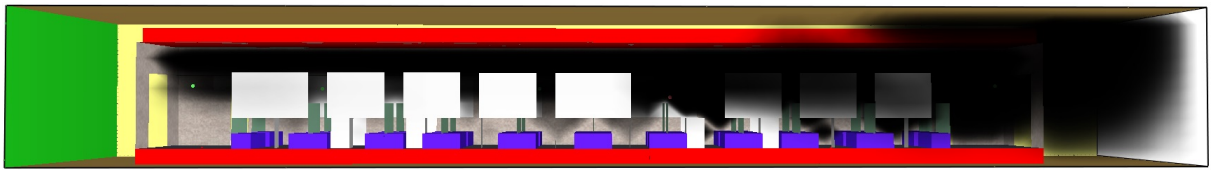
Figure 6.4: temperature at 1100 seconds in the middle of the seats



(a) At 30 seconds



(b) At 400 seconds



(c) At 1100 seconds

Figure 6.5: Soot spreads

6.3 A more realistic model

In order to get a more realistic model, we also allow the wall and floor to burn. This is done through a direct pyrolysis model in which the ignition temperature and HRRPUA are in according with [1-2] (Andreini, Da Soghe, Facchini, Giusti) who have achieved their results from cone calorimeter test:

	Ignition temperature (^{o}C)	HRRPUA (kW/m^2)
Floor	415	160
Wall	395	190

For the seats we use the indirect approach with the following data, always taken in according with [1-2]:

Material	Heat of combustion (kJ/kg)	Heat of reaction (kJ/kg)	byproducts
Fabric	$1{,}5{\cdot}10^4$	1000	100% reaction fuel
Foam	$2{,}5{\cdot}10^4$	1750	100% reaction fuel

FDS compel user to adopt a grid which has the same dimensions of the object that could burn. This must be bear in mind particularly for these kind of simulation where the ratio between the size of inflammable and non-flammable is elevated. In this simulation we set the windows to open at 600 ^{o}C.[1]. In addition we allow the exit doors to open after 60 seconds in order to simulate the condition in an emergency egress.[2] Therefore the prominent features of this simulation are:

- 3 carriages simulated within a tunnel having a cross section of 31 m^2;
- lateral doors open after 60 second on the platform size[3];
- the ignition source is not characterized by a constant HRRPUA but its trapezoidal whit a peak value of 2 MW/m^2, and leasts 600 second (10 minutes) as show in the graph:

[1] An exact temperature at which thermal fracturing in glass occur is not theoretically predictable because there are a lot of factors which determine it. The correct approach is therefore experimental and we take this value of reference from T.J.Shields,G.W.H.Silicock e S.K.Hassani The behaviour of Double Glazing in an Enclosure Fire

[2] Also in a tunnel, an ETR1000 maintains a speed of 300 Km/h at which it takes 70 seconds to a complete stop.

[3] In reality after 60 second also the doors between the carriages open. This will be useful later for further consideration.

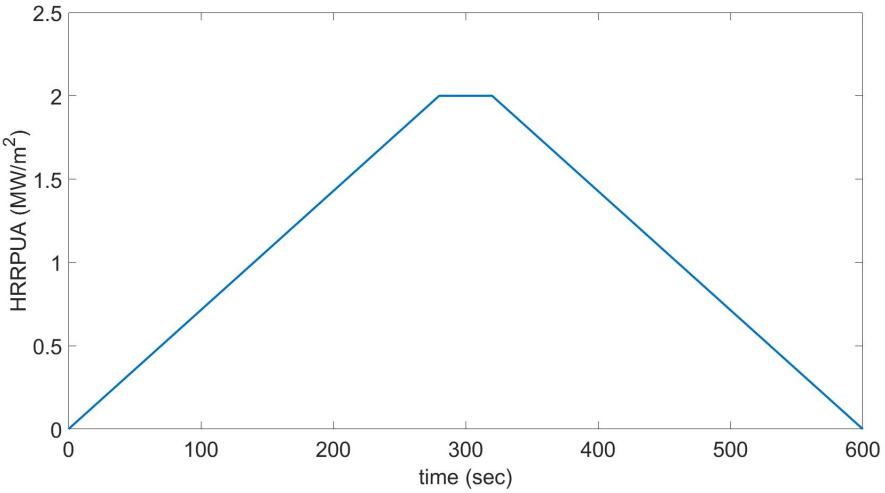


Figure 6.6: Graph of heat release rate per unit area

This is in order to simulate the real behaviour of a real ignition source. The ignition source is placed in the middle of the mid coach and has got an area equal to 0,30 m^2;

- the boundary conditions on the tunnel permit an air flux of 31 m^3/s which means that the air mean speed is of 1 m/s within the tunnel;
- we simulate 1200 seconds and the number of cells is equal to 780000. The simulation takes about four days to be carried out.

