

# HARSIA PROJECT

## TASK 2 REPORT

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## Disclaimer

The analysis presented below is the technical opinion of the UGent team (Dr. Georgios Maragkos and Prof. Bart Merci), based on their professional experience and expertise in the context of fire simulations with CFD, and based on the available information as provided at the date of writing this report. The findings of the analysis are the result of careful consideration of the available information and are subject to change if new information on the accident were to be disclosed.

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# 1 INTRODUCTION

After having analyzed the information, as made available by Mr. Costas Lakafossis, of the railway accident that took place in Tempi, Greece, on 28 February 2023, the aim of this report is for the UGent team (Dr. Georgios Maragkos and Prof. Bart Merci) to assess the validity of the CFD simulations that have been performed for the scenario. The CFD code Fire Dynamics Simulator (FDS), version 6.8, was used for the simulations of all the input files discussed in the report. The reviewed FDS input files are presented in the appendix.

The choice of the CFD code itself is deemed reasonable because FDS is currently the state-of-the-art CFD code, widely used for modelling of fire-related scenarios in the context of fire safety engineering. The considered FDS version is also fairly recent and hence up-to-date (i.e., 6.9.1 is the latest version). A detailed review of the different aspects (i.e., models, input data, boundary conditions, etc.) of the FDS input files, as provided by Mr. Costas Lakafossis, that were used for the CFD simulations is presented below. Emphasis is given on whether the choices made in the CFD simulations are reasonable and/or verifiable, based on the available information for the Tempi accident as provided to the UGent team. In the end, some general conclusions are provided for all the CFD scenarios considered.

## 2 ANALYSIS OF CFD SCENARIOS

A brief overview of the CFD scenarios reads:

- ✓ **Scenario Case06\_03**: involves the release of liquid fuel (n-pentane) from two fire sources and the formation of a fire ball,
- ✓ **Scenario Case02\_01\_new**: illustrates the ignition of a benzene fuel source,
- ✓ **Scenario Case04\_05b**: illustrates the lack of ignition of a silicone oil fuel source.

### 2.1 Scenario Case06\_03

The main objective of this scenario is to estimate the total amount of fuel required in order to replicate the fire ball as observed in the video footage.

- **Size of computational domain** (length x width x height): 160 m x 100 m x 80 m.

This is deemed a reasonable and verifiable choice based on the available video footage (i.e., the maximum diameter of the fire ball, as observed from the video, is on the order of 80 m). Therefore, the size of the domain is considered large enough to enable the undisrupted injection of fuel and the creation of the fire ball.

- **Geometry**: Two different fire sources are considered. The primary fire source injects fuel horizontally towards an inclined surface placed approximately 2 m away. A second fire source, positioned 10 m upstream of the primary fire source, injects fuel with a 45° angle upward.

From the video footage and other information on the Tempi accident, as made available to the UGent team, it cannot be verified whether the chosen geometry resembles, to within a reasonable degree of accuracy, what actually occurred in reality during the Tempi accident. In addition, it is unclear why the second fire source, injecting fuel in the same direction as the primary fire source (but from 10 m upstream), is needed in the simulations.

- **Grid size:** Local grid refinement (i.e., stretched 0.25 m x 0.25 m x 0.1 m grid size close to the fire sources and uniform 0.5 m grid size away from the fire sources).

An overview of the considered local grid refinement and the cell size near the fuel sources is presented in Figure 1. In general, the use of cubic (uniform) cells is recommended in order to accurately capture turbulence and mixing which will, in turn, affect combustion. The use of local grid refinement and stretched cells can potentially affect the CFD solution (i.e., particularly in locations where there is a big jump in grid sizes). The aspect ratio (2.5) is higher than the value that can potentially lead to numerical instabilities as mentioned in the FDS documentation (i.e., a value of 2 is mentioned in the FDS user's guide [1]). Combined with some velocity oscillations observed in the flow field (see comment later), it is unclear whether the chosen mesh and grid sizes are reasonable to accurately simulate the scenario. Ideally, a grid sensitivity study needs to be performed to illustrate that the CFD predictions are grid-insensitive (i.e., the grid size does not significantly affect the shape/size of the predicted fire ball). Justification of the appropriate grid size can also be made a priori and a posteriori based on widely accepted criteria and metrics from the literature.

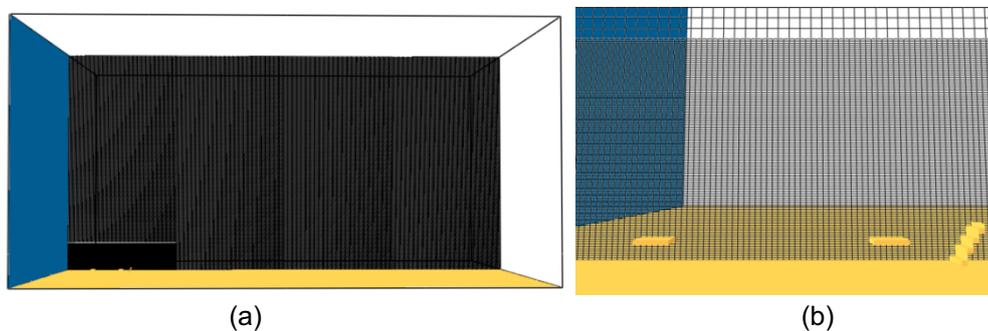


Figure 1. Illustration of the (a) computational domain / mesh and (b) local grid refinement region used in the simulation of scenario Case06\_03.

- **Running time:** 30 s.

This is deemed a reasonable choice. The prescribed running time is sufficiently long to simulate the injection of the fuel and for the creation of the fire ball. The chosen value would have also been sufficient for having an established wind profile over the entire domain. However, this was not considered in the simulations (see point on “Initial conditions - Velocity” below).

- **Model selection:** default FDS models (in VLES mode).

This is deemed a reasonable choice. FDS using the default models has been validated by NIST for a wide range of fire scenarios [2].

- **Initial conditions**

- Ambient temperature: default FDS value (i.e., 20°C).

Given the time and date of the accident (i.e., 28 Feb 2023 – at approximately 23:21 EET) and the available meteorological data from nearby weather stations (i.e., Larissa), the choice is not deemed entirely reasonable, as ambient temperature was most likely

much lower. However, the impact of this parameter on the actual shape/size of the fire ball is not expected to be significant.

- Velocity: still air (0 m/s).

This is not deemed a reasonable choice. As a consequence of this choice, there is no established wind-induced flow field inside the computational domain at the moment of the first fuel injection (see Figure 2). The simulation should allow for at least 1 flow through time to allow for any initial transient effects to have left the computational domain. Hence, the fuel injection inside the computational domain should ideally start after at least  $t = L/u = (160 \text{ m}) \times (10 \text{ m/s}) = 16 \text{ s}$  or when the wind-induced flow field has visibly reached the right side of the computational domain.

