**Wildland-Urban Interface Virtual Essays Workbench**

**WUIVIEW**

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PBD Virtual Lab
WUIVIEW

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Civil Protection

# Technical Note TN 6.1
# Main specifications of CFD codes for WUIVIEW activities

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**Abstract**

CFD simulations will be the core activity of the WUVIEW performance based fire safety analysis. The purpose of this document is to provide WUIVIEW partners with a general overview of the CFD codes to be used in the Action. The general simulation framework is described, particularly highlighting data inputs and scenario description requirements, to be developed in subsequent WUIVIEW WPs. This TN provides the technical foundations and main specifications of the databases to be designed within the WUIVIEW working program (ongoing action by UPC).

*(1) Draft / Final*
*(2) Public / Restricted / Internal*

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# 1. Introduction

CFD simulations will be the core activity of the WUVIEW performance based fire safety analysis. We will rely on a well-established fire protection engineering methodology (Performance-Based Design, PBD), which is based on cutting-edge fire simulations techniques, to get insights on the response to fire of typical building systems and materials. Models used will be of CFD (Computational Fluid Dynamics) nature, which deliver information on key variables for risk management (temperatures, heat and smoke exposure on people and assets, etc.).

The purpose of this document is to provide WUIVIEW partners with a general overview of the CFD codes to be used in the Action. The general simulation framework will be described, particularly highlighting data inputs and scenario description requirements, to be developed in subsequent WUIVIEW WPs.

# 2. General overview to CFD codes: FDS and FLUENT

Computational Fluid Dynamics (CFD) is used to solve fluid dynamics problems that cannot be solved analytically. CFD takes advantage of the ever increasing computing power available nowadays and powerful numerical schemes that allow finding approximate solutions to systems of partial differential equations. This approach has made possible the calculation of mass, heat and momentum fluxes that would otherwise be impossible to estimate. These properties have awarded CFD tools a privileged position in science and engineering, and they are currently employed in a wide variety of fields including hydrodynamics, aerodynamics, combustion and heat transfer frameworks.

Due to its nature, CFD constitutes a very powerful tool in fire safety science and engineering, where most problems involve the analysis of physical and chemical phenomena that interact with each other in a wide range of spatial and temporal scales. Among the broad variety of available codes, we choose to use FDS and FLUENT for the following reasons.

Fire Dynamics Simulator (FDS) is a large-eddy simulation (LES) code for low-speed flows, with an emphasis on smoke and heat transport from fires. It has been developed by the National Institute of Standards and Technology (NIST) of the Unites States Department of Commerce, in cooperation with VTT Technical Research Centre of Finland[1]. FDS is being actively developed and maintained at present. It is open-source, which has allowed substantial testing and validation by third parties. Currently, it is the most accepted standard in the international fire safety science and engineering community. It is widely employed to design building fire protection strategies and its use is recommended in several guides of Performance-Based Design (PBD).

FDS includes a fairly easy to use interface that facilitates defining parameters, running simulations and analyzing results without having to understand or compile the code. Furthermore, its open nature has promoted its coupling with more powerful graphical user interfaces that provide additional capabilities for the definition of simulation geometries. Some examples of such interfaces, which we may use, are BlenderFDS and PyroSim. BlenderFDS is a plugin for Blender, a popular open-source 3D computer graphics software. Pyrosim is proprietary software developed by Thunderhead Engineering specifically as an FDS accessory tool.

On the other hand, ANSYS Fluent is a commercial CFD program developed for fluid dynamics analysis. It is part of a larger suite of numerical engineering tools which include, among others, structural analysis and electronics. It was firstly released in the 1970s and it has since then evolved to exploit the ever increasing computing capacity. At present, it is widely used in the aerospace and automotive industries.

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[1] FDS official webpage: https://pages.nist.gov/fds-smv/

# 3. Working with FDS

The general workflow in FDS is based on the following steps: firstly, the user must define a simulation scenario. Along with the geometry, thermal properties can be assigned to all existing objects. Additionally, fires can be introduced and parametrized following a variety of approaches that will be discussed below. This scenario is accompanied by a set of numerical parameters that will control the simulation. Finally, the user must specify which output variables are to be recorded in which location and at which frequency.