With this simulation we gain insight in the following point:

- The temperature is not excessive elevated. This is due to the fact that respect to the preceding simulations, we have had more mass to heat up (the concrete of the tunnel and more carriage);
- Due to what aforementioned there is not possibility of serious structural damage for the tunnel (spalling) because it occurs above 1000 ^oC;
- The most relevant danger is for the persons due to the toxic gas contained in the soot;
- We have seen that also with the doors between the carriages open, the fire remain limited in the carriage where he is spawned. Also the

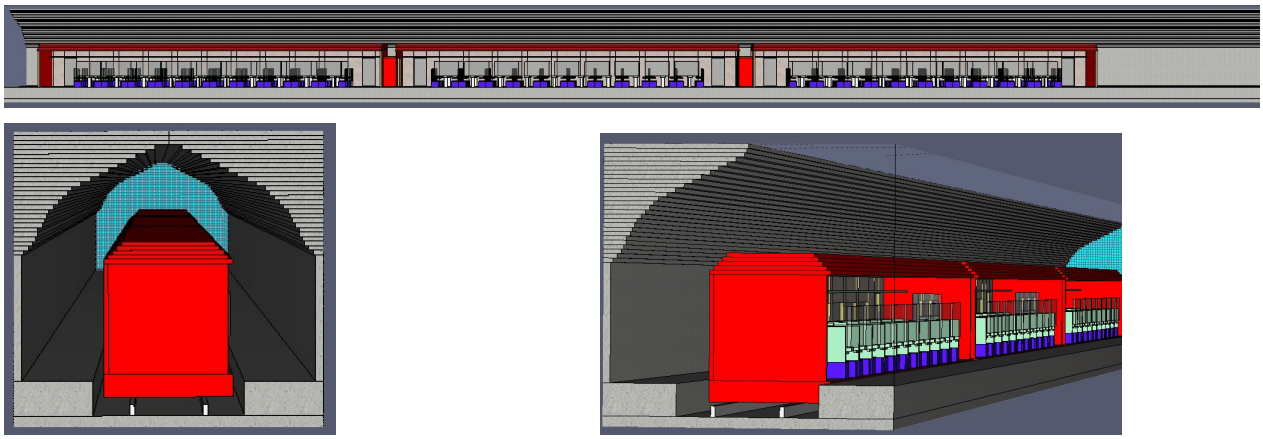
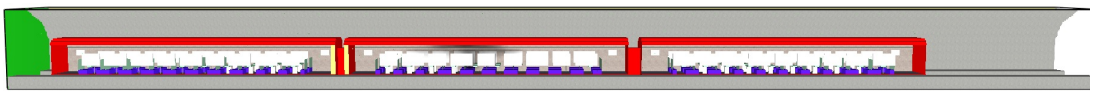
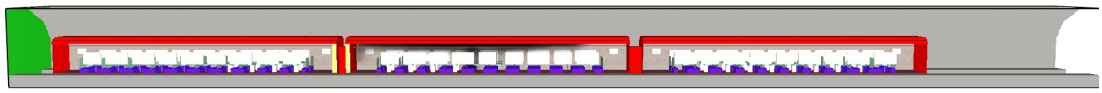


Figure 6.7: The model on PyroSim

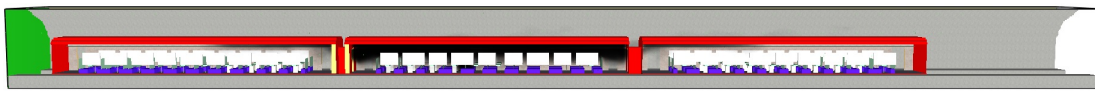
temperature in adjacent coaches is low. From this, we deduce that is necessary to have a fine grid in the carriage where fire is produced and we should take a coarser grid in the others carriage, because there the flames do not propagate. It should take advantage from this idea for saving time due to a lesser number of cells.