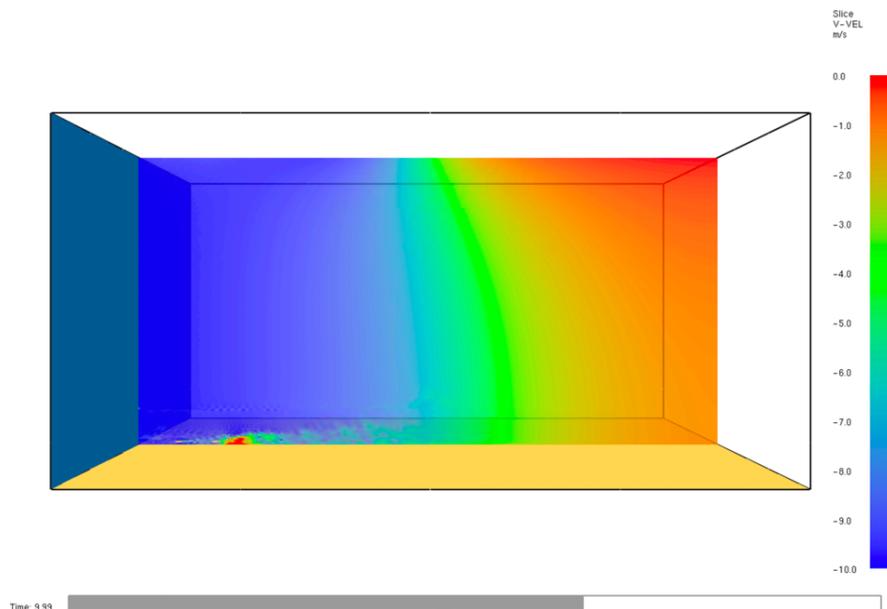


Figure 2. Velocity profile inside the computational domain just before the first fuel injection in the simulation of scenario Case06\_03.

- Relative humidity: default FDS value (i.e., 40%).

Given the time and date of the accident (i.e., 28 Feb 2023 – at approximately 23:21 EET) and the available meteorological data from nearby weather stations (i.e., Larissa), the choice is not deemed entirely reasonable, as the relative humidity was most likely higher. However, the impact of this parameter on the actual shape/size of the fire ball is not expected to be significant.

- **Boundary conditions**

- Velocity: prescribed constant and uniform velocity of 10 m/s over one boundary of the computational domain.

The modelling of the wind is not very realistic and hence is not deemed reasonable: there is no consideration of velocity variation as a function of height (although this is typically accounted for in atmospheric type of flows); and no velocity fluctuations are applied at the boundary to represent the turbulence in the wind velocity profile.

Moreover, the modelling of the wind profile in the simulations can have a noticeable and potentially significant effect on the predicted shape/size of the fire ball. This aspect requires further attention and would require a sensitivity study, using different approaches for modelling wind in the simulations.

The imposed wind velocity magnitude cannot be verified due to lack of officially recorded meteorological data at the exact location of the accident. Rather, the wind velocity magnitude has been estimated from testimonies of people present in the accident [3] which, inevitably, introduces a high degree of uncertainty. The imposed velocity magnitude is expected to have a significant effect on the predicted shape/size of the fire ball. This aspect requires further attention and would require a sensitivity study, using different wind velocity values in the simulations.

In addition, some (unphysical) velocity oscillations are observed in the simulations near the fuel sources and at the height of the local grid refinement. This could be related to the aspect ratio of the cells, as mentioned above. An illustration of such oscillations, taken at time  $t = 5\text{ s}$  in the simulations, is presented in Figure 3. These oscillations have been observed during the entire time period before fuel injection occurs, and it is unclear what effect they have on the predicted shape/size of the fire ball.

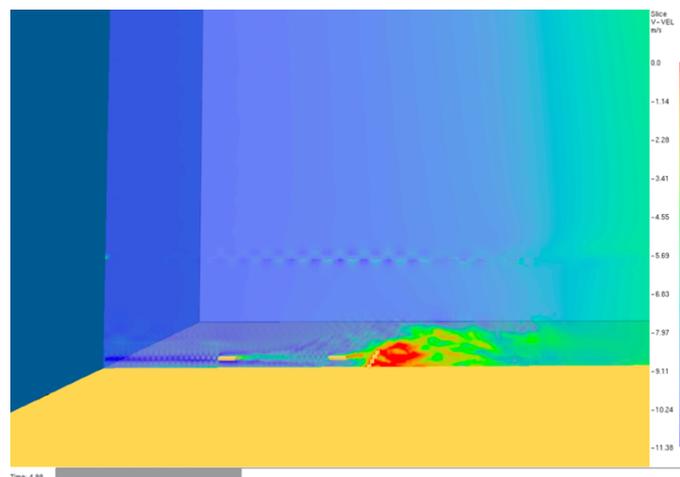


Figure 3. Illustration of some (unphysical) velocity oscillations near the fuel sources during the simulation of scenario Case06\_03 (photo taken at time  $t = 5\text{ s}$ ).

- **Fuel:** liquid n-pentane ( $C_5H_{12}$ ).

The choice of liquid n-pentane as a potential fuel is deemed reasonable. Given the way FDS handles combustion (i.e., use of infinitely fast chemistry), setting the auto-ignition temperature (AIT) of the fuel to  $0^\circ\text{C}$ , as was done in the simulations, will essentially allow for the ignition and combustion of any combustible (liquid/gas) fuel introduced in the CFD simulations. This type of modelling can be considered reasonable if ignition is not the main focus of the work but instead the goal is to roughly estimate the total amount of fuel that could result in the fire ball as observed in the video footage. However, this type of modelling cannot be used for reverse engineering in order to determine what type of fuel was present during the scenario, nor as to whether a certain (liquid/gas) fuel would ignite or not. According to [4], the heat of combustion for liquid

n-heptane is  $\Delta H_c = 42 \text{ MJ/kg}$ , the CO yield in well-ventilated combustion is  $y_{CO} = 0.008$ , and the soot yield is  $y_{soot} = 0.033$  for n-pentane. While the choice for the heat of combustion is reasonable (i.e.,  $44 \text{ MJ/kg}$ ), significantly higher values have been assigned for the CO (i.e.,  $0.05$ ) and soot (i.e.,  $0.1$ ) yields in the CFD simulations. Nevertheless, the choice of these parameters is not expected to have a significant effect on the predictions of the resulting shape/size of the fire ball.