## 3.1. Geometry, materials and computational domain

FDS allows the definition of objects (OBSTs) that are made of surfaces (SURFs), which in turn can be composed of materials (MATLs). Each of these components can have their own properties, which may affect the overall behavior of every specific instance existing in the domain. For example, a wall would be an object whose faces can be made of the same or different types of surface. In the case of a house façade, the outer and inner faces will be different. This can be accounted for in FDS.

From the thermal point of view, object surfaces can be considered adiabatic or they can be populated with thermal properties: density (kg/m$^3$), conductivity (W·m$^{-1}$·K$^{-1}$), emissivity (-) and specific heat (kJ·kg$^{-1}$·K$^{-1}$). Conductivity and specific heat can be defined as a function of temperature, whereas density and emissivity must take constant values.

Once the scenario geometry has been defined, all objects must be included in a computational domain which definition is of utmost importance. Decisions in the design of the computational domain will affect simulation convergence, validity of results and computation time. In order to keep computation times affordable, usually a trade-off must be found between domain size, simulation length and level of detail.

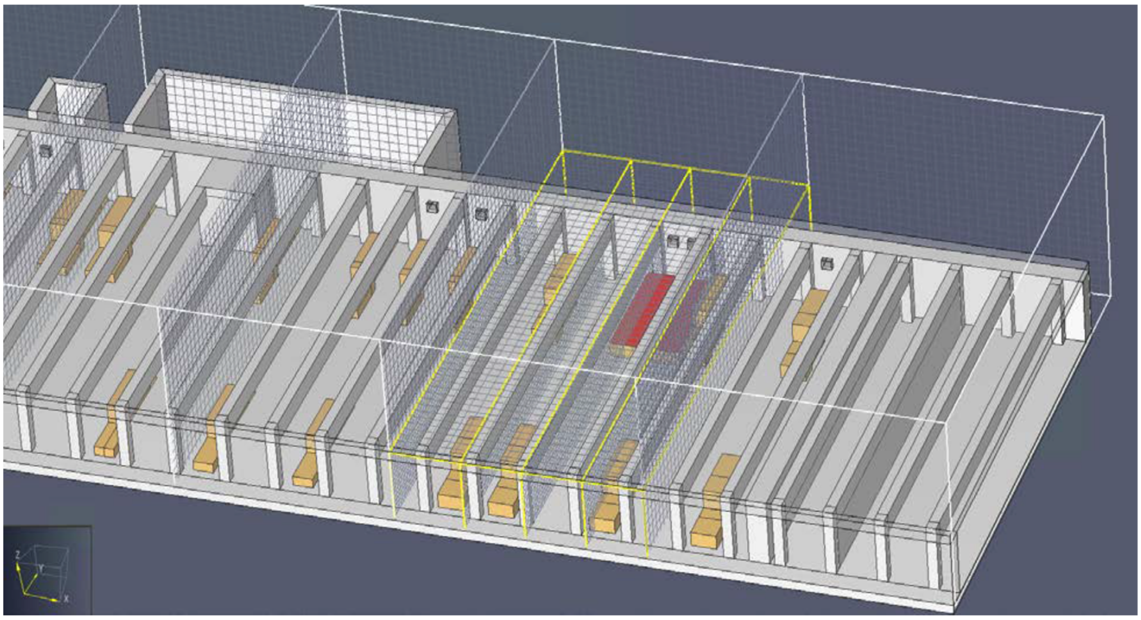

*Figure 1. Example of FDS valid geometry and associated computational domain.*

For the moment, FDS can only work on structured –i.e. orthogonal– grids, which has serious implications for object geometry. All object boundaries will automatically be adjusted to the computational grid as soon as the simulation begins. Therefore, it is good practice to align object boundaries with computational meshes beforehand, as illustrated in Figure 1. This fact also implies that any oblique or curvilinear surface will be approximated through stair-like surfaces as exemplified in Figure 2. However, the newest version of FDS allows modelling objects with other geometries than cubes (e.g. circular surfaces and cones can be used), which could be of great interest when modeling natural residential fuels.