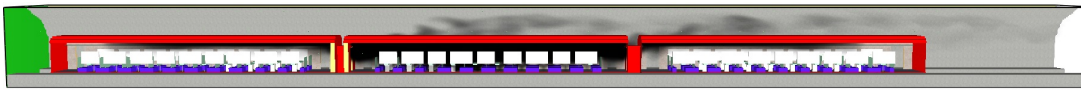
(a) At 20 seconds



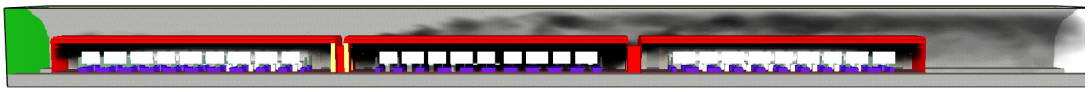
(b) At 50 seconds



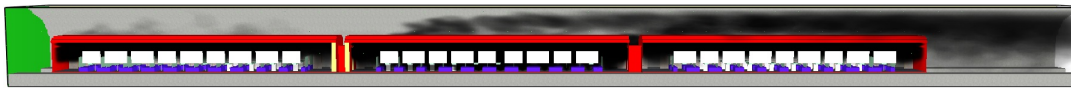
(c) At 120 seconds



(d) At 160 seconds



(e) At 220 seconds



(f) At 300 seconds

(g) At 500 seconds

(h) At 1000 seconds

Figure 6.8: The dynamics of soot

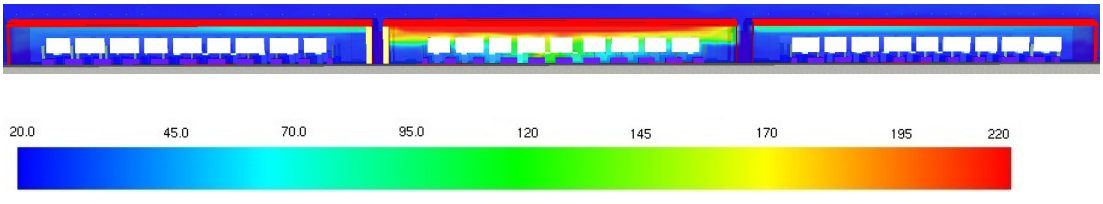


Figure 6.9: The peak temperature

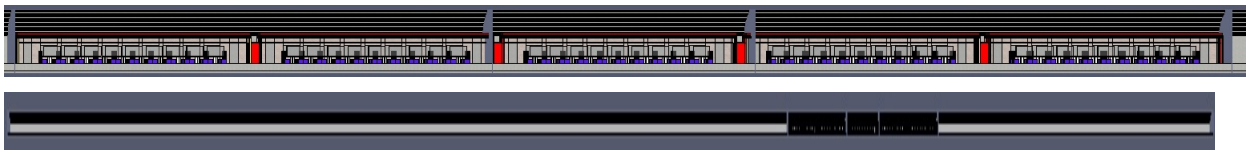


Figure 6.10: The model on PyroSim of the 5 carriages within 1 km long tunnel

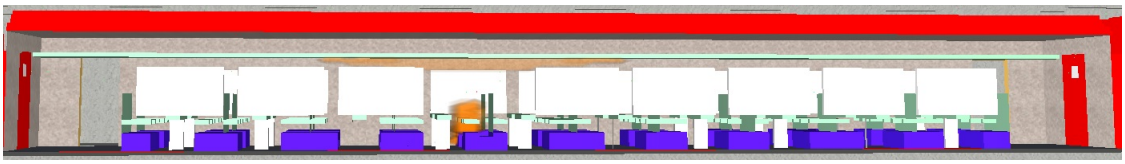
6.4 Accurate train convoy simulations

Taken advantage from what we learnt in the previous simulation, we simulate the fire of a train convoy composed by 5 carriages within a 1 km long tunnel. We accomplish this purpose using more meshes with different dimension of cells. Precisely we adopt 5 meshes:

- The mesh that contains the middle coach, where the fire is produce, has cells of 9×30×9.21 cm. This mesh includes also 1 meters of the adjacent carriages and is made of 475500 cells;
- Two symmetrical meshes abutted on the aforementioned that contains the other four carriages plus 1 meters of tunnel alone. This meshes are coarser and have 87500 cells each one of 27×49×18.43 cm;
- Other 2 meshes adjoined to the previous to complete the discretization. These meshes have cells of 27×90.13×18.43 cm and have not the same length because the train convoy is not in the middle of the tunnel, but 650 meters from one extreme and 220 meters from the other. The former is made of 472500 cells and the latter of 201250.

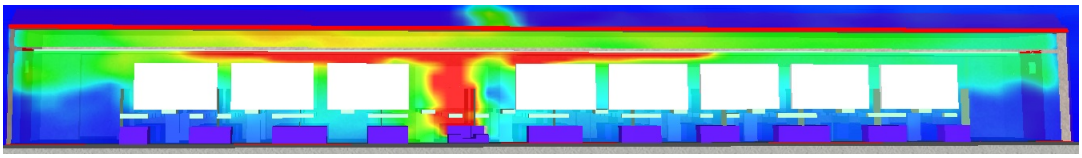
FDS compel the user to adopt different meshes that have the ratio between adjacent side equal to an integer number. In total we have got 1 417500 cells about twofold of the previous simulation. We can say that in this manner, we have swap details with size. This is legitimate because we have seen that an elevated number of nodes is necessary and valuable only where there are flames and combustion reactions. Respect to the last simulation we do not allow the doors between carriages to open, because in a real egress these doors remain closed, and this is revealed favourable for limiting the fire in the coach where it is spawned. In addition we study two separated scenarios: one in which there is the usually 1 m/s of average wind speed and another where the extremes are simply open which imply air at rest. Simulating 1200 seconds these kind of simulations require about one week (of real time) of computation.