- **Fuel injection method:** prescribed particle mass flux (with droplets with a constant diameter of  $500 \mu\text{m}$ ) from a given area with a specified injection velocity. Primary injection velocity with a particle mass flux of  $4273.5 \text{ kg/m}^2/\text{s}$  from a  $0.3 \text{ m}^2$  area (with an injection velocity of  $20 \text{ m/s}$ ) and a secondary injection with a particle mass flux of  $952.3 \text{ kg/m}^2/\text{s}$  from a  $0.3 \text{ m}^2$  area (with an injection velocity of approximately  $10 \text{ m/s}$  with a  $45^\circ$  angle upward).

The case is essentially modelled as a spray combustion scenario (i.e., injected liquid n-pentane droplets with a given velocity). Given the unknowns and uncertainties involved in the Tempi accident, it cannot be verified whether it is a reasonable choice or not. It is also unclear whether the considered fuel injection areas (i.e.,  $1.5 \text{ m} \times 0.2 \text{ m} = 0.3 \text{ m}^2$ ) are a reasonable choice for the scenario at hand. The choice of  $500 \mu\text{m}$  as droplet diameter can be considered reasonable for large (coarse) spray droplets. However, a sensitivity study on this choice would be needed to demonstrate that this parameter does not (significantly) affect the resulting shape/size of the fire ball.

Estimation of the total injected fuel mass inside the computational domain (based on the input data of the Case06\_03.fds file in the appendix):

- Primary fuel source:  $m_1 = \dot{m}_1 A_1 t_1 = 4273.5 \frac{\text{kg}}{\text{m}^2 \text{s}} \times 0.3 \text{ m}^2 \times 1.25 \text{ s} \approx 1600 \text{ kg}$
- Secondary fuel source:  $m_2 = \dot{m}_2 A_2 t_2 = 952.3 \frac{\text{kg}}{\text{m}^2 \text{s}} \times 0.3 \text{ m}^2 \times 3.5 \text{ s} \approx 1000 \text{ kg}$
- Total mass:  $m = m_1 + m_2 = 1600 \text{ kg} + 1000 \text{ kg} = 2600 \text{ kg}$

Based on an empirical correlation for fire balls [5], approximately  $2600 \text{ kg}$  would be needed to produce a spherical fire ball with a maximum diameter of  $80 \text{ m}$  (i.e., size similar to the one observed in the video footage of the Tempi accident [3]). This value is comparable to the total amount of fuel used in the simulations, hence, it is deemed a reasonable choice/starting point for the CFD study. Nevertheless, the potential impact of the considered total amount of fuel in the simulations on the shape/size of the fire ball needs to be demonstrated. A brief sensitivity study on this aspect, carried out by the UGent team, using half and double the amount of fuel, did not reveal significant qualitative differences in the resulting shape/size of the fire ball. Thus, CFD is a valuable tool for providing a rough estimate of the potential total amount of fuel required to replicate the fire ball, as observed in the video footage, but it cannot be easily used to precisely determine it. It also remains unclear whether the treatment of the fire source as a spill plume (i.e., without high injection velocity) would resemble (or not) the results obtained with current fuel injection method.

**Notes:** Simulations with the provided FDS input files give rise to some warnings that require attention:

- WARNING: Problem with units compatibility of SPATIAL\_STATISITIC VOLUME INTEGRAL with the QUANTITY MASS FRACTION

## 2.2 Scenario Case02\_01\_new and scenario Case04\_05b

The main objective of these two scenarios is to illustrate that the consideration of a benzene fire source can ignite and replicate the observed fire ball in the video footage, while a silicone oil fire source would fail to ignite. Hence, these two scenarios are discussed and analyzed together in this section.

In scenario Case02\_01\_new, liquid benzene fuel is injected horizontally from a (2 m x 1.5 m = 3 m<sup>2</sup>) fire source with a prescribed mass flux. The injected fuel flows above a horizontal heat source (gas temperature above the heat source > 500°C), positioned approximately 2.5 m away, in order to ignite the fuel. In scenario Case04\_05b, liquid silicone oil droplets are injected horizontally from a (2 m x 1.5 m = 3 m<sup>2</sup>) fire source with a prescribed particle mass flux and a given velocity. The injected fuel droplets hit a vertical surface, positioned approximately 2.5 m away, which acts as a heat source (gas temperature near the heat source > 500°C) in order to ignite them. The geometry of the fuel and heat sources in the two scenarios is presented in Figure 4. The scenario involving the benzene fire source (Case02\_01\_new) successfully ignites and creates a large horizontal fire ball. On the other hand, the scenario involving the silicone oil fire source (Case04\_05b) does not ignite.

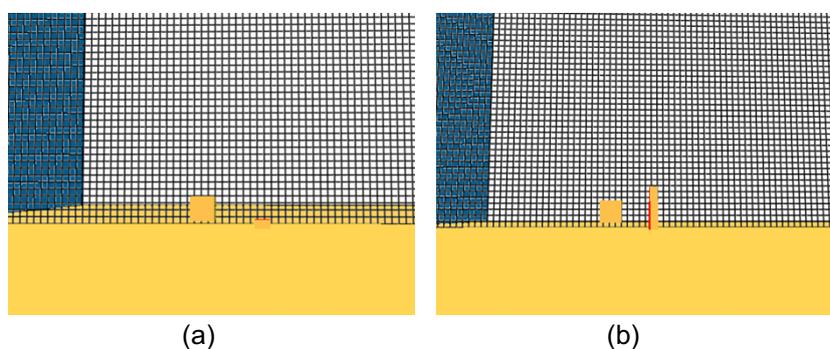


Figure 4. Mesh and geometry of the fire and heat sources used in the simulations for scenario (a) Case02\_01\_new and (b) Case04\_05b.

The comments and analysis regarding the size of computational domain, running time, model selection, initial conditions and boundary conditions (for velocity only), as previously reported for the Case06\_03 file, also apply here as well. It is noted that the computational domain for the benzene case (Case02\_01\_new) has a height of 60 m (not 80 m as the previous cases), but that is not an important issue because the resulting fire ball is issued horizontally. A uniform grid size (0.5 cm) is used in both scenarios. This choice can be considered reasonable for simulating large-scale fires or pollutant dispersion scenarios but can be potentially (too) coarse for accurately simulating spray combustion scenarios involving ignition and fire sources with limited number of cells across their diameter. A grid sensitivity study would be required to demonstrate that the CFD predictions are indeed grid-insensitive (i.e., the grid size does not significantly affect the ignition and the shape/ size of the predicted fire ball).