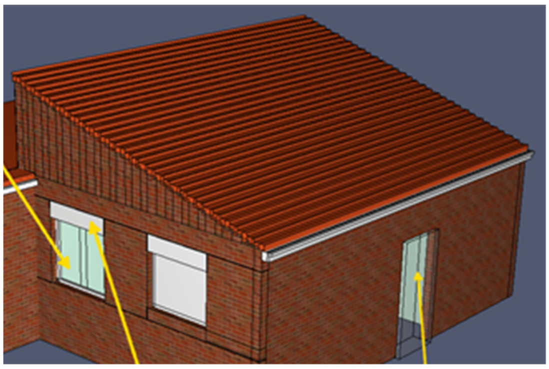

*Figure 2. Example of FDS geometry limitations. Surfaces not aligned with the computational mesh, such as this roof, will be approximated by stair-like surfaces.*

## 3.2. Fire source prescription

The most frequent case of use of FDS includes prescription of the fire source. This is usually accomplished through the external definition of its Heat Release Rate (HRR) as a function of time. The HRR(t) curve must be assigned to an object of a given volume and surface area. In this regard, there is a significant amount of experimental work performed by the fire engineering community, which can be very helpful in estimating HRR(t) curves of common burning objects. The user must indicate which surfaces “burn” and distribute the heat release rate per unit area accordingly. HRR per unit area (HRRPUA) is defined in units of kW/m$^2$. Additionally, a single gaseous fuel must be defined with its heat of combustion ($\Delta H_C$). FDS uses HRR(t) and $\Delta H_C$ values to compute the Mass Loss Rate MLR(t) of gaseous fuel that must leave each burning surface to provide the prescribed HRR(t). Alternatively, the user can input Mass Loss Rate (MLR) per unit area (in units of kg s$^{-1}\cdot$ m$^{-2}$) curves from which FDS derive HRR. Even if various solid burning surfaces can co-exist in an FDS scenario, computational limitations restrict the number of gaseous fuels to one. In normal conditions, the correct amount of gaseous fuel is emitted from the surface and burned provided that there is enough available oxygen. However, there are cases (e.g. in under-ventilated conditions) in which not all gaseous fuel is burned at the expected rate. This may result in an effective HRR curve below the values prescribed by the user. Therefore, actual HRR should always be confirmed upon simulation completion.

From the input point of view, the only input information needed to compute thermal transfer from the fire consists in HRR(t) and the heat of combustion of the gaseous fuel. Additionally, chemical information about gaseous fuel components and their combustion reactions can help in modelling the concentration of combustion products and smoke.

## 3.3. Fire source simulation

Alternatively, fire can be predicted instead of prescribed. This approach is not as thoroughly validated and it presents additional numerical challenges, but in turn it constitutes a powerful tool to simulate burning vegetation.

In order to predict the HRR curve, a complete set of physical and chemical properties must be defined for all combustible materials. These properties include fuel load (distributed in particles type, e.g. foliage, branches from 0 -3 mm, branches from 3 – 6 mm, etc.) mean density, thermal conductivity and heat capacity of fuel the fuel, fuel particles shape (which can be spherical or cylindrical) and dimensions, surface area-to-volume ratio, moisture content and information about the pyrolysis and combustion processes. The latter is typically provided in the form of Arrhenius coefficients.

These fuel particles must be distributed in the computational domain following a pre-defined shape and volume. If during the simulation they are ignited by an external heat source, these materials will burn following the defined pyrolysis and combustion reactions. Similarly to solid objects, the shape that burnable vegetation can take is limited in FDS. Typically, only cubes, cones and cylinders can be defined. Different particle categories can be defined to replicate the experimental mass distribution among different particle diameters.

## 3.4. Environmental variables

Inputs regarding ambient temperature (°C), Relative Humidity (%), wind speed profile ($m\ s^{-1}$ over z axis) and wind speed main direction should be also set when using CFD tools.

## 3.5. Outputs

Desired outputs must be specified during scenario design in FDS. Amongst the wealth of information produced during simulations, only pre-defined variables will be tracked at specified locations, and their values stored for posterior analysis. Virtually any variable used in the calculations can be exported to spreadsheets files (normally in CSV format), including temperatures, species concentrations, velocities, mass and heat fluxes, as well as their radiative and convective components. Their values can be visualized in a) specific domain points, b) 2D slices orientated along the three Cartesian axes and c) on solid surfaces.

Outputs can be displayed graphically for visualization and analyzed quantitatively in post-processing steps. Typically, we will measure air temperatures, heat fluxes received by critical components and concentrations of smoke and other combustion product gases. This will allow us to assess aspects such as heat impact on building systems, structure survivability, sheltering capacity, etc. Simulation results will then be compared to predefined performance criteria (e.g. threshold temperatures for materials melting/cracking; pain triggering heat dosages for fire responders and/or civilians, tenability conditions in terms of smoke exposures, etc.).