(a) At 300 seconds when the the plateu is reached



(b) At 650 seconds when the windows is broken and the ignition source is quenched

(c) At 1150 seconds the fire is stable



(d) Indicative value of themperaturein the half of the carriage

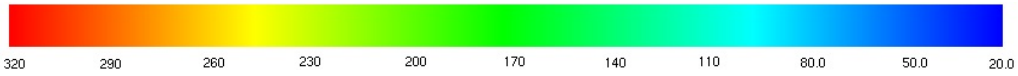


Figure 6.11: The coach where fire take place in scenario with the airflow

6.4.1 Scenario with the airflow

A flux of 31 m^3/s assure on a 31 m^2 of tunnel frontal section an average speed equal to 1 m/s. This value could be attain in presence of a normal wind, if this is in the longitudinal direction, or in presence of a forced convection (which in long tunnel is very frequent). Except for persons in the middle coach, the principal threat is not the temperature but the soot. How easily attended, due to the presence of the airflow, the soot is pushed out. Within the soot the harmfuller species is the carbon monoxide. How reported in chapter 2, only 667 ppm are extremely dangerous, and we take as dangerous an exposure above 100 ppm for more then 10 minutes.[4] The data about

[4]World Health Organization recommendations

of the CO concentration (kg_{CO}/kg_{air}) in the proximity of the door and the platform are reported.

A possible egress strategy

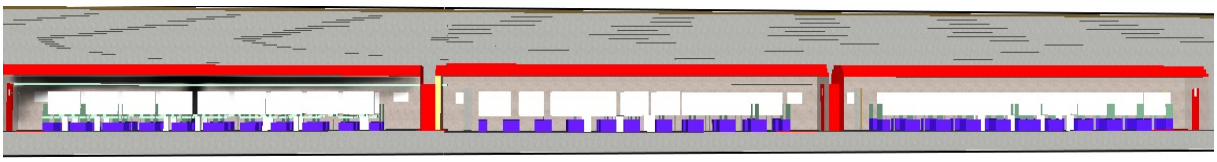
We have seen that the main danger is the noxious gas in the soot. The soot reaches out of the convoy (on the platform) a maximum temperature of 42 ^oC which is not too high. Due to airflow the first and second carriages are not invested by the soot. Absolutely, the third carriage, where the the fire is generated, has to be evacuated for first[5]. For persons in this coach, it is convenient to move upwind because they are already exposed to the soot and in this way they have a shorter distance to travel for arriving in a zone with fresh air. Persons in carriage one and two are protected by any danger because both the soot and the fire are not able to reach them. Therefore they have no urgency and should evacuate with order and calm. For subjects in the fourth and fifth carriages, we could devise an egress strategy that take into account their health conditions and bodily capacities, namely :

- Persons who have a normal mobility: these persons are able to evacuate without difficulties. After the doors open, the soot takes at least 50 seconds to reach the fourth carriage. People, thus, should have enough time to get off the train and move in the same direction of the wind. In addition, taking into consideration that the speed of the soot is about 1 m/s and that people move faster that it do[6] , if they are in advantage the soot never get to reach them. Through the data of CO concentration and the smokeview's results, we can state that if people evacuate by two minutes after the train has made a complete stop they will not incur in serious risk. In the worst case that people getting off and find themselves in the middle of the smoke, they should go through it in a few seconds because the gas concentration is not enough to provoke any effects;

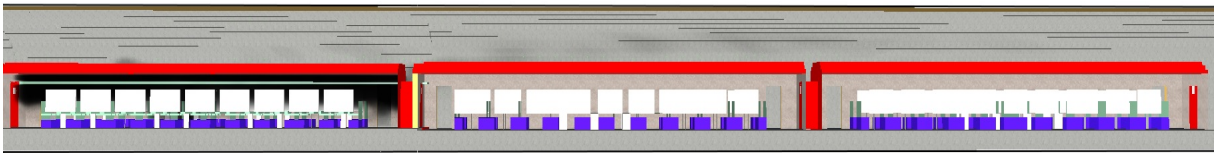
- Persons who have an impaired mobility: persons who cannot walk normally, for instance the elderly, should evacuate for first or they could stay in the carriage until the fire is quenched by firefighters, in fact we have seen that for 20 minutes at least (the time simulated) the fire does not spread in the other carriage;

[5]fig.6.15 show the extremely high value of CO.

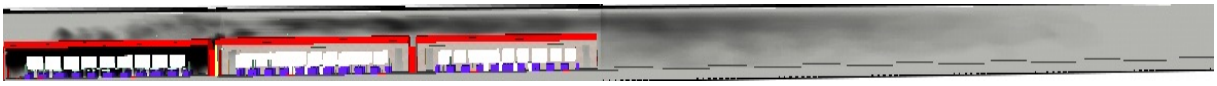
[6]The preferred walking speed at which humans chose to walk in normal condition felling comfortable is about 1,4 m/s