The main comments after reviewing the two above-discussed FDS input files are the following:

- The benzene scenario (Case02\_01\_new) does not use exactly the same setup as the silicone oil scenario (Case04\_05b) (see Figure 4). More specifically, there is difference between a horizontal hot surface and a vertical hot surface for ignition. Hence, a direct comparison between the two scenarios is effectively impossible. In order to make a fair comparison, the exact same setup is required, with only the fuel changed.

- The way the heat source has been set up in the simulations of both scenarios (Case02\_01\_new and Case04\_05b) is not the most typical approach used in modelling (i.e., not imposing a surface temperature but rather a heat flux). More specifically, a net heat flux of 1000 kW/m<sup>2</sup> and a heat transfer coefficient of 1000 W/m<sup>2</sup>/K have been defined, which led to a maximum surface temperature at the heat source on the order of 1700°C. The resulting gas temperature in the vicinity of the heater surface is then on the order of 500°C or higher. The resulting surface temperature, and subsequent gas temperature in its vicinity, as well as the duration of the heat source, are important with respect to fuel ignition. It is unclear whether the current way of modelling the fuel ignition is realistic, based on what actually happened during the accident. Ideally, a sensitivity study on the influence of the heat source temperature needs to be performed, considering a range of values that could have occurred during the accident due to, e.g., external heat source, sparks due to collision, or other.
- The auto-ignition temperature (AIT), a parameter defined in the FDS input file, corresponds to the physical AIT in case of spontaneous ignition (i.e., in the absence of an ignition source). In the context of the Tempi train accident, piloted ignition of the fire ball is deemed likely (i.e., due to hot sparks due to the high mechanical friction due to the impact, or due to an initial small flame). In such cases, the AIT parameter should ideally be lowered to the fire point of the fuel, in order to mimic the presence of the pilot ignition source. The value for the AIT parameter used for benzene in scenario Case02\_01\_new (298°C) is much higher than the range of fire points reported in the literature [4] and hence is a conservative choice (i.e., if ignition is observed in the simulations, then ignition is to be expected in reality as well). The value used for silicone oil in scenario Case04\_05b, though, is 450°C, whereas the silicone oil (Bayer Baysilone M50 EL) used in the transformers of the trains has a reported fire point of approximately 350°C [6]. This is not a conservative choice, and hence this is not deemed a reasonable choice. Moreover, simulations of scenario Case04\_05b, with exactly the same setup and only changing the AIT value from 450°C to 350°C, leads to ignition of the silicone oil fuel source (simulations carried out by the UGent team). It should be noted that if the accident was supposed not to involve a pilot ignition, and hence the AIT parameter should indeed correspond to the auto-ignition temperature of the fuel (and not its fire point), the value of 298°C chosen for benzene is significantly lower than the value reported in the literature (i.e., 560°C [4]). With the latter value, the benzene fire source in scenario Case02\_01\_new with the exact same input file does not ignite (simulations carried out by the UGent team). In short, if the AIT parameter is given a realistic value of the real AIT as reported in the literature, neither benzene nor silicone oil ignite in the simulations with the set-up at hand. On the other hand, if a realistic value for the fire point is used for the AIT parameter in the simulations, both fuels ignite with the set-up at hand.
- The prescribed critical flame temperature for both fuels (i.e.,  $T_{CFT} = 1900^{\circ}\text{C}$ ) appears to be significantly higher than the ones reported in the literature (e.g.,  $T_{CFT} = 1537^{\circ}\text{C}$  [4] for benzene). Hence this is not deemed a reasonable choice. Even though the effect of this parameter is deemed to be less important than the prescribed AIT value, a sensitivity study on the influence of this parameter should also be considered in the simulations.

In general, the ignition source (i.e., the gas temperature in its vicinity) will be important with respect to (liquid/gas) fuel ignition. The CFD user should be aware of the importance of the AIT parameter in the modelling with FDS. It is worth noting that FDS suggests decreasing the AIT value in case of very coarse meshes (e.g., cell size >10 cm) in the simulations because naturally the flame temperature cannot be accurately predicted on such grids. The grid used in the simulations of both scenarios is

much coarser (i.e., 50 cm). There are also other important modelling aspects (e.g., related to radiation and extinction modelling among others) to consider when modelling ignition of (liquid/gas) fuels.

**Notes:** Simulations with the provided FDS input files give rise to some warnings that require attention:

- WARNING: SPEC SiliconOil\_SimpleFormula is not in the table of pre-defined species. Any unassigned SPEC variables in the input were assigned the properties of nitrogen.
- WARNING: Droplet heat transfer is not predicted when a droplet is on a SURF with a specified ADIABATIC, NET\_HEAT\_FLUX, or CONVECTIVE\_HEAT\_FLUX.
- WARNING: Problem with units compatibility of SPATIAL\_STATISITIC VOLUME INTEGRAL with the QUANTITY MASS FRACTION

### 3 CONCLUSIONS

A brief summary of the main conclusions of the report reads:

- The version (6.8) of FDS with the current input file (Case06\_03) could in principle be used for reverse engineering in order to roughly estimate the required amount of fuel involved in the incident that led to the observed fire ball. However, it must be acknowledged that there are several significant uncertainties, including the wind conditions and the location, size, type and injection method of the initial fire source(s), among others.
- Determination of the amount of fuel that led to the fire ball (or a range of possible values for the amount of fuel) from CFD simulations requires a more comprehensive sensitivity study than what has been provided to the UGent team for review.
- The following settings are not deemed suitable, with potentially significant impact on the CFD simulation results, and require further investigation in the simulations:
  - grid cell size in all scenarios,
  - velocity boundary condition and fuel injection method in scenario Case06\_03,
  - AIT parameter and heat source characteristics in scenarios Case02\_01\_new and Case04\_05b.
- The following settings are not deemed suitable, with expected only little impact on the CFD simulation results, and it is recommended to adjust these settings in future CFD simulations:
  - ambient temperature and relative humidity in all scenarios,
  - time of fuel injection in scenario Case06\_03,
  - critical flame temperature in scenarios Case02\_01\_new and Case04\_05b.
- Given the overall uncertainties, it is not deemed possible to determine the type of (liquid/gas) fuel that led to the fire ball with a reasonable degree of reliability from the CFD simulations.
- The ignition of a (liquid/gaseous) fuel will strongly depend on the initial and boundary conditions of the problem, the type and characteristics of the ignition source, as well as on the defined thermophysical properties of the fuels and the selected models in the CFD simulations. With the current setups (Case02\_01\_new, Case04\_05b), no concrete statements regarding the potential ignition (or not) of liquid fuels can be made. A more comprehensive sensitivity study is needed by incorporating the correct thermophysical properties of the fuels and by examining the influence of the heat source, among others.