## 3.6. Coupling of FDS with external tools

Due to FDS limitations in terms of geometry description, we intend to couple it with external tools such as BlenderFDS and Pyrosim. Pyrosim can be used as standalone application to define ad-hoc geometries and easily import them into FDS. On the other hand, BlenderFDS serves as a bridge with a good number of 3D design tools. Blender FDS allows importing .FBX files, which constitute the current standard in 3D graphical design. This will boost the usability of our virtual workbench, since practically any 3D geometry designed with state-of-the-art third-party software will be importable in our framework.

## 3.7. WUIVIEW information flow to work with FDS

*In order to perform a fire safety analysis with FDS within the WUIVIEW Action, information generated and gathered from different work packages (i.e. WP2, WP3, WP4 and WP5) should be used. Figure 3 depicts an information flow diagram in which the links with the different WUIVIEW deliverables can be observed. Input data for FDS simulations shall firstly come from D5.1 "Inventory of pattern scenarios". Building systems and materials, burning elements, geometry and environmental variables (*

Table 1) should be defined in WP5 and transferred as a simulation scenario following the procedures detailed in last section.

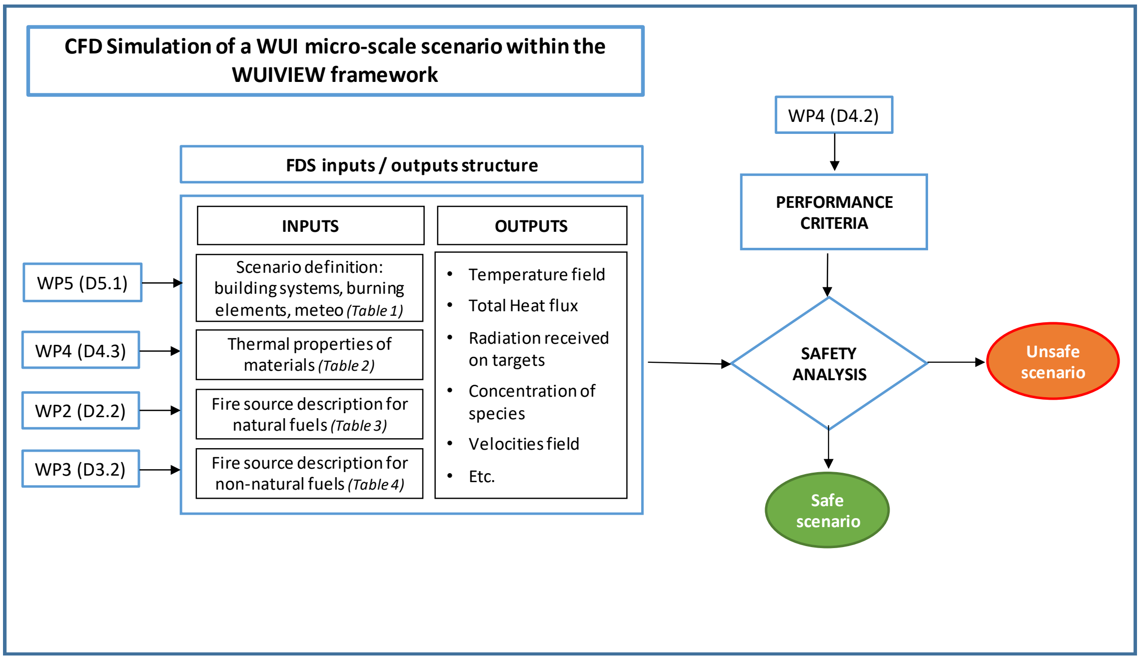

*Figure 3. Information flow diagram for fire safety analysis with FDS.*

*Table 1. FDS scenario definition, to be gathered and classified in WP5 – D5.1*

| Category | Description |
|---|---|
| **Scenario definition** (WP5 - D5.1) | Building system components and materials |
| | Fire source element: type and geometry |
| | Meteorological conditions: Temperature (°C), relative humidity (%), 10 m wind speed (m/s) and direction (°) |