(a) At 50 seconds



(b) At 110 seconds



(c) At 200 seconds

(d) At 300 seconds

(e) At 500 seconds

(f) At 700 seconds

(g) At 1000 seconds

(h) A wider view

Figure 6.12: The dynamics of Soot with airflow

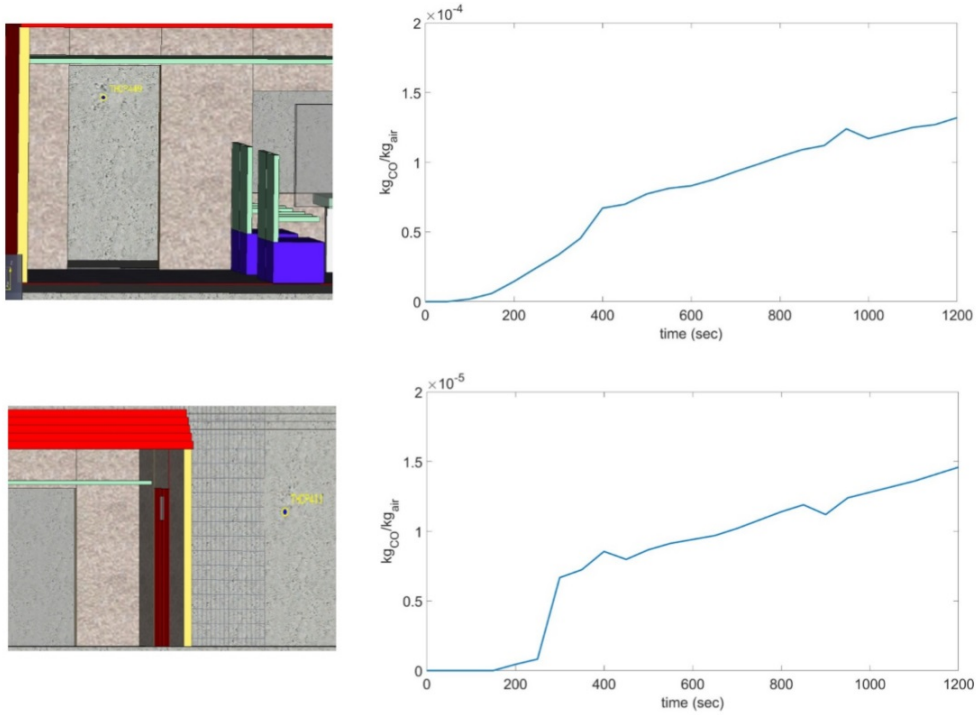
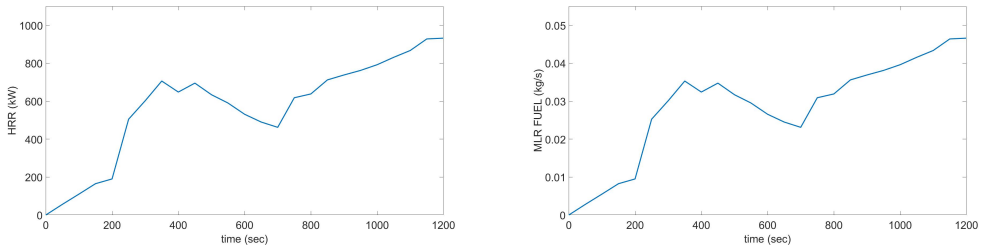


Figure 6.13: Carbon monoxide concentration with airflow



(a) HRR values (b) FUEL burnt

Figure 6.14: Scenario with airflow

We evaluate how much time the evacuation should take before that a person loses consciousness due to the concentration of toxic gas. For this purpose we use the Stewart's formula[7]:

$$t = \frac{COHb\%}{3,317 \cdot 10^{-}5 \cdot (ppm_{CO})^{1,036} \cdot V} \tag{6.1}$$

where

- t: time express in minutes necessary to a human body for having a given COHb%;
- COHb%: percentage of carboxyhemoglobin in blood flow. We take this value equal to 30 namely the value which persons risk of fainting;
- ppm$_{CO}$: CO air concentration express in parts-per-million. We take the highest value detected on the platform (at an high of 1.8 meters) i.e. 150 ppm ;
- V : average respiratory rate express in l/min. We take 20 l/min namely the value in the middle of doing some physical activity.

all these data give us an underestimated value, in favour of safety:

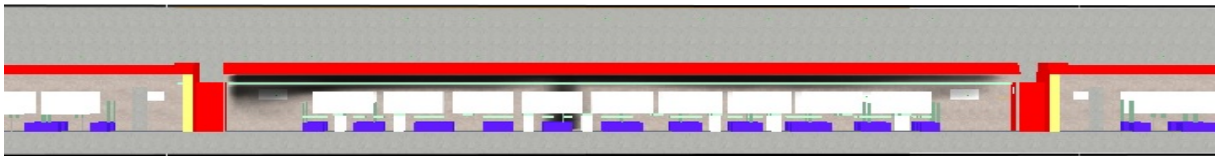
$$t = \frac{30}{3,317 \cdot 10^{-}5 \cdot (150)^{1,036} \cdot 20} = 251,7 \cong 4h$$

From this we deduce that the people have got enough time to evacuate or to be rescued if they are not able to move.