## REFERENCES

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- [2] S. H. J. F. R. M. M. V. E. M. K. McGrattan, „Fire Dynamics Simulator Technical Reference Guide Volume 3: Validation,” NIST Special Publication 1018-3 (Sixth Edition), 2025.
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- [4] C. Beyler, „Chapter: Flammability Limits of Premixed and Diffusion Flames,” in *SFPE Handbook of Fire Protection Engineering (5th edition)*, New York, Springer, 2016, pp. 2-175, 2-183, 3-134.
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- [6] B. AG, „Bayer silicones Baysilone fluids brochure,” [Online]. Available: <https://dcproducts.com.au/wp-content/uploads/2020/12/BayerBaysiloneFluidsBrochure.pdf>. [Geopend 23 January 2025].

## APPENDIX: FDS INPUT FILES

The FDS input files which were reviewed in the report are included in this section.

- **Scenario Case06\_03**

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MONODISPERSE=.TRUE.,  
QUANTITIES='PARTICLE VELOCITY',  
AGE=10.0/

&REAC ID='NAPHTHA-TK',  
FUEL='N-PENTANE',  
AUTO\_IGNITION\_TEMPERATURE=0.0,  
CO\_YIELD=0.05,  
SOOT\_YIELD=0.1,  
HEAT\_OF\_COMBUSTION=4.4E+4/

&SURF ID='AirBlow',  
RGB=26,114,176,  
VEL=-10.0,

TAU\_V=-1.0/

&SURF ID='BlowNAPHTHA',  
RGB=26,74,25,  
VEL=-20.0,  
RAMP\_V='BlowNAPHTHA\_RAMP\_V',  
MASS\_FRACTION=1.0,  
SPEC\_ID='N-PENTANE',  
TAU\_MF=1.0,  
PART\_ID='NAPHTHADrops',  
NPPC=10,  
PARTICLE\_MASS\_FLUX=4273.5,  
RAMP\_PART='BlowNAPHTHA\_RAMP\_PART'/

&RAMP ID='BlowNAPHTHA\_RAMP\_V', T=10.0, F=0.0/  
&RAMP ID='BlowNAPHTHA\_RAMP\_V', T=10.1, F=1.0/  
&RAMP ID='BlowNAPHTHA\_RAMP\_V', T=10.6, F=1.0/  
&RAMP ID='BlowNAPHTHA\_RAMP\_V', T=12.0, F=0.0/  
&RAMP ID='BlowNAPHTHA\_RAMP\_PART', T=10.0, F=0.0/  
&RAMP ID='BlowNAPHTHA\_RAMP\_PART', T=10.1, F=1.0/  
&RAMP ID='BlowNAPHTHA\_RAMP\_PART', T=10.6, F=1.0/  
&RAMP ID='BlowNAPHTHA\_RAMP\_PART', T=12.0, F=0.0/

&SURF ID='BlowNAPHTHA\_2nd',  
RGB=26,155,15,  
VEL=-7.1,  
RAMP\_V='BlowNAPHTHA\_2nd\_RAMP\_V',  
VEL\_T=0.0,7.1,  
MASS\_FRACTION=1.0,  
SPEC\_ID='N-PENTANE',  
TAU\_MF=1.0,  
PART\_ID='NAPHTHADrops',  
NPPC=10,  
PARTICLE\_MASS\_FLUX=952.3,  
RAMP\_PART='BlowNAPHTHA\_2nd\_RAMP\_PART'/

&RAMP ID='BlowNAPHTHA\_2nd\_RAMP\_V', T=12.0, F=0.0/  
&RAMP ID='BlowNAPHTHA\_2nd\_RAMP\_V', T=12.1, F=1.0/  
&RAMP ID='BlowNAPHTHA\_2nd\_RAMP\_V', T=15.9, F=1.0/  
&RAMP ID='BlowNAPHTHA\_2nd\_RAMP\_V', T=16.0, F=0.0/  
&RAMP ID='BlowNAPHTHA\_2nd\_RAMP\_PART', T=12.0, F=0.0/  
&RAMP ID='BlowNAPHTHA\_2nd\_RAMP\_PART', T=12.5, F=1.0/  
&RAMP ID='BlowNAPHTHA\_2nd\_RAMP\_PART', T=15.5, F=1.0/  
&RAMP ID='BlowNAPHTHA\_2nd\_RAMP\_PART', T=16.0, F=0.0/

&OBST ID='Barrel', XB=10.5,12.0,48.0,49.5,0.8,1.0/  
&OBST ID='Barrel', XB=10.5,12.0,58.0,59.5,0.8,1.0/  
&OBST ID='wall 30deg.stl', XB=10.25,12.25,45.75,46.0,0.0,0.0/

&OBST ID='wall 30deg.stl', XB=10.25,12.25,45.75,46.0,0.2,0.2/  
&OBST ID='wall 30deg.stl', XB=10.25,12.25,45.5,45.75,0.5,0.5E/  
&OBST ID='wall 30deg.stl', XB=10.25,12.25,45.5,45.75,0.7,0.7/  
&OBST ID='wall 30deg.stl', XB=10.25,12.25,45.25,45.5,0.9,0.9/  
&OBST ID='wall 30deg.stl', XB=10.25,12.25,45.25,45.5,1.1,1.1E/  
&OBST ID='wall 30deg.stl', XB=10.25,12.25,45.0,45.25,1.3,1.3/  
&OBST ID='wall 30deg.stl', XB=10.25,12.25,45.0,45.25,1.5,1.5/  
&OBST ID='wall 30deg.stl', XB=10.25,12.25,46.0,46.0,0.0,0.2/  
&OBST ID='wall 30deg.stl', XB=10.25,12.25,45.75,45.75,0.0,0.7/  
&OBST ID='wall 30deg.stl', XB=10.25,12.25,45.5,45.5,0.5,1.1/  
&OBST ID='wall 30deg.stl', XB=10.25,12.25,45.25,45.25,0.9,1.5/  
&OBST ID='wall 30deg.stl', XB=10.25,12.25,45.0,45.0,1.3,1.7/  
&OBST ID='wall 30deg.stl', XB=10.25,10.25,45.75,46.0,0.0,0.2/  
&OBST ID='wall 30deg.stl', XB=10.25,10.25,45.5,45.75,0.5,0.7/  
&OBST ID='wall 30deg.stl', XB=10.25,10.25,45.25,45.5,0.9,1.1/  
&OBST ID='wall 30deg.stl', XB=10.25,10.25,45.0,45.25,1.3,1.5/  
&OBST ID='wall 30deg.stl', XB=12.25,12.25,45.75,46.0,0.0,0.2  
&OBST ID='wall 30deg.stl', XB=12.25,12.25,45.5,45.75,0.5,0.7/  
&OBST ID='wall 30deg.stl', XB=12.25,12.25,45.25,45.5,0.9,1.1/  
&OBST ID='wall 30deg.stl', XB=12.25,12.25,45.0,45.25,1.3,1.5/