*Regarding thermal properties of materials, those shall come from D4.3 "Data base on thermal properties and fire protection characteristics of building materials and systems". Table 2 specifies the particular properties that the database should gather. Input data concerning natural fuels acting as fire sources in FDS should come from D2.2 "Excel database on natural fuels burning characteristics".*

Table 3 gathers the different properties to be collected. Similarly, data on fire sources coming from non-natural fuels should be found in D3.2 "Excel database on artificial fuels burning characteristics". Table 4 specifies the information to be collected on non-natural fuel fire sources. Note that tables 2-4 are actually specifying the main fields that WUIVIEW databases (to be developed under WP2, WP3 and WP4) should contain. Those will hence be the basis for database design (on going action by UPC).

*Table 2. FDS needed inputs for thermal properties of materials, to be gathered and classified in WP4 – D4.3*

| Property | | Description | Units |
|---|---|---|---|
| Thermal properties of materials | **Material type** | Generic type of the material (e.g. plastic, wood, metal) | n.a. |
| | **Material sub-type** | Specific type of the material | n.a. |
| | $\rho$ | Material density | kg/m$^3$ |
| | $k$ | Thermal conductivity[1] | W·m$^{-1}$·K$^{-1}$ |
| | $C_p$ | Specific heat[1] | J·kg$^{-1}$·K$^{-1}$ |
| | $\varepsilon$ | Emissivity | - |

[1] A *k(T) or $C_p$(T)* function can be implemented in FDS, so a mathematical expression (or a table of values) is preferred if available. If not, *k* or $C_p$ at a given temperature should be detailed.

*Table 3. FDS needed inputs for a natural fuel fire source, to be gathered and classified in WP2 – D2.2*

| Property | | Description | Units |
|---|---|---|---|
| Natural Fuel fire source description | **Fuel type** | Type of natural fuel (e.g. tree, hedge, shrub, etc.) | n.a. |
| | **Specie** | Scientific name | n.a. |
| | $\rho_o$ | Density of the natural material on dry basis | kg/m$^3$ |
| | $k$ | Thermal conductivity of the natural material[1] | W·m$^{-1}$·K$^{-1}$ |
| | $C_p$ | Specific heat of the natural material[1] | J·kg$^{-1}$·K$^{-1}$ |
| | $\varepsilon$ | Emissivity of the natural material | - |
| | $\Delta H_C$ | Heat of combustion of volatiles | kJ/kg |
| | **Particles distribution** | Mass percentage on dry basis for different diameter classes | % |
| | ***MC*** | Moisture content in dry basis for each defined diameter class | % |
| | $\sigma$ | Surface-are-to-volume ratio for each defined diameter class | m$^{-1}$ |
| | **Adopted geometry** | Geometry that best fits the object | n.a. |
| | **Dimensions** | Height, width, depth, diameter, total volume, etc. | m |
| | $\rho_b$ | Bulk density of the natural fuel on dry basis | kg/m$^3$ |
| | **Burning area** | Surfaces of the fuel in contact with the exterior | m$^2$ |
| | **Mass Loss Rate MLR(t)** | Experimental curve of mass of pyrolised gases leaving solid surfaces per unit time | kg/s |

| | | | |
|---|---|---|---|
| | **Heat Release Rate HRR(t)** | Experimental firepower curve | kW/s |

[1] A *$k(T)$ or $C_p(T)$* function can be implemented in FDS, so a mathematical expression (or a table of vaues) is preferred if available. If not, *$k$* or $C_p$ at a given temperature should be detailed.

*Table 4. FDS needed inputs for a non-natural fuel fire source, to be gathered and classified in WP3 – D3.2*

| **Property** | | **Description** | **Units** |
|---|---|---|---|
| Natural Fuel fire source description | **Category** | Generic classification of the burning object (e.g. "appliance") | n.a. |
| | **Object** | Specific type of object (e.g. TV monitor) | n.a. |
| | $\rho$ | Density of the material | $kg/m^3$ |
| | $k$ | Thermal conductivity of the material[1] | $W \cdot m^{-1} \cdot K^{-1}$ |
| | $C_p$ | Specific heat of the material[1] | $J \cdot kg^{-1} \cdot K^{-1}$ |
| | $\varepsilon$ | Emissivity of the non-natural material | - |
| | $\Delta H_C$ | Heat of combustion of volatiles | kJ/kg |
| | **Adopted geometry** | Geometry (or group of geometries) that best fits the object | n.a. |
| | **Dimensions** | Height, width, depth, diameter, total volume, etc. | m |
| | **Burning area** | Surfaces of the fuel in contact with the exterior | $m^2$ |
| | **Mass Loss Rate MLR(t)** | Experimental curve of mass of pyrolised gases leaving solid surfaces per unit time | kg/s |
| | **Heat Release Rate HRR(t)** | Experimental firepower curve | kW/s |