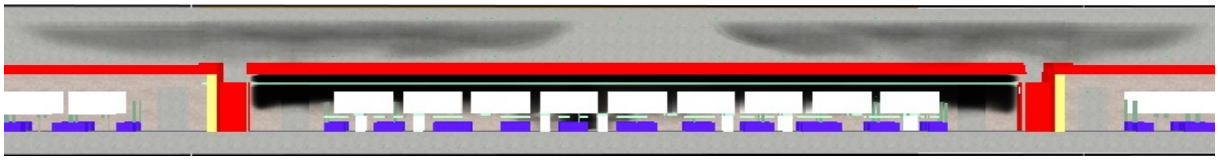
6.4.2 Scenario without airflow

In this scenario, there is not any forced flow within the tunnel. The motion of air is only convective, namely, generated by buoyancy force due to the difference of density which is in turn due to the difference of temperature provoked by the fire. How derives from data the velocity of the soot is of 0,3 m/s and the scenario is almost symmetric namely there is the same flow's development on backward and forward. Furthermore due to lack of any forced motion, the soot move forward remaining in the upper part of the tunnel and starts to descend 200 meters far from the convoy. Obviously, except for the ventilation, all the other parameters remain the same. Another consideration is that both the temperature and the gas concentration in the soot are lower.

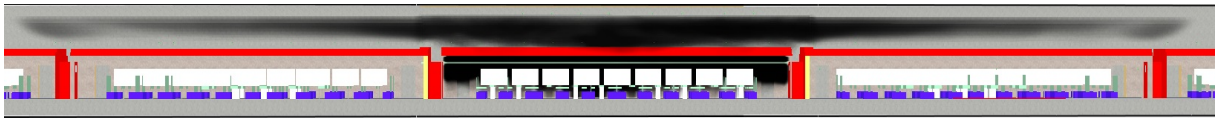
[7]Peterson JE e Stewart RD,1970



(a) At 50 seconds



(b) At 110 seconds



(c) At 200 seconds

(d) At 300 seconds

(e) At 500 seconds

(f) At 700 seconds

(g) At 1000 seconds

Figure 6.15: The dynamics of soot without airflow

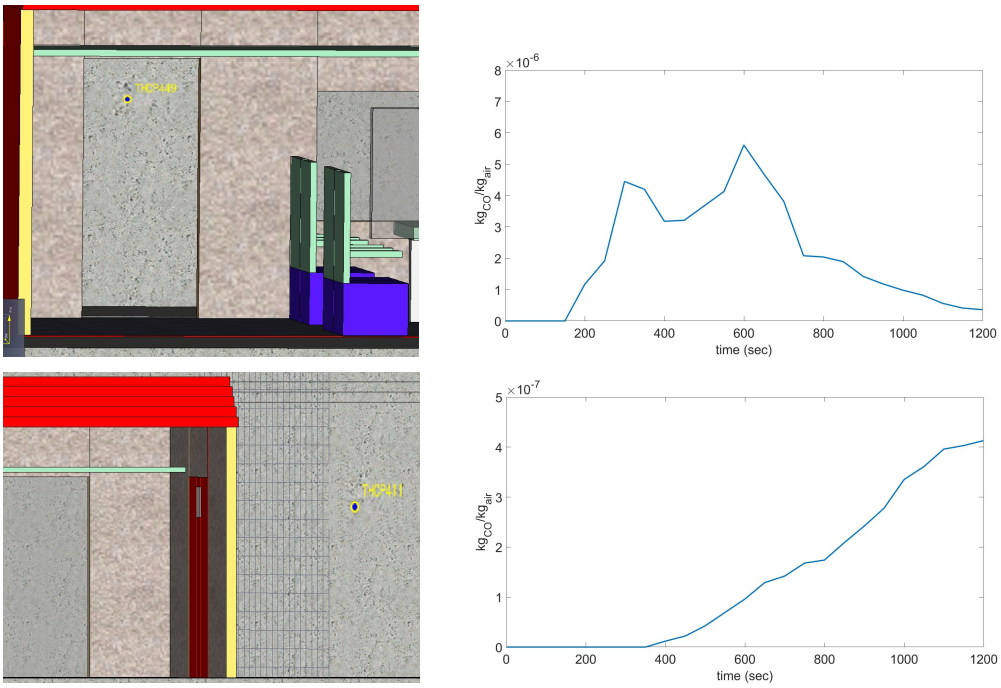
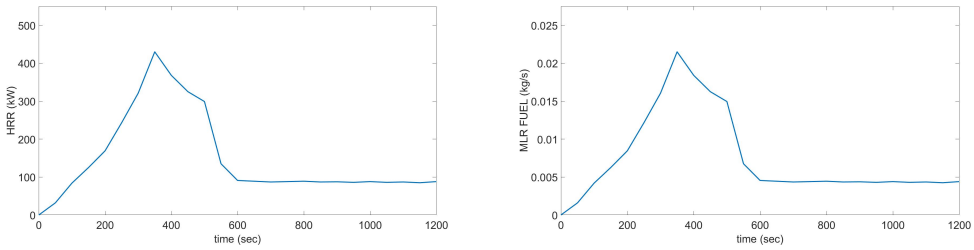