&VENT ID='NAPTHAvent01', SURF\_ID='BlowNAPHTHA', XB=10.5,12.0,48.0,48.0,0.8,1.0/  
&VENT ID='Vent01', SURF\_ID='OPEN', XB=-40.0,60.0,-90.0,70.0,80.0,80.0/  
&VENT ID='Vent02', SURF\_ID='OPEN', XB=60.0,60.0,-90.0,70.0,0.0,80.0/  
&VENT ID='Vent03', SURF\_ID='OPEN', XB=-40.0,60.0,-90.0,-90.0,0.0,80.0/  
&VENT ID='Vent04', SURF\_ID='OPEN', XB=-40.0,-40.0,-90.0,69.75,0.0,79.75/  
&VENT ID='Vent05', SURF\_ID='AirBlow', XB=-40.0,60.0,70.0,70.0,0.0,80.0/  
&VENT ID='NAPTHAvent02', SURF\_ID='BlowNAPHTHA\_2nd', XB=10.5,12.0,58.0,58.0,0.8,1.0/

&SLCF QUANTITY='TEMPERATURE', ID='Temp', PBX=15.0/  
&SLCF QUANTITY='VELOCITY', VECTOR=.TRUE., ID='Air', PBX=15.0/  
&SLCF QUANTITY='VELOCITY', VECTOR=.TRUE., ID='AirX', PBX=11.5/  
&SLCF QUANTITY='VOLUME FRACTION', SPEC\_ID='N-PENTANE', ID='NAPHTHA', PBX=15.0/  
&SLCF QUANTITY='VOLUME FRACTION', SPEC\_ID='N-PENTANE', ID='NAPHTHA', PBX=11.5/

&DEVC ID='[Species: N-PENTANE] Volume Fraction\_MEAN', QUANTITY='VOLUME FRACTION',  
SPEC\_ID='N-PENTANE', SPATIAL\_STATISTIC='MEAN', XB=0.0,1.0,0.0,1.0,0.0,1.0/  
&DEVC ID='[Species: N-PENTANE] Volume Fraction\_VOLUME MEAN', QUANTITY='VOLUME  
FRACTION', SPEC\_ID='N-PENTANE', SPATIAL\_STATISTIC='VOLUME MEAN',  
XB=0.0,1.0,0.0,1.0,0.0,1.0/  
&DEVC ID='[Species: N-PENTANE] Volume Fraction\_MAX', QUANTITY='VOLUME FRACTION',  
SPEC\_ID='N-PENTANE', SPATIAL\_STATISTIC='MAX', XB=0.0,1.0,0.0,1.0,0.0,1.0/  
&DEVC ID='[Species: N-PENTANE] Mass Flux\_MEAN', QUANTITY='MASS FLUX', SPEC\_ID='N-  
PENTANE', SPATIAL\_STATISTIC='MEAN', XB=0.0,1.0,0.0,1.0,0.0,1.0/  
&DEVC ID='[Species: N-PENTANE] Mass Flux\_MAX', QUANTITY='MASS FLUX', SPEC\_ID='N-  
PENTANE', SPATIAL\_STATISTIC='MAX', XB=0.0,1.0,0.0,1.0,0.0,1.0/

&DEVC ID='[Species: N-PENTANE] Mass Fraction\_VOLUME INTEGRAL', QUANTITY='MASS FRACTION', SPEC\_ID='N-PENTANE', SPATIAL\_STATISTIC='VOLUME INTEGRAL',  
XB=0.0,1.0,0.0,1.0,0.0,1.0/  
&DEVC ID='[Species: N-PENTANE] Mass Fraction\_MASS INTEGRAL', QUANTITY='MASS FRACTION', SPEC\_ID='N-PENTANE', SPATIAL\_STATISTIC='MASS INTEGRAL',  
XB=0.0,1.0,0.0,1.0,0.0,1.0/  
&DEVC ID='[Species: N-PENTANE] Mass Fraction\_MEAN', QUANTITY='MASS FRACTION', SPEC\_ID='N-PENTANE', SPATIAL\_STATISTIC='MEAN', XB=0.0,1.0,0.0,1.0,0.0,1.0/

&TAIL /

- **Scenario Case02\_01\_new**

Case02\_01\_new.fds

Generated by PyroSim 2023.3.1206

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&HEAD CHID='Case02\_01\_new'/  
&TIME T\_END=30.0/  
&DUMP DT\_RESTART=10.0, DT\_SL3D=0.25/  
&MISC CFL\_MAX=0.8/

&MESH ID='MESH-01', IJK=40,80,120, XB=-40.0,-20.0,-90.0,-50.0,0.0,60.0, MPI\_PROCESS=0/  
&MESH ID='MESH-02', IJK=40,80,120, XB=-40.0,-20.0,-50.0,-10.0,0.0,60.0, MPI\_PROCESS=1/  
&MESH ID='MESH-03', IJK=40,80,120, XB=-40.0,-20.0,-10.0,30.0,0.0,60.0, MPI\_PROCESS=2/  
&MESH ID='MESH-04', IJK=40,80,120, XB=-40.0,-20.0,30.0,70.0,0.0,60.0, MPI\_PROCESS=3/  
&MESH ID='MESH-05', IJK=40,80,120, XB=-20.0,0.0,-90.0,-50.0,0.0,60.0, MPI\_PROCESS=4/  
&MESH ID='MESH-06', IJK=40,80,120, XB=-20.0,0.0,-50.0,-10.0,0.0,60.0, MPI\_PROCESS=5/  
&MESH ID='MESH-07', IJK=40,80,120, XB=-20.0,0.0,-10.0,30.0,0.0,60.0, MPI\_PROCESS=6/  
&MESH ID='MESH-08', IJK=40,80,120, XB=-20.0,0.0,30.0,70.0,0.0,60.0, MPI\_PROCESS=7/  
&MESH ID='MESH-09', IJK=40,80,120, XB=0.0,20.0,-90.0,-50.0,0.0,60.0, MPI\_PROCESS=8/  
&MESH ID='MESH-10', IJK=40,80,120, XB=0.0,20.0,-50.0,-10.0,0.0,60.0, MPI\_PROCESS=9/  
&MESH ID='MESH-11', IJK=40,80,120, XB=0.0,20.0,-10.0,30.0,0.0,60.0, MPI\_PROCESS=10/  
&MESH ID='MESH-12', IJK=40,80,120, XB=0.0,20.0,30.0,70.0,0.0,60.0, MPI\_PROCESS=11/  
&MESH ID='MESH-13', IJK=40,80,120, XB=20.0,40.0,-90.0,-50.0,0.0,60.0, MPI\_PROCESS=12/  
&MESH ID='MESH-14', IJK=40,80,120, XB=20.0,40.0,-50.0,-10.0,0.0,60.0, MPI\_PROCESS=13/  
&MESH ID='MESH-15', IJK=40,80,120, XB=20.0,40.0,-10.0,30.0,0.0,60.0, MPI\_PROCESS=14/  
&MESH ID='MESH-16', IJK=40,80,120, XB=20.0,40.0,30.0,70.0,0.0,60.0, MPI\_PROCESS=15/  
&MESH ID='MESH-17', IJK=40,80,120, XB=40.0,60.0,-90.0,-50.0,0.0,60.0, MPI\_PROCESS=16/  
&MESH ID='MESH-18', IJK=40,80,120, XB=40.0,60.0,-50.0,-10.0,0.0,60.0, MPI\_PROCESS=17/  
&MESH ID='MESH-19', IJK=40,80,120, XB=40.0,60.0,-10.0,30.0,0.0,60.0, MPI\_PROCESS=18/  
&MESH ID='MESH-20', IJK=40,80,120, XB=40.0,60.0,30.0,70.0,0.0,60.0, MPI\_PROCESS=19/