[1] A *$k(T)$ or $C_p(T)$* function can be implemented in FDS, so a mathematical expression (or a table of vaues) is preferred if available. If not, *$k$* or $C_p$ at a given temperature should be detailed.

# 4. Working with FLUENT

FLUENT software will be mainly used in WUIVIEW as a simulation tool to explore the fire impact (i.e thermal and fluid-dynamic response of the vessel and its content) on LPG tanks at the WUI microscale.

The system domain (in this case the tank lading – both liquid and vapor space - and its steel wall) is discretized in small elements creating a computational grid as showed in Figure 4. It is therefore necessary to define the tank geometry (diameter, length and wall thickness).

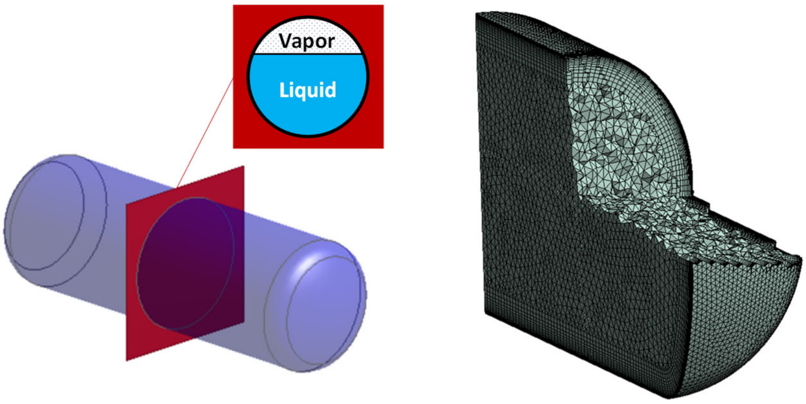

*Figure 4. Example of tank geometry and computational grid.*

Then, the governing equations for mass, momentum (including turbulent quantities) and energy are solved for the tank lading and the solid wall (energy equation only). Further details on the model setup can be found in Scarponi et al. (2018).

The CFD model requires the definition of appropriate boundary and initial conditions (initial temperature, pressure and degree of filling). In the CFD approach presented here, the boundary condition (at time $t$ and at point $\vec{x}$ on the external tank wall) reproducing the radiative and convective heat transfer with the exterior is expressed according to Eq. (1).

$$\dot{q}"(\vec{x},t) = \sigma\varepsilon_w\left(T_{BB,eq}(\vec{x},t)^4 - T_w(\vec{x},t)^4\right) + h_g(\vec{x},t)\left(T_g(\vec{x},t) - T_w(\vec{x},t)\right) \qquad \text{Eq. (1)}$$

$$T_{BB,eq}(\vec{x},t) = \sqrt[4]{\frac{I(\vec{x},t)}{\sigma}} \qquad \text{Eq. (2)}$$

Here, $\dot{q}"$(W/m$^2$) is the heat flux through the external surface of the tank wall, $\sigma$ (=5.67 x 10$^{-8}$ W·m$^{-2}$·K$^{-4}$) is the Stefan-Boltzman constant, $\varepsilon_w$ (-) is the emissivity of the wall and $T_w$ (K) is the wall temperature. $T_{BB,eq}$ (K) is the equivalent black body temperature (representative of the incident radiation hitting the tank surface). Values of the incident radiation *I* (W/m$^2$) *(*representing the radiative contribution of both the fire and the ambient), the temperature of the gases (air, flame, smoke) $T_g$ (K) in contact with the surface and the convective heat transfer coefficient $h_g$ (W·m$^{-2}$·K$^{-1}$) need to be specified according to the fire scenario characteristics.