Figure 6.16: Carbon monoxide concentration without airflow



(a) HRR values (b) FUEL burnt

Figure 6.17: Scenario with airflow

A possible egress strategy

Also in this case the worst situation is for the mid coach where the fire is generated. Due to the lack of longitudinal ventilation the fire spread less and both the noxious species and the temperature are lower. Thus, this scenario is less severe than previous. The conditions for the first, second, fourth and fifth coaches are symmetrical. Second and fourth coaches commence to be invested by the smoke after 30 seconds that the door open and are completely reached by the soot after 250 seconds. This interval should be enough for the major part of people to evacuate and in addition the smoke tend to rise, thus under 2 meters the air is relatively clean. As a rule the third carriage must be evacuated for first. People in the first and second cars should egress forwards and those in the fourth and fifth cars should egress backwards. We also know that the smoke move forward with a speed of 0.3 m/s, therefore people could move easily faster than it do. As showed by the data, on the platform, the level of CO is under 100 ppm.

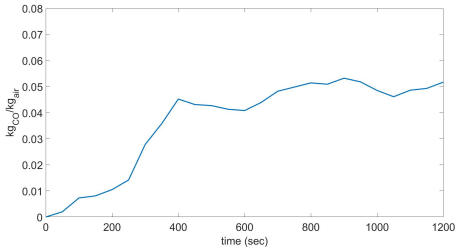
6.4.3 A comparison between the two scenarios

The phenomenology of these two scenario is quite different and all is due to the ventilation which in the first scenario permits a more growth of the fire. This should be corroborated by the data of concentration and temperature within the third coach fig. 6.15 and fig. 6.16. So we must wonder what is the cause of this behaviour. In my personal opinion, an explanation is the following: We know that the combustion is a chemical reaction with reagents the "fuel" and oxygen and the "soot'' as product. Every reaction, in a close system, tend to reach a dynamics equilibrium, and when it is reached there are not any variations in concentration of both reagents and products.[8] But our system is open and therefore it can exchange matter with the surrounding. In particular, it can discharge the soot (namely the products), and thus if there is a ventilation as it is in the first scenario, the discharge is very efficient and the equilibrium is never reached. A little more formal argumentation could be done in terms of equilibrium constant[9] and Le Châtelier's principle[10]. At the equilibrium the ratio between concentration of products and reactants will be equal to the equilibrium constant. However if we perturb the equilibria, in this case by means of ventilation we remove products from the system, the ratio between products and reagents concentration diminishes and the only way to reach the value of the constant equilibrium again is through the production of other products. In this manner the combustion is continually sustained and improved. In the second scenario, the discharge is natural, and it does not result as in the first. Therefore we can conclude that the ventilation is an extremely important parameter that influences the whole development of the fire both in terms of intensity and in terms of duration.

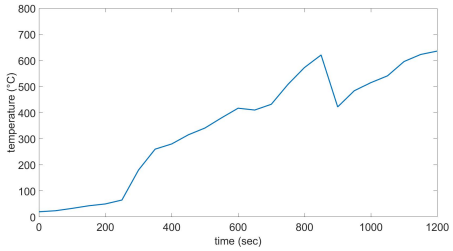
[8] Of course the exact amount of reagents and products depends on the temperature but this is a qualitative reasoning.

[9] The definition of constant equilibrium could be looked up on chapter 3.

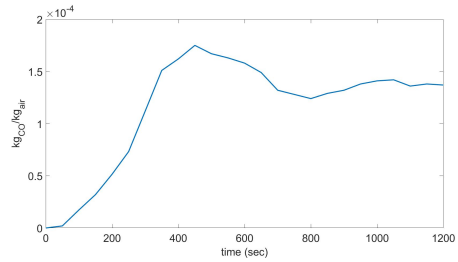
[10] Le Châtelier's principle stated that: When any system at equilibrium is subjected to change in concentration, temperature, volume, or pressure, then the system readjust itself to counteract the effect of the applied change and a new equilibrium is established.