&SPEC ID='LiquidFuel', FYI='Liquid Benzene', FORMULA='C6H6', DENSITY\_LIQUID=879.0,  
SPECIFIC\_HEAT\_LIQUID=1.5, VAPORIZATION\_TEMPERATURE=80.0,  
MELTING\_TEMPERATURE=5.0, HEAT\_OF\_VAPORIZATION=433.0/

&REAC ID='FDS6 BENZENE\_TK',  
FYI='FDS6 Predefined',

FUEL='LiquidFuel',  
CRITICAL\_FLAME\_TEMPERATURE=1900.0,  
AUTO\_IGNITION\_TEMPERATURE=298.0,  
CO\_YIELD=0.067,  
SOOT\_YIELD=0.181,  
HEAT\_OF\_COMBUSTION=4.01E+4/

&DEVC ID='TIMER->OUT', QUANTITY='TIME', XYZ=-40.0,-90.0,0.0, SETPOINT=1.0/

&SURF ID='AirBlow',  
RGB=26,114,176,  
VEL=-10.0,  
TAU\_V=-1.0/

&SURF ID='BlowLiquid',  
RGB=204,204,0,  
MASS\_FLUX=600.0,  
SPEC\_ID='LiquidFuel',  
RAMP\_MF='BlowLiquid\_RAMP\_MF'/

&RAMP ID='BlowLiquid\_RAMP\_MF', T=10.0, F=0.0/  
&RAMP ID='BlowLiquid\_RAMP\_MF', T=10.5, F=1.0/  
&RAMP ID='BlowLiquid\_RAMP\_MF', T=11.5, F=1.0/  
&RAMP ID='BlowLiquid\_RAMP\_MF', T=12.0, F=0.0/

&SURF ID='Flame',  
COLOR='RED',  
HEAT\_TRANSFER\_COEFFICIENT=1000,  
NET\_HEAT\_FLUX=1000,  
RAMP\_Q='Flame\_RAMP\_Q'/

&RAMP ID='Flame\_RAMP\_Q', T=0.0, F=0.0/  
&RAMP ID='Flame\_RAMP\_Q', T=7.0, F=7.5/  
&RAMP ID='Flame\_RAMP\_Q', T=9.5, F=1.0/  
&RAMP ID='Flame\_RAMP\_Q', T=14.0, F=1.0/  
&RAMP ID='Flame\_RAMP\_Q', T=14.5, F=0.0/

&OBST ID='Barrel', XB=10.5,12.5,48.0,49.5,0.5,2.0/  
&OBST ID='Obstruction', XB=11.0,12.0,44.5,45.5,5.551115E-17,0.4, SURF\_ID='INERT'/

&VENT ID='BlowerVent', SURF\_ID='BlowLiquid', XB=10.5,12.5,48.0,48.0,0.5,2.0/  
&VENT ID='Vent01', SURF\_ID='OPEN', XB=-40.0,60.0,-90.0,70.0,60.0,60.0/  
&VENT ID='Vent02', SURF\_ID='OPEN', XB=60.0,60.0,-90.0,70.0,0.0,60.0/  
&VENT ID='Vent03', SURF\_ID='OPEN', XB=-40.0,60.0,-90.0,-90.0,0.0,60.0/  
&VENT ID='Vent04', SURF\_ID='OPEN', XB=-40.0,-40.0,-90.0,70.0,0.0,60.0/  
&VENT ID='Vent05', SURF\_ID='AirBlow', XB=-40.0,60.0,70.0,70.0,0.0,60.0/  
&VENT ID='Sparks', SURF\_ID='Flame', XB=11.0,12.0,44.5,45.5,0.4,0.4, DEVC\_ID='TIMER->OUT'/

&SLCF QUANTITY='TEMPERATURE', ID='Temp', PBY=45.0/

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&SLCF QUANTITY='VELOCITY', VECTOR=.TRUE., ID='Air', PBX=15.0/
&SLCF QUANTITY='VELOCITY', VECTOR=.TRUE., ID='AirX', PBX=11.5/
&SLCF QUANTITY='VOLUME FRACTION', SPEC_ID='LiquidFuel', ID='Benzene', PBX=15.0/
&SLCF QUANTITY='VOLUME FRACTION', SPEC_ID='LiquidFuel', ID='Benzene', PBX=11.5/
&SLCF QUANTITY='TEMPERATURE', ID='Slice', PBX=11.5/

&DEVC ID='[Species: LiquidFuel] Mass Flux_MEAN', QUANTITY='MASS FLUX',
SPEC_ID='LiquidFuel', SPATIAL_STATISTIC='MEAN', XB=-40.0,60.0,-90.0,70.0,0.0,60.0/
&DEVC ID='[Species: LiquidFuel] Mass Flux_MAX', QUANTITY='MASS FLUX', SPEC_ID='LiquidFuel',
SPATIAL_STATISTIC='MAX', XB=-40.0,60.0,-90.0,70.0,0.0,60.0/
&DEVC ID='[Species: LiquidFuel] Mass Fraction_VOLUME INTEGRAL', QUANTITY='MASS
FRACTION', SPEC_ID='LiquidFuel', SPATIAL_STATISTIC='VOLUME INTEGRAL', XB=-40.0,60.0,-
90.0,70.0,0.0,60.0/
&DEVC ID='[Species: LiquidFuel] Mass Fraction_MASS INTEGRAL', QUANTITY='MASS FRACTION',
SPEC_ID='LiquidFuel', SPATIAL_STATISTIC='MASS INTEGRAL', XB=-40.0,60.0,-90.0,70.0,0.0,60.0/