The definition of such parameters can be done following different approaches, depending on available data, accuracy required and organizational factors such as time, costs and computational resources. There are mainly three options to define *I*, $h_g$ and $T_g$:

1) Direct definition: $I$, $h_g$ and $T_g$ are prescribed by the analyst. This option will be used in the WUIVEIW framework, basically in a preliminary phase, to get orders of magnitude of our variables of interest.
2) Solid flame model: the flame is modelled as a solid body with an assigned emissive power (Figure 5). This method requires to calculate the view factor between the solid body representing the fire and the flame. It is necessary to assign a fire curve (i.e. defining a transient emissive power curve) to the solid flame surface. This requires literature or experimental data. The solid flame model allows to obtain a spatial and temporal distribution of the incident radiation. However, the gas temperature and the convective heat transfer coefficient must be defined based on experience and/or empirical formulas. This option will be mainly used in the WUIVIEW framework in scenarios involving fire spread through unmanaged plots or through wild fuels.

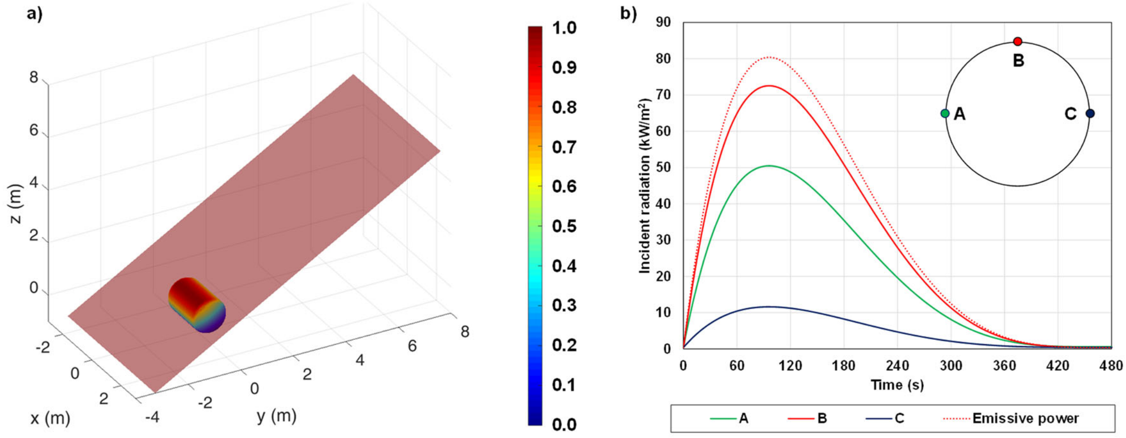

*Figure 5. Example of solid flame modelling approach. a) View factors between the tank and a plane representing the flame. b) Example of emissive power curve and the resulting incident radiation on three different points on the tank wall surface.*

3) Fire source simulation: FDS is used to simulate the fire source. Spatial and temporal distribution of $I$, $h_g$ and $T_g$ on the tank wall are hence obtained as FDS outputs. A Matlab routine is used to transform FDS outputs to Fluent inputs. Figure 6 presents an example of a FDS simulation with six trees burning in the proximity of a LPG tank and the resulting incident radiation on the tank front side. This option will be used in scenarios with burning residential fuels of different nature (either natural or non natural). Either a prescription or a combustion simulation of the fire source will be possible when working with natural fuels. Only fire prescription will be used when working with non-natural fuels.