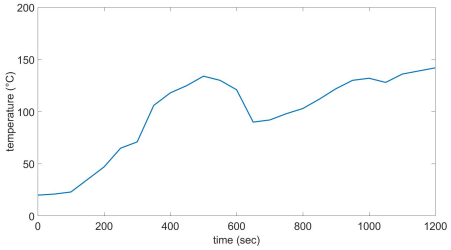
(a) CO concentration with airflow



(b) Temperature with airflow



(c) CO concentration with no airflow



(d) Temperature with no airflow

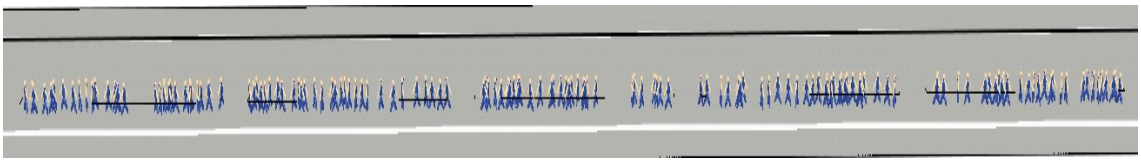
Figure 6.18: A comparison between concentration and temperature within the middle carriage in the two scenarios

6.5 EVAC

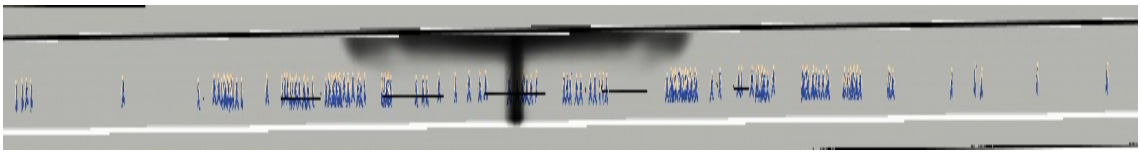
Evac is an evacuation simulation module for FDS developed and maintained by VTT Technical Research Centre of Finland, which is fully embedded in Fire Dynamics Simulator (FDS) .

6.5.1 The underlying theory

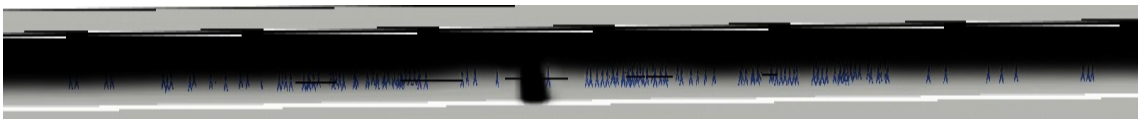
EVAC exploits a planar model to simulates persons as rigid disk characterized by a mass and a moment of inertia. The different value of mass and moment of inertia allows to distinguish the population in man, woman, elderlies and children. This subject are solicited by an ambient force due to the interaction among the subject and the surrounding and a social force that is due to parameters as the concentration of smoke and visibility. Each kind of subject has got in addition a maximum speed. The principal parameters that we can model are the amount of each kind of subject, their initial position and the probability that they know where the exits are.



(a) At the beginning



(b) After 120 secondos



(c) After 500 seconds

Figure 6.19: EVAC applied to a tunnel

6.5.2 Some Considerations

Here we report some consideration about the performance of EVAC. We have seen that this software is adapted to simulate the behaviour of people during an egress from a big environment with only few obstacles. It could managed a large number of persons (over 100) but the size of the structure which hosts them, should be large and empty. I have tried unsuccessfully to simulate an evacuation of a convoy. The problem which i found is that the people hinder each other and they get stuck within the coaches. Therefore i tried to simulate only the evacuation of tunnel allowing the people to stay only on platform. The platform has revealed itself as narrow passage anyway, in fact peoples hamper each other also in this case. We could state that to simulate the behaviour of persons in a complex general geometry is very difficult, in fact VTT suggests to carry out a statistical analysis by means of more simulations. The clues and models behind this software are great anyway. Here we report some pictures of a tunnel evacuation, where we can see the improper behaviour of persons.

We have seen that EVAC is not very responsive and in this simulation people does not evacuate properly. Surely a development of the software will bring about a more realistic dynamics of people and also EVAC will become an evaluable tools in fire analysis as FDS it is.

Conclusions

The present thesis project shows that FDS is appropriate to simulate also complex geometries with self-propagating fires such as train convoy in a tunnel. The results of simulations in simplified geometries, have highlighted that fires tend to spread towards the openings. In addition, we have shown that in the simulation of train cars, the environment is extremely important in determining the fire dynamics even inside a car and therefore is mandatory to simulate also the surrounding and not only the car interior. Most precious results are obtained relative to the whole convoy within the tunnel 1 km long. Analyzing two scenarios, one with and other without ventilation, we have seen that this factor strongly influences the fire intensity. With ventilation, the fire is stronger and therefore along with an higher temperature, there is a greater production of toxic gas. Furthermore the smoke moves only in the wind direction because he is not able to move upwind, however the soot will occupy the whole tunnel cross section. On the opposite, without the ventilation, concentration of harmful gas is lower and together with the fact that soot tends to rise, on the platform we have less than 100 ppm of CO. We can state that for the tunnel, in the case of passenger train, there is no risk for its structural integrity because the temperature in close proximity of the ceiling are lower than 300 ^{o}C. We have suggested an egress strategy on both the scenarios and taking into account all the results, we can claim that this kind of fires are manageable.

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