TECHNICAL REPORT

# ISO/TR 16730-3

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# Fire safety engineering — Assessment, verification and validation of calculation methods —

## Part 3: Example of a CFD model

*Ingénierie de la sécurité incendie — Évaluation, vérification et validation des méthodes de calcul —*

*Partie 3: Exemple d'un modèle CFD*

Reference number
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# Foreword

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The committee responsible for this document is ISO/TC 92, *Fire safety*, Subcommittee SC 4, *Fire safety engineering*.

ISO 16730 consists of the following parts, under the general title *Fire Safety Engineering — Assessment, verification and validation of calculation methods*:

— *Part 3: Example of a CFD model*

— *Part 5: Example of an Egress model* (Technical report)

The following parts are under preparation:

— Part 2: *Example of a fire zone model* (Technical report)

— Part 4: *Example of a structural model* (Technical report)

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# Fire safety engineering — Assessment, verification and validation of calculation methods —

# Part 3: Example of a CFD model

## 1 Scope

ISO 16730-1 describes what the contents of a technical documentation and of a user's manual should be for an assessment, if the application of a calculation method as engineering tool to predict real-world scenarios leads to validated results. The purpose of this part of ISO 16730 is to show how ISO 16730-1 is applied to a calculation method, for a specific example. It demonstrates how technical and users' aspects of the method are properly described in order to enable the assessment of the method in view of verification and validation.

The example in this part of ISO 16730 describes the application of procedures given in ISO 16730-1 for a computational fluid dynamics (CFD) model (ISIS).

The main objective of the specific model treated in this part of ISO 16730 is the simulation of a fire in an open environment or confined compartments with natural or forced ventilation system.

## 2 Normative references

The following documents, in whole or in part, are normatively referenced in this document and are indispensable for its application. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 16730-1, *Fire safety engineering — Assessment, verification and validation of calculation methods — Part 1: General*

## 3 General information on the CFD model considered

The name given to the CFD model considered in this part of ISO 16730 is "ISIS". The computer code ISIS, developed by The French Institute for Radiological Protection and Nuclear Safety (IRSN) and defined as a computational fluid dynamic model (also called CFD or field model), is based on a coherent set of models that can be used to simulate a fire in large and mechanically ventilated compartments. This kind of configuration involving complex flows requires an accurate physical modelling and efficient numerical methods. Usually, the spatial and time scales encountered in fires are very disparate and the coupling between phenomena is very strong.

The verification and validation phases of the code are two distinct processes which are constantly updated based on the last code developments. The verification phase employs a wide range of techniques such as the comparison to an analytical solution for model problems, the use of manufactured solution, and the comparison to benchmark result. The validation process is based on the so-called building-block approach including first-unit problems, sub-system cases, and then large-scale realistic fire experiments. This process allows dividing a complex engineering system into several simpler cases. Consequently, the validation guide of this code[1] includes laminar, turbulent, and fire cases and contains a total of 18 test cases.

## 4 Methodology used in this part of ISO 16730

For the calculation method considered, checks based on ISO 16730-1 and as outlined in this part of ISO 16730 are applied. This part of ISO 16730 lists in Annexes A and B the important issues to be checked in a left-hand column of a two-column table. The issues addressed are then described in detail and it is shown how these were dealt with during the development of the calculation method in the right-hand column of Annexes A and B, where Annex A covers the description of the calculation method and Annex B covers the complete description of the assessment (verification and validation) of the particular calculation method. Annex C describes a worked example, and Annex D adds a user's manual.

# Annex A
(informative)

# Description of the calculation method

## A.1 Purpose

| | |
|---|---|
| Definition of problem solved or function performed | — The main objective of this calculation method is to simulate a fire in an open environment or confined compartments with natural or forced ventilation system.<br>— The basic modelling relies on a low Mach number formulation of the Navier-Stokes equations combined with a turbulent combustion model adapted for variable density flow. |
| (Qualitative) description of results of the calculation method | — Output includes<br>— gas temperature in the fire room and neighbouring rooms,<br>— pressure variation during the fire,<br>— inlet and outlet mass flow rates in the admission and extraction branches of the compartment,<br>— heat flux received by a wall,<br>— oxygen depletion in the compartment, and<br>— combustion products in the compartment and target rooms. |
| Justification statements and feasibility studies | The effect of the fire growth process on the ventilation network is a major concern for Fire Safety Analysis. Consequently, the model has been developed to allow the coupling between a ventilation network and a fire in a mechanically ventilated compartment. Pressure variations in the fire compartment are also connected on the ventilation network and can cause reverse flows in the inlet or exhaust branches. This critical scenario is also of major interest for Fire Safety Analysis. |

## A.2 Theory

| | |
|---|---|
| Underlying conceptual model (governing phenomena) | Physical modelling in this calculation method is based on classical local conservations laws for physical quantities such as mass, momentum (in a low-speed flow formulation), energy, and species concentrations. Governing formulae in the case of a fire simulation describe a turbulent reactive flow with radiative transfers. |
| Theoretical basis of the phenomena and physical laws on which the calculation method is based | This field model is a Reynolds-Averaged Navier-Stokes (RANS) model with a two-formula closure for turbulent flow.<br>The scalars fluxes are modelled by the gradient diffusion assumption and buoyancy effects are considered in turbulence production terms. The combustion model is based on the conserved scalar approach and assumes a fast chemistry. It relies on a modified eddy break up model for non-premixed combustion. |

## A.3 Implementation of theory

| | |
|---|---|
| Governing formulae | The set of governing formulae are described in detail in References [2] and [5].<br>To simulate a fire in a confined compartment, the following governing formulae are solved:<br>— RANS equations;<br>— two-formula turbulence closure ($k$-$\varepsilon$);<br>— mixture fraction (combustion process);<br>— fuel mass fraction;<br>— enthalpy;<br>— radiation transfers;<br>— Bernoulli equations for inlet and exhaust branches.<br>The density of the reactive mixture is defined using the ideal gas law (equation of state of perfect gas) and the mean molecular weight of individual species of the mixture. |