&TAIL /
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- **Scenario Case04\_05b**

Case04\_05b.fds

Generated by PyroSim 2023.3.1206

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```
&HEAD CHID='Case04_05b'/
&TIME T_END=30.0/
&DUMP DT_RESTART=10.0, DT_SL3D=0.25/
```

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&MESH ID='MESH-01', IJK=40,80,160, XB=-40.0,-20.0,-90.0,-50.0,0.0,80.0, MPI_PROCESS=0/
&MESH ID='MESH-02', IJK=40,80,160, XB=-40.0,-20.0,-50.0,-10.0,0.0,80.0, MPI_PROCESS=1/
&MESH ID='MESH-03', IJK=40,80,160, XB=-40.0,-20.0,-10.0,30.0,0.0,80.0, MPI_PROCESS=2/
&MESH ID='MESH-04', IJK=40,80,160, XB=-40.0,-20.0,30.0,70.0,0.0,80.0, MPI_PROCESS=3/
&MESH ID='MESH-05', IJK=40,80,160, XB=-20.0,0.0,-90.0,-50.0,0.0,80.0, MPI_PROCESS=4/
&MESH ID='MESH-06', IJK=40,80,160, XB=-20.0,0.0,-50.0,-10.0,0.0,80.0, MPI_PROCESS=5/
&MESH ID='MESH-07', IJK=40,80,160, XB=-20.0,0.0,-10.0,30.0,0.0,80.0, MPI_PROCESS=6/
&MESH ID='MESH-08', IJK=40,80,160, XB=-20.0,0.0,30.0,70.0,0.0,80.0, MPI_PROCESS=7/
&MESH ID='MESH-09', IJK=40,80,160, XB=0.0,20.0,-90.0,-50.0,0.0,80.0, MPI_PROCESS=8/
&MESH ID='MESH-10', IJK=40,80,160, XB=0.0,20.0,-50.0,-10.0,0.0,80.0, MPI_PROCESS=9/
&MESH ID='MESH-11', IJK=40,80,160, XB=0.0,20.0,-10.0,30.0,0.0,80.0, MPI_PROCESS=10/
&MESH ID='MESH-12', IJK=40,80,160, XB=0.0,20.0,30.0,70.0,0.0,80.0, MPI_PROCESS=11/
&MESH ID='MESH-13', IJK=40,80,160, XB=20.0,40.0,-90.0,-50.0,0.0,80.0, MPI_PROCESS=12/
&MESH ID='MESH-14', IJK=40,80,160, XB=20.0,40.0,-50.0,-10.0,0.0,80.0, MPI_PROCESS=13/
&MESH ID='MESH-15', IJK=40,80,160, XB=20.0,40.0,-10.0,30.0,0.0,80.0, MPI_PROCESS=14/
&MESH ID='MESH-16', IJK=40,80,160, XB=20.0,40.0,30.0,70.0,0.0,80.0, MPI_PROCESS=15/
&MESH ID='MESH-17', IJK=40,80,160, XB=40.0,60.0,-90.0,-50.0,0.0,80.0, MPI_PROCESS=16/
&MESH ID='MESH-18', IJK=40,80,160, XB=40.0,60.0,-50.0,-10.0,0.0,80.0, MPI_PROCESS=17/
&MESH ID='MESH-19', IJK=40,80,160, XB=40.0,60.0,-10.0,30.0,0.0,80.0, MPI_PROCESS=18/
&MESH ID='MESH-20', IJK=40,80,160, XB=40.0,60.0,30.0,70.0,0.0,80.0, MPI_PROCESS=19/
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&SPEC ID='SiliconOil\_SimpleFormula', FORMULA='C3H10O1.5', DENSITY\_LIQUID=963.0,  
SPECIFIC\_HEAT\_LIQUID=1.46, VAPORIZATION\_TEMPERATURE=150.0,  
MELTING\_TEMPERATURE=-50.0, HEAT\_OF\_VAPORIZATION=300.0/

&PART ID='SiliconOilDrops',  
SPEC\_ID='SiliconOil\_SimpleFormula',  
DIAMETER=500.0,  
MONODISPERSE=.TRUE.,  
QUANTITIES='PARTICLE VELOCITY',  
AGE=10.0/

&REAC ID='SiliconFuel\_TK',  
FUEL='SiliconOil\_SimpleFormula',  
CRITICAL\_FLAME\_TEMPERATURE=1900.0,  
AUTO\_IGNITION\_TEMPERATURE=450.0,  
CO\_YIELD=4.0E-3,  
SOOT\_YIELD=0.2,  
HEAT\_OF\_COMBUSTION=1.7E+4/

&DEVC ID='TIMER->OUT', QUANTITY='TIME', XYZ=-40.0,-90.0,0.0, SETPOINT=1.0/

&SURF ID='AirBlow',  
RGB=26,114,176,  
VEL=-10.0,  
TAU\_V=-1.0/

&SURF ID='Flame',  
COLOR='RED',  
HEAT\_TRANSFER\_COEFFICIENT=1000.0,  
NET\_HEAT\_FLUX=1000.0,  
RAMP\_Q='Flame\_RAMP\_Q'/

&RAMP ID='Flame\_RAMP\_Q', T=0.0, F=0.0/  
&RAMP ID='Flame\_RAMP\_Q', T=7.0, F=7.5/  
&RAMP ID='Flame\_RAMP\_Q', T=9.5, F=1.0/  
&RAMP ID='Flame\_RAMP\_Q', T=14.0, F=1.0/  
&RAMP ID='Flame\_RAMP\_Q', T=14.5, F=0.0/

&SURF ID='BlowLiquid',  
RGB=204,204,0,  
VEL=-10.0,  
MASS\_FRACTION=1.0,  
SPEC\_ID='SiliconOil\_SimpleFormula',  
RAMP\_MF='BlowLiquid\_RAMP\_MF',  
PART\_ID='SiliconOilDrops',  
NPPC=10,  
PARTICLE\_MASS\_FLUX=600.0,  
RAMP\_PART='BlowLiquid\_RAMP\_PART'/

&RAMP ID='BlowLiquid\_RAMP\_MF', T=10.0, F=0.0/

&RAMP ID='BlowLiquid\_RAMP\_MF', T=10.5, F=1.0/  
&RAMP ID='BlowLiquid\_RAMP\_MF', T=11.5, F=1.0/  
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