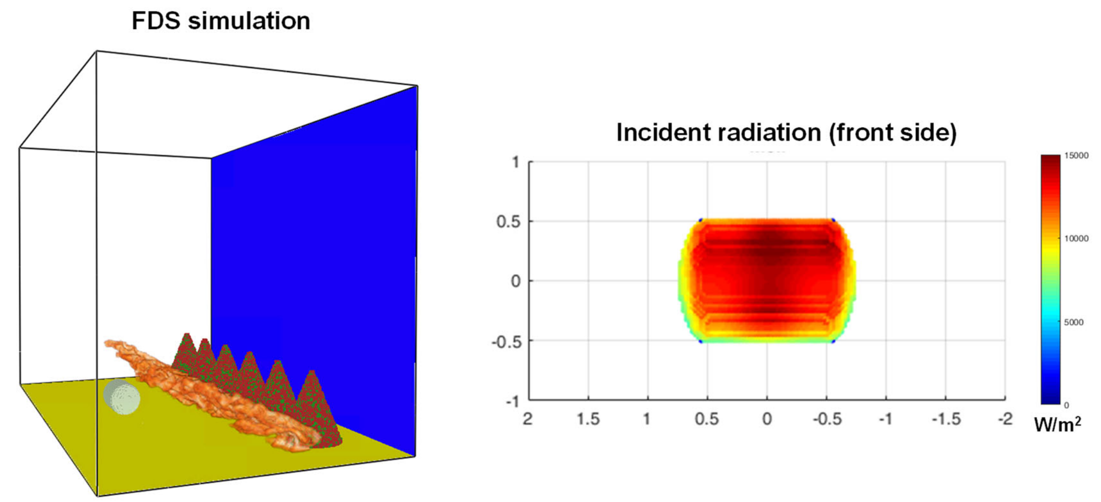

*Figure 6. Example of fire simulator approach. Left: FDS simulation considering six trees burning in the proximity of a tank. Right: Incident radiation on the tank front side at a given instant of time.*

CFD simulation of fire exposure to LPG tanks may provide different kind of results. The most useful for the purpose of the WUIVIEW project are the pressurization curve and the temperature distribution on the external wall. In fact, the combination of pressure increase and mechanical weakening of the tank shell above 400 °C represent a treat for tank integrity.

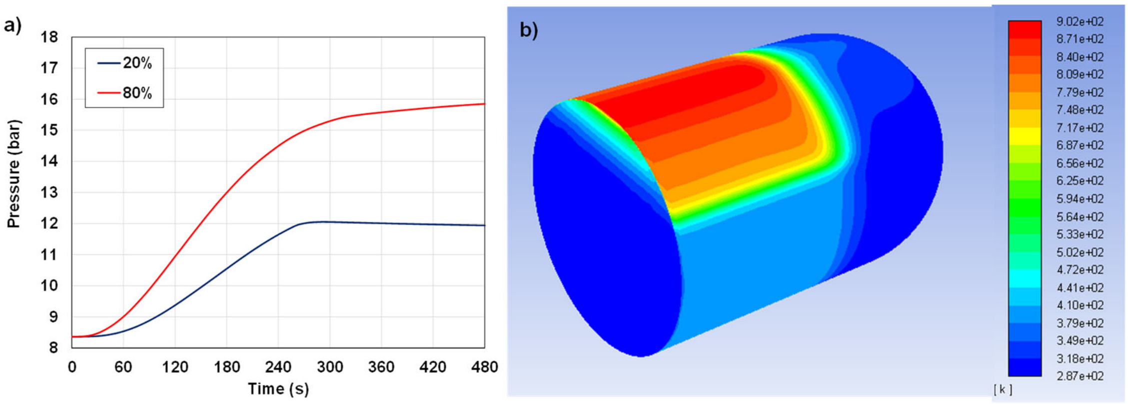

*Figure 7. Example CFD results obtained with Fluent. a) Pressurization curves for a tank with a 20 % (blue curve) and 80 % (red curve) initial filling degree. b) Temperature distribution on the external tank wall.*

The required inputs for a Fluent simulation are summarized in Table 5.

*Table 5. Description of the information required for FLUENT simulations within WUIVIEW and its source..*

| Required input | Source |
|---|---|
| **Tank diameter (m)** | Tank manufacturer for synthetic cases / scenario definition from forensic studies (WP5) |
| **Tank length (m)** | Tank manufacturer for synthetic cases / scenario definition from forensic studies (WP5) |
| **Tank wall thickness (mm)** | Tank manufacturer for synthetic cases / scenario definition from forensic studies (WP5) |
| **PRV set point (bar)** | Tank manufacturer for synthetic cases / scenario definition from forensic studies (WP5) |
| **$I$, $h_g$ and $T_g$** | Direct definition / solid flame model / FDS simulation |

CFD simulations can be carried out both in 3D or in 2D. This second option allows to save a considerable amount of computational time (a 3D simulation considering a 1 m diameter by 2 m length tank for 8 min of fire exposure takes approximately one month on an Intel® Core™ i7-7700 CPU @ 3.60GHz using 8 cores in parallel). However, it is only applicable when the fire condition can be assumed to be uniform along the tank axis.

# 5. References

Scarponi, G.E., Landucci, G., Heymes, F., Cozzani, V., 2018. Experimental and numerical study of the behavior of LPG tanks exposed to wildland fires. Process Saf. Environ. Prot. 114, 251–270.