| | |
|---|---|
| Mathematical techniques, procedures, and computational algorithms employed, with references to them | The balance formulae for scalars (species, enthalpy, etc.) are discretized in time and in space using a finite volume method to obtain schemes that achieve a good compromise between the calculation time and accuracy and ensure that unknowns stay within their physical boundaries; second-order up winding techniques are used to accurately take into account fast spatial variations in unknowns, without stability loss. The Navier-Stokes equations are discretized in space using a finite element technique that satisfies the compatibility properties between velocity and pressure necessary for stability. Unlike finite volume schemes with staggered meshes, this technique also makes it easy to use meshes that are locally unstructured due to the geometry involved or refinement. To ensure coherence with the finite volume discretization, the approximation selected is low-order and conforming.[10] The temporal discretization is performed with a fractional step scheme such that in Reference [11]. This semi-implicit scheme allows large time-step while each formula is solved in sequence.<br><br>The model is based on the scientific computing development platform PELICANS, which is available as open-source software (https://gforge.irsn.fr/gf/project/pelicans). PELICANS offers a library of software components, consisting of "building blocks" for implementing numerical methods. The model is entirely parallelized via this platform, for both the assembly and solution of discrete systems. |
| Identification of each assumption embedded in the logic; limitations on the input parameters that are caused by the range of applicability of the calculation method | — structured mesh;<br><br>— hydrodynamic model: low Mach number assumption;<br><br>— molecular diffusion: each species of the mixture have the same mass diffusion coefficient;<br><br>— heat capacity: only constant heat capacity is used;<br><br>— turbulence model: RANS formulation, Boussinesq approximation for the eddy viscosity, simple gradient diffusion hypothesis, constant turbulent Prandtl, or Schmidt number;<br><br>— combustion model: non-premixed combustion, unity Lewis approximation;<br><br>— heat transfer model: 1D heat conduction in walls;<br><br>— radiation model: gray media assumption, no diffusion in the Radiative Transfer Equation. |
| Discussion of precision of the results obtained by important algorithms, and, in the case of computer models, any dependence on particular computer capabilities | In general, the results given by the model for the simulation of a fire in a confined compartment are in good agreement with the measurements. An error of the order of 10 % to 20 % is observed for temperature, species mass fraction, wall heat flux, pressure, and ventilation flow rate variations. |
| Description of results of the sensitivity analyses | Work described in Reference [12]. |

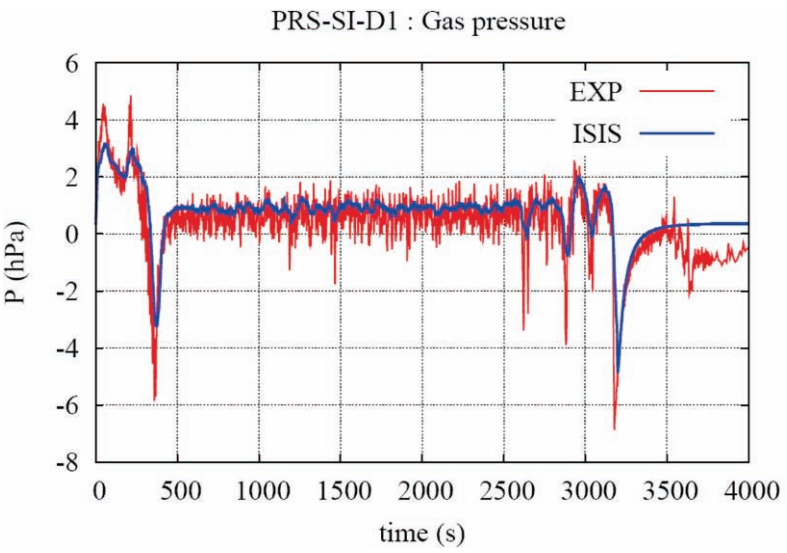
## A.4 Input

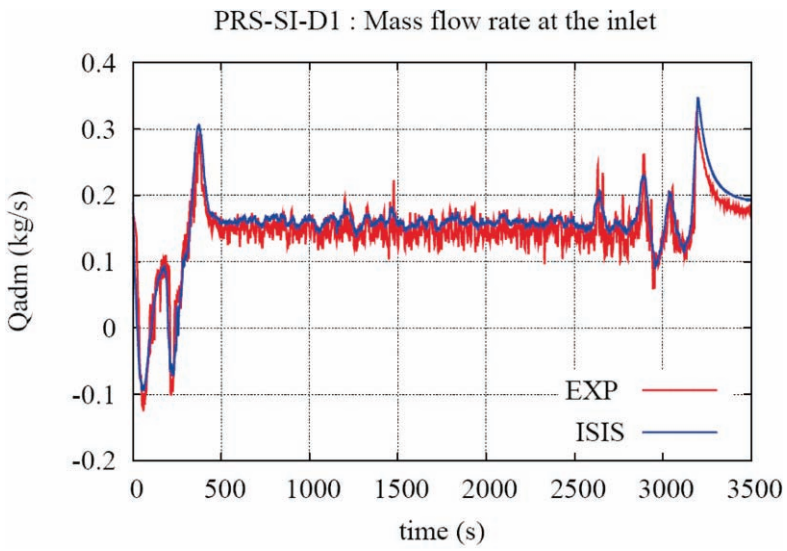
| | |
|---|---|
| Required input | — geometry;<br>— mesh;<br>— time-step;<br>— thermophysical properties (for fuel, walls, insulation);<br>— initial conditions;<br>— boundary conditions;<br>— resistance of the inlet and exhaust branches. |
| Source of the data required | — Data for geometry, time, and space discretization are user's input.<br>— Material properties should be taken from test or literature. |
| For computer models: any auxiliary programs or external data files required | LINUX distribution with<br>— gcc 4 (or newer version),<br>— GNU make 3.77 (or newer version),<br>— PERL 5.6 (or newer version), and<br>— Java 1.5.0 (or newer version).<br>Postprocessing tools are<br>— Meshtv,<br>— OpenDX,<br>— GMV,<br>— PARAVIEW, or<br>— FIELDVIEW.<br>Mesh generation with ISIS or<br>— Emc2,<br>— Mefisto,<br>— Gambit, or<br>— GMSH. |
| Provide information on the source, contents, and use of data libraries for computer models | Data libraries concerning fuel properties or walls or insulation materials can be found in SFPE Handbook of Fire Protection Engineering. |

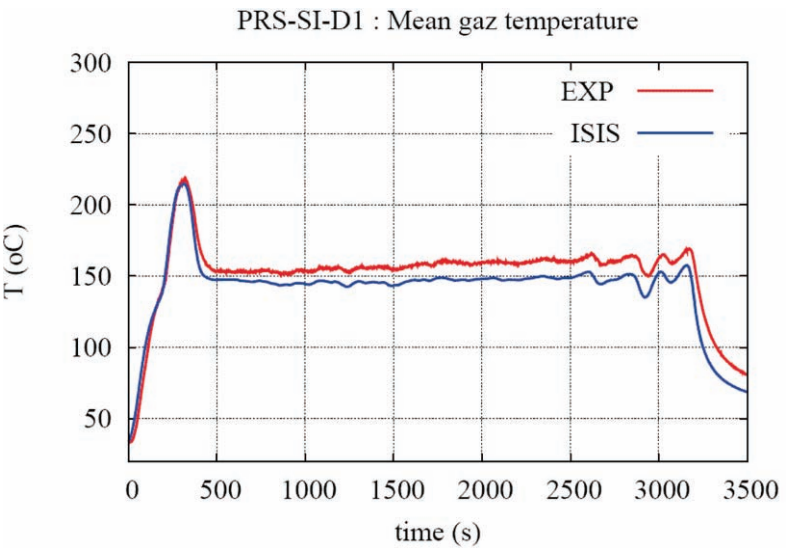
# Annex B
(informative)

# Complete description of the assessment (verification and validation) of the calculation method

| | |
|---|---|
| (Quantitative) results of any efforts to evaluate the predictive capabilities of the calculation method in accordance with Clause 5 of ISO 16730-1 | The verification process of the code is presented in Reference [5]. About 20 cases are performed and include comparisons to analytical solutions, manufactured solutions, and benchmark cases. Some of these examples can be found in References [4], [5], [10], and [11].<br>The validation process used for the assessment of the fire model is described in Reference [1]and an example is given in References [5] and [6].<br>The validation guide[1] contains 18 test cases:<br>— laminar cases (5)<br>— 3D backward-facing step<br>— laminar diffusion flame of methane<br>— 2D laminar jet<br>— radiation heat transfers in a 3D idealized furnace<br>— convection and radiation in a 3D differentially heated cavity<br>— turbulent cases (10)<br>— turbulent flow with a square obstacle<br>— natural convection in an enclosed cavity<br>— thermal plumes<br>— 2D buoyant diffusion flame<br>— turbulent jet flame I: no coupling between the flow and the soot<br>— turbulent jet flame II: coupling between the flow and the soot<br>— 2D cartesian turbulent jet<br>— radiative transfers in a turbulent piloted jet flame<br>— radiative transfers in a turbulent sooty flame<br>— pyrolysis of polymethylmethacrylate (PMMA) in a cone calorimeter<br>— fire cases (3)<br>— LIC1.14 test<br>— PRISME Source test PRS-SI-D1<br>— PRISME Source tests PRS-SI-D3<br>An example of a quantitative comparison is given for a confined fire test performed at the IRSN Fire Test Laboratory. Pressure, admission flow rate, and mean gas temperature calculated by the model are plotted versus time and compared to experimental measurements. |



| | |
|---|---|
| References to reviews, analytical tests, comparison tests, experimental validation, and code checking already performed [If, in case of computer models, the validation of the calculation method is based on beta testing, the documentation should include a profile of those involved in the testing (e.g. were they involved to any degree in the development of the calculation method or were they naive users; were they given any extra instruction that would not be available to the intended users of the final product, etc.)] | Verification: References [4], [5], [10], and [11]<br>Validations: References [1],[4],[5],[6],[7],[8], and[9] |
| The extent to which the calculation method meets this part of ISO 16730 | The V&V process for this particular model meets the requirements of ISO 16730-1. |

# Annex C
(informative)

# Worked example

## C.1 General

The example below is taken from Reference [1].

The simulation of a real-scale experimental fire is addressed in this Annex. This test has been performed at IRSN, as a part of an experimental program performed to provide data for the validation of computational tools simulating fires in mechanically ventilated compartments, with first application to nuclear power plant. This test turns out to be particularly difficult, for essentially two reasons. The first one is that the large-scale geometry of the studied problem and the duration of the transient of interest make the computational requirements considerable; the first concern is then to assess the code stability and convergence for such systems. Second, the flow results from an intricate coupling between nonlinear phenomena, as turbulence, combustion, and buoyancy effects; separate validation of each single model is then clearly out of reach, and relied for this purpose on the previously described building-block approach. In the same direction, note in addition that the knowledge of initial and boundary conditions, together with the characterization of the flow, is necessarily less comprehensive than in experiments carried out at the laboratory scale, which even reinforces the interest of validating each "elementary" model using simpler experiments.

## C.2 Problem description

The experiment consists in a confined ethanol pool fire in a compartment mechanically ventilated with a metal cupboard close to the fire. The schematic diagram of the compartment fire is shown in Figure C.1. The dimensions are for the $x$, $y$, and $z$ directions, respectively, $Lx$ = 9 m, $Ly$ = 6 m, and $Lz$ = 7,5 m. The different walls, the floor, and the ceiling are 0,25-m thick concrete walls. The compartment is connected to a ventilation network including a forced ventilation supply inlet and a forced ventilation exhaust vent (Figure C.1) with dimensions of 0,3 $m^2$ and 0,4 $m^2$, respectively. The ventilation rate is 5 $h^{-1}$ and the depression –200 Pa. The pool fire is a square of surface 1 $m^2$ and height 0,13 m, located at the centre of the compartment. The fire heat release rate, defined as the product of the fuel mass loss rate and the heat of combustion of ethanol, reaches 563 kW during the stationary combustion phase Figure C.2.

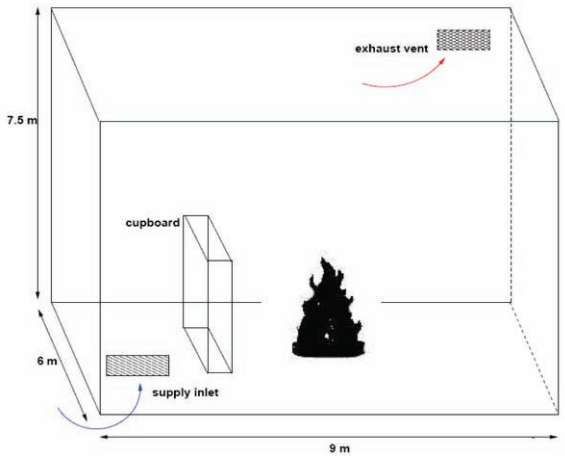



**Figure C.1 — Experimental fire case geometry**

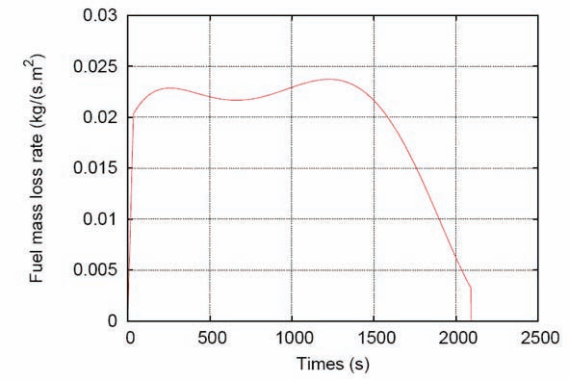



**Figure C.2 — Fuel mass loss rate in the experimental fire case**

The system describing the turbulent reactive flow in the low Mach number regime is presented below. The approximation turbulence resorts to the mass-weighted averaging, also called the Favre averaging. A modified $k$-$\varepsilon$ model based on the Boussinesq hypothesis and the eddy viscosity model is used for turbulence closure. To model the turbulent combustion process, a fast chemistry assumption and the conserved scalar approach are used; the mixture fraction variable $z$ and the fuel mass fraction $Y_F$ are kept as unknowns variables. Removing for short in the notations the Favre or Reynolds turbulence averaging operators, governing formulae read:

— mass balance:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathrm{v} = 0 \tag{C.1}$$

— momentum balance:

$$\frac{\partial \rho \mathrm{v}}{\partial t} + \nabla \cdot \left( \rho \mathrm{v} \otimes \mathrm{v} \right) = -\nabla p + \nabla \cdot \tau + \left( \rho - \rho_0 \right) g \tag{C.2}$$

— turbulent kinetic energy balance:

$$\frac{\partial \rho k}{\partial t} + \nabla \cdot \rho \mathrm{v} k = \nabla \cdot \left( \frac{\mu_e}{\sigma_k} \nabla k \right) + G_k + G_b - \rho \varepsilon \tag{C.3}$$

— viscous dissipation balance:

$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot \rho \mathrm{v} \varepsilon = \nabla \cdot \left( \frac{\mu_e}{\sigma_\varepsilon} \nabla \varepsilon \right) + \frac{\varepsilon}{k} \left( c_{\varepsilon 1,1} G_k + c_{\varepsilon 1,2} G_b - c_{\varepsilon 2} \rho \varepsilon \right) \tag{C.4}$$

— enthalpy balance:

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot \rho \mathrm{v} h = \nabla \cdot \left( \frac{\mu_e}{\sigma_h} \nabla h \right) + \frac{dP_{th}}{dt} \tag{C.5}$$

— mixture fraction balance:

$$\frac{\partial \rho z}{\partial t} + \nabla \cdot \rho \mathrm{v} z = \nabla \cdot \left( \frac{\mu_e}{\sigma_z} \nabla z \right) \tag{C.6}$$

— fuel mass fraction balance:

$$\frac{\partial \rho Y_F}{\partial t} + \nabla \cdot \rho \mathrm{v} Y_F = \nabla \cdot \left( \frac{\mu_e}{\sigma_{Y_F}} \nabla Y_F \right) + \dot{\omega}_F \tag{C.7}$$

The Reynolds stress tensor, $\tau$, appearing in the momentum formula, is expressed as:

$$\tau = \mu_e \left( \nabla \mathrm{u} + \nabla^t \mathrm{u} - \frac{2}{3} (\nabla \cdot \mathrm{u}) \mathrm{I} \right) - \frac{2}{3} \rho k \mathrm{I} \tag{C.8}$$

Turbulent production terms are defined as:

$$G_k = \tau \otimes \nabla \mathrm{v} \tag{C.9}$$

$$G_b = \frac{\mu_t}{\rho \sigma_g} \nabla \rho \cdot g \tag{C.10}$$

where the term $G_b$ stands for the generation and destruction of turbulence due to buoyancy forces. In multicomponent mixtures, the density of the mixture is evaluated by:

$$\rho = \frac{P_{th} W}{R_u T} \tag{C.11}$$

with

$$\frac{1}{W} = \sum_{k=1}^{N} \frac{Y_k}{W_k} \tag{C.12}$$

where $W$ is the mean molar weight of the mixture and $Y_k$ and $W_k$, respectively, stand for the mass fraction and the atomic weight of species $k$ (i.e. fuel, etc.). The fuel burning rate is calculated according to:

$$\dot{\omega}_F = -C_{\mathrm{EBU}} \rho \frac{\varepsilon}{k} \min \left( Y_F, \frac{Y_O}{s} \right) \tag{C.13}$$

where $C_{\mathrm{EBU}}$ is a model constant commonly taken of the order of four but which can be modelled by a viscous mixing model; here, the first option, $C_{\mathrm{EBU}} = 4$, is used. To deal with radiative losses, the so-called Markstein model is used, so the specific enthalpy is linked to the temperature by the following relation:

$$h = c_p (T - T_0) + \Delta H_c (1 - \chi_r) Y_F \tag{C.14}$$

where $T_0$ is a reference temperature, $\Delta H_c$ is the heat of combustion and $\chi_r$ is the fraction of energy of combustion lost by radiative transfer; $\chi_r$ is set to 0,25 in this simulation. The model constants have the following standard values:

$$c_\mu = 0{,}09 \quad c_{\varepsilon 1,1} = 1{,}44 \quad c_{\varepsilon 2} = 1{,}92 \quad c_{\varepsilon 1,2} = 1{,}44$$

$$\sigma_k = 1 \qquad \sigma_\varepsilon = 1{,}3 \qquad \sigma_h = \sigma_z = \sigma_{Y_F} = 0{,}71$$

The thermodynamic pressure of the room is computed by solving a simplified (0D) momentum balance formula for the system composed of the confined compartment and the ventilation network. In this

modelling, a Bernoulli general equation describes each branch *i* of the network, which is, in this particular case, connected to the compartment:

$$\frac{L_i}{S_i}\frac{\partial Q_i}{\partial t} = P_{th} - P_{\text{node},i} - f \tag{C.15}$$

where $Q_i$ is the flow rate in the branch *i*, $P_{\text{node},i}$ is the pressure at extremity of the branch which is not located at the compartment wall, and *f* is an aerodynamic resistance. The geometrical dimensions $L_i$ and $S_i$ are, respectively, the length and the surface of the branch *i*. This system shall be supplemented by the overall mass balance formula of the compartment:

$$\int_{\Omega}\frac{\partial}{\partial t}\left(\frac{P_{th}W}{RT}\right) + \sum_i Q_i = 0 \tag{C.16}$$

Geometrical and material properties are gathered in the following tables:

— gas mixture:

  dynamic viscosity: $\mu = 1{,}68 \times 10^{-5}$ kg/(m·s)

  thermal conductivity: $\lambda = 0{,}018$ W/(m·K)

  specific heat: $c_p = 1\,100$ J/(kg·K)

  Prandtl number: $Pr = 0{,}71$

  heat of combustion: $\Delta H_c = 2{,}56 \times 10^7$ J/kg

— concrete walls:

  density: $\rho_w = 2\,430$ kg/m$^3$

  thermal conductivity: $\lambda_w = 1{,}5$ W/(m·K)

  specific heat: $c_{p,w} = 736$ J/(kg·K)

  walls thickness: $e_w = 0{,}25$ m

— metal cupboard:

  density: $\rho_c = 7\,801$ kg/m$^3$

  thermal conductivity: $\lambda_c = 43$ W/(m·K)

  specific heat: $c_{p,c} = 473$ J/(kg·K)

  walls thickness: $e_c = 0{,}25$ m

Initial conditions are given by:

$$V = p = h = z = Y_F = 0 \tag{C.17}$$

$$k = 10^{-12}\ \text{m}^2/\text{s}^2 \tag{C.18}$$

$$\varepsilon = 10^{-9}\ \text{m}^2/\text{s}^3 \tag{C.19}$$

$T = 290$ K; $\rho = \rho_{air}$ (C.20)

To define the boundary conditions, three different surfaces are considered:

— Fire: $v = (0, 0, w_F)$; $h = \Delta H_c (1 - \chi_r)$; $z = Y_F = 1$; $k = 0{,}1\ w_F^2$; $\varepsilon = C_\mu k^{3/2}/l_\varepsilon$

where $w_F$ is function of the fuel mass loss rate; $w_F = m_F/\rho_F$; and $l_\varepsilon = 0{,}07L^*$ with $L^*$ a characteristic length scale, equivalent to fire radius.

— Walls: conduction in walls is accounted for in the energy balance equation. A log-law wall function is used for the momentum and turbulence balance formulae.

— Supply inlet and exhaust vent: a prescribed velocity is computed to match the flow rate in each branch; fuel is supposed to remain in the compartment.

## C.3 Numeric

Various non-uniform grid are tested with 8 500, 68 000, and 240 000 meshes named thereafter mesh1, mesh2, and mesh3. Numerical parameters and main features of the numerical scheme are gathered in the following table.

| | |
|---|---|
| Initial time | 0 |
| Final time | mesh1: 2 800 s; mesh2: 1 000 s; mesh3: 250 s |
| Time-step | mesh1, mesh2: $\Delta t = 0{,}1$ s; mesh3: $\Delta t = 0{,}05$ s |
| Solution algorithm | semi-implicit fractional step scheme implemented for transport formulae for $k$, $\varepsilon$, $h$, $z$, and $Y_F$ variables; implicit coupling between the $k$-$\varepsilon$ two formulae and the two transport formulae for $z$ and $Y_F$ is obtained by a fixed point algorithm |
| Time discretization | first order (backward Euler) scheme |
| Spatial discretization | upwinding approximation for the convective terms of the $k$-$\varepsilon$ and Navier-Stokes equations |

## C.4 Results

### Thermodynamic pressure and mass flow rate

The evolution of the thermodynamic pressure in the compartment fire as a function of time (see Figure C.3) is in a good agreement with the experiment data. During the combustion stationary phase, the calculated pressure oscillates around −2 hPa and the amplitude of the oscillations is less strong than in the experiment. A strong overpressure at ignition and a weak depression at extinction are observed in both cases. The evolution of mass flow rate at the supply inlet according to time is shown in Figure C.4. It stabilizes around 0,7 kg/s after a short period corresponding to the ignition phase. The mass flow rate at exit, not shown here, is almost identical. These results lie in the uncertainty range of the experimental data.

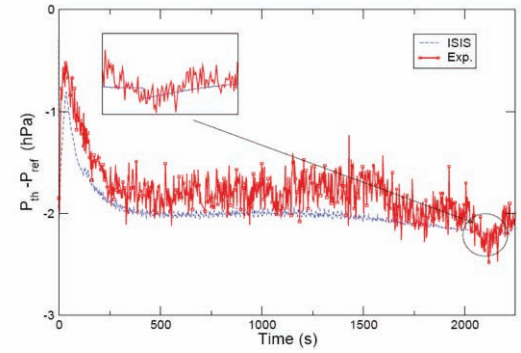



**Figure C.3 — Thermodynamic pressure vs. time**

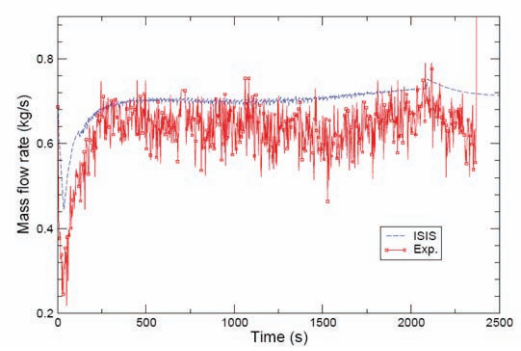



**Figure C.4 — Mass flow rate at admission vs. time**

### Temperature in the plume region

The evolution of temperature with time in the plume region, 3 m above the fire, obtained with mesh1 is presented for the whole transient in Figure C.5. After the time $t$ = 250 s, both the computed and experimental temperatures oscillate around similar values until the end of fire. The predicted peak of temperature in the early transient, not observed in experiments, could be due to the absence of models in the code to simulate combustion in the transition from the laminar to the turbulent flow regime, as occurs at ignition. Figure C.6 points out strong temporal variations of temperature corresponding to a rotation of the flame around its axis. This flame rotational behaviour is also observed in experiments with an almost equal frequency.

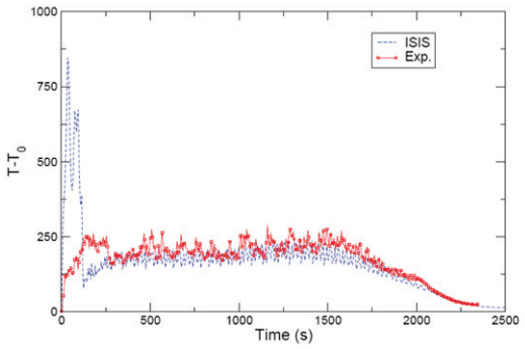



**Figure C.5 — Temperature vs. time to 3 m above the fire**

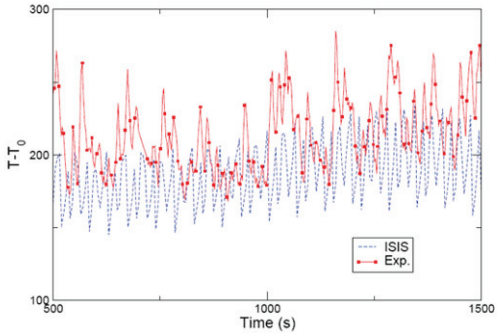



**Figure C.6 — Temperature vs. time to 3 m above the fire**

# Annex D
(informative)

# User's manual

## D.1 General

The example below is taken from Reference [3].

This tutorial presents the case of a fire in a room with an open door. In this example, the combustion module is not used and the flame is modelled by a volumetric heat release rate at the level of the fire.

The complete input file is found in the directory "tutorial/RoomFire" within the ISIS root directory. It can be edited using the series of commands below:

source < ISIS_DIR > /bin/init.csh or . < ISIS_DIR > /bin/init.sh

cd < ISIS_DIR > /ISIS/tutorial/RoomFire

xisis data.pel

Objectives:

— generate a mesh for a simple 3D domain and define a door;

— define a turbulent flow;

— define a volumetric heat source at the level of the fire.

## D.2 Description

A fire in a room is simulated by a volumetric heat release rate generated at the level of the fire. The room is connected to the exterior by an open door. This test case is widely cited in the literature; refer to the experimental work in Reference [13], and the numerical work in Reference [14].

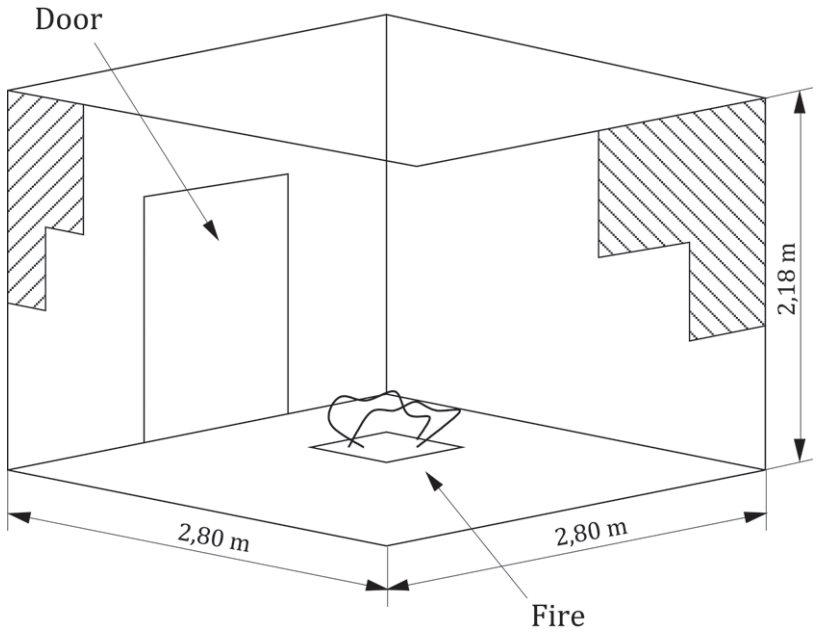



**Figure D.1 — Room configuration**

## D.3 Mesh definition

The first step is to define the mesh.

It is started by choosing the type of geometry. This example involves 3D Cartesian computation.

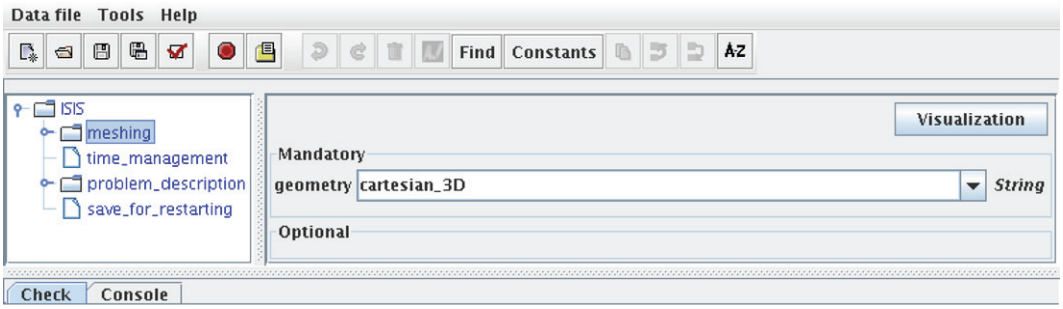



**Figure D.2 — Geometry**

The PELICANS "GE_BoxWithBoxes" internal mesh generator is used to create a mesh for the domain. The mesh description simply involves defining the "vertices_coordinates_0" input for the *x* direction, the "vertices_coordinates_1" input for the *y* direction, and the "vertices_coordinates_2" input for the *z* direction.

The fire is represented by a volumetric heat source in the centre of the room with a volume of 0,3 m × 0,3 m × 0,3 m.

In the *x* direction, a mesh for [0;2,80] shall be generated, taking into account the mesh for the fire. Thus, four mesh cells are placed between the walls and the fire, and one cell in the fire:

```
vertices_coordinates_0 =   (regular_vector(0.00, 4, 1.25) <<
        regular_vector(1.25, 1, 1.55) <<
        regular_vector(1.55, 4, 2.80))
```

In the *y* direction, a mesh for segment [0;2,80] shall be generated, taking into account the mesh for the fire and the door. Three mesh cells are placed between the walls and the door, one between the door and the fire, and one in the fire:

```
vertices_coordinates_1 =   (regular_vector(0.00, 3, 1.03) <<
        regular_vector(1.03, 1, 1.25) <<
        regular_vector(1.25, 1, 1.55) <<
        regular_vector(1.55, 1, 1.77) <<
        regular_vector(1.77, 3, 2.80))
```

In the *z* direction, a mesh for segment [0;2,18] shall be generated, taking into account the mesh for the fire and the door. One mesh cell is placed in the fire, five between the fire and the top of the door, and one above the door:

```
vertices_coordinates_2 =   (regular_vector(0.00, 1, 0.30) <<
        regular_vector(0.30, 5, 1.83) <<
        regular_vector(1.83, 1, 2.18))
```

An intentionally coarse mesh with 9 × 9 × 7 = 567 mesh cells, each cell having a characteristic size of around 30 cm, is obtained.

## D.4 Choosing a time-step

In the example, a time-step of 0,25 s and a final time of 20 s are chosen.

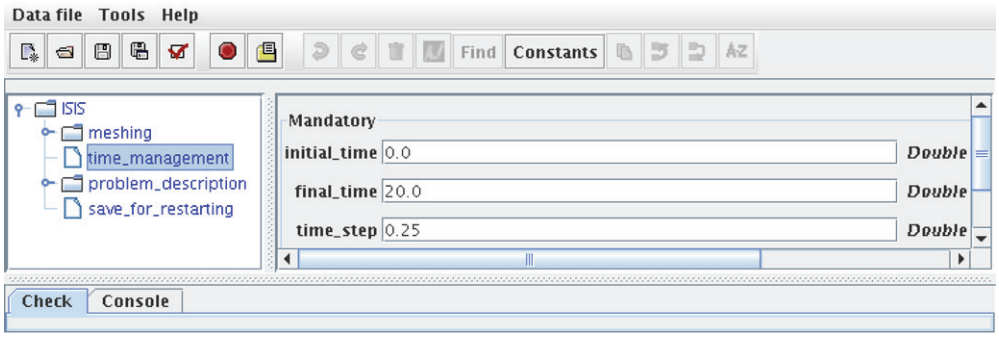



**Figure D.3 — "time_management" menu**

## D.5 Defining the problem of interest

This example involves a turbulence calculation: "low_mach" is selected for *Navier_Stokes, energy_balance* is activated, and "k_epsilon" is chosen for *turbulence_model*.

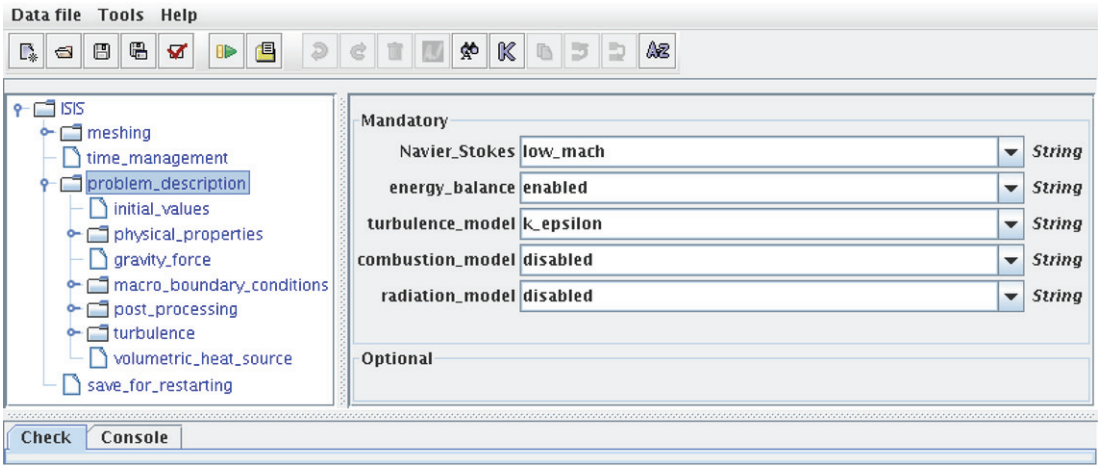



**Figure D.4 — Defining the problem of interest**

## D.6 Defining the initial value of unknowns

In the next step, the initial value of the fields is defined. The type of flow selected defines the unknowns for the problem and thus the initial unknown values needed to set are as follows.

— Because the fluid is at rest in the beginning, a zero initial value is imposed for velocity.

— For enthalpy, the law $H = c_p\ (T - T_0)$ is chosen where $T_0$ is the initial fluid temperature; initial enthalpy is thus set at 0;

— Finally, an initial value for the $k$ and $\varepsilon$ fields is provided, 0,001 in this case.

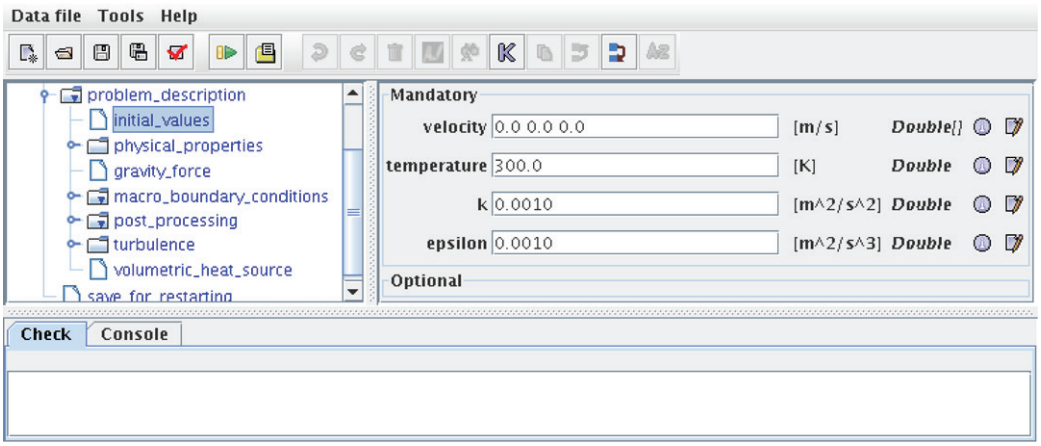



**Figure D.5 — Initial values**

## D.7 Defining fluid properties

The type of problem also defines the fluid properties to be specified, in this example the laws for density, laminar viscosity, conductivity, specific heat, and enthalpy.

For density, the "dilatable" law is chosen, for which $\rho T = \rho_0 T_0$. The reference density, $\rho_0 = 1$, and the temperature, $T_0 = 300$, shall then be entered.

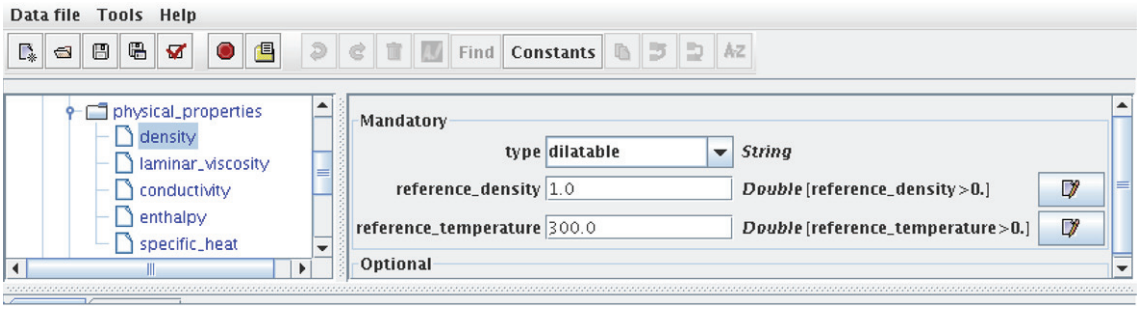



**Figure D.6 — Density: $\rho T$ = constant**

The other laws are defined in the same way:

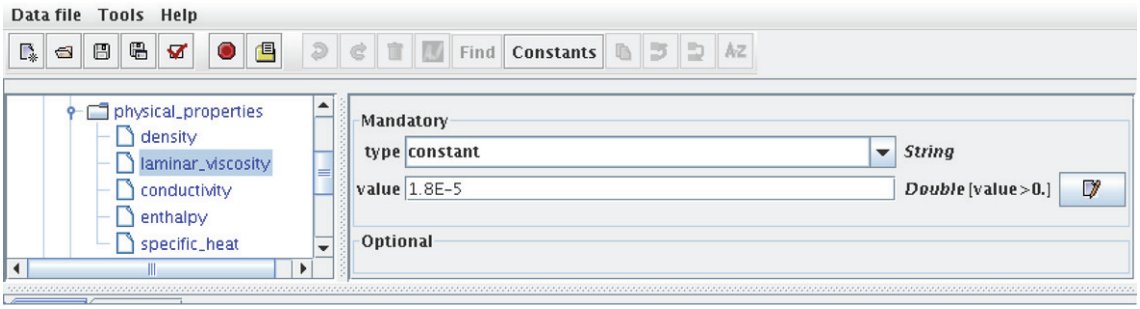



**Figure D.7 — Constant laminar viscosity**

## D.8 Defining gravity

The next step is to define the gravity field, and how gravity is handled in the formulae (standard or Boussinesq approach). The term assembled in the momentum conservation formula is $(\rho - \rho_0)\, g$, so, the reference density $\rho_0$ is also needed to be defined in this Annex.

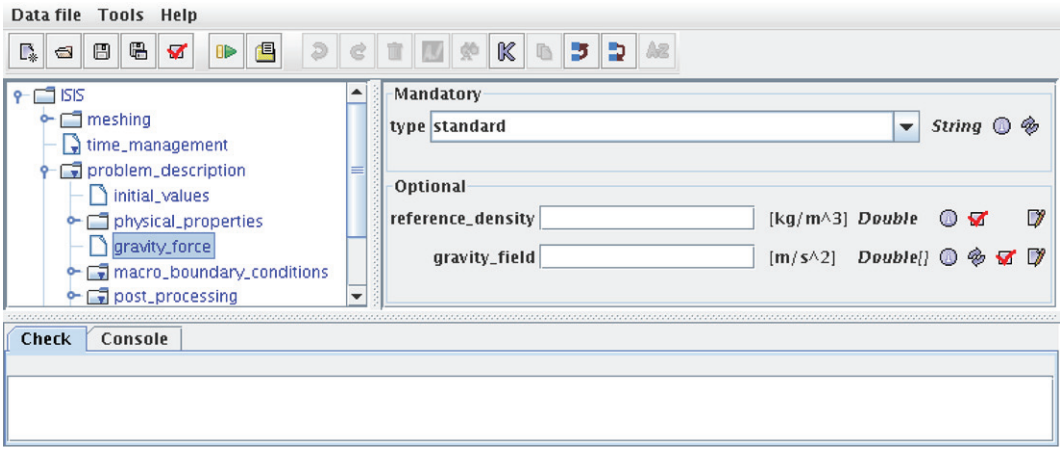



**Figure D.8 — Gravity:** $(\rho - \rho_0)\, g$

## D.9 Defining boundary conditions

To define the boundary conditions, the regions at the outer reaches of the domain where these conditions apply shall first be defined. Regardless of the mesh generator chosen during the mesh building stage, it shall specify the external boundaries by "colouring" them (each part of the boundary receives a label called a "colour"). The various colours defined in the mesh shall then be grouped into "macrocolours" for which the boundary conditions are applied.

In this case, the PELICANS "GE_BoxWithBoxes" internal mesh generator defines four colours: "top", "bottom", "left", and "right". They are grouped under the macrocolour "walls". This is done in "meshing/macro_colors".

The door, where specific boundary conditions apply, is also needed to be defined. To do so, the "GE_Colorist" module, which allows colouring part of the vertices, faces, or mesh cells, is used. The optional "GE_Colorist" section in "meshing/GE_Meshing" is first created (by right-clicking). Then, a part of the boundary is coloured by adding the optional "faces" section and defining a new colour, "door_colour". Next, the button at the end of the line is clicked to open the constant definition menu. There a Boolean expression is entered, as a function of the vector "$DV_X" composed of coordinates at the centre of the

boundary faces, that is true for faces contained in the door. The PELICANS expression in_box($DV_X, < x0 y0 z0 > , < x1 y1 z1 > ) is used, which returns true if

$$x0 < \$DV\_X(0) < x1;\ y0 < \$DV\_X(1) < y1;\ \text{and}\ z0 < \$DV\_X(2) < z1. \tag{D.1}$$

With this function, the door formula is:

```
(in_box($DV_X,
vector(2.8-l.e-06, 1.03, 0.00),
vector(2.8+1.e-06, 1.77, 1.83)))
```

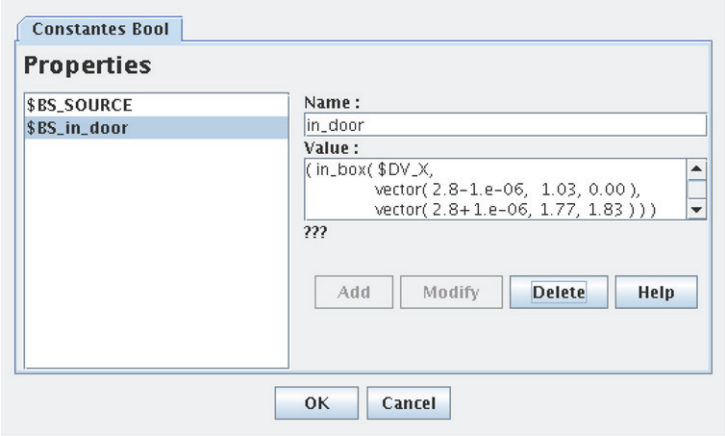



**Figure D.9 — Defining the Boolean variable "in_door"**

NOTE The question marks in the previous figure indicate that the "in_door" variable cannot be assessed, as it depends on the "$DV_X" variable which, when the code is run, takes the coordinate values for all the centres of the boundary faces in the domain.

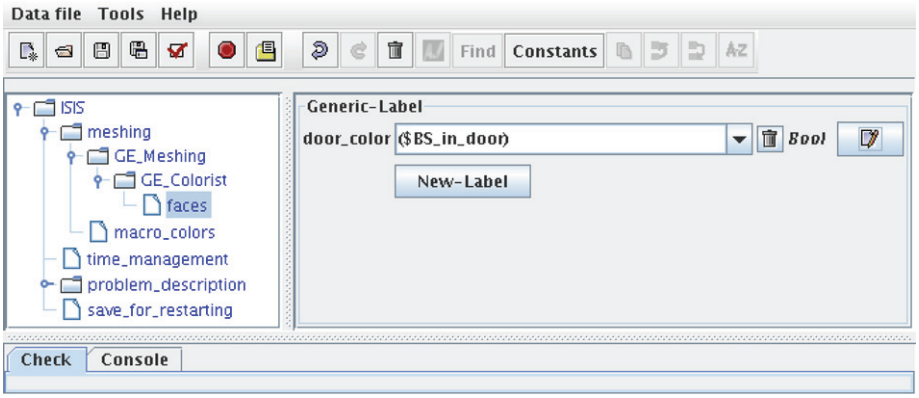



**Figure D.10 — Defining "door_color"**

The final step is to define the two corresponding macrocolours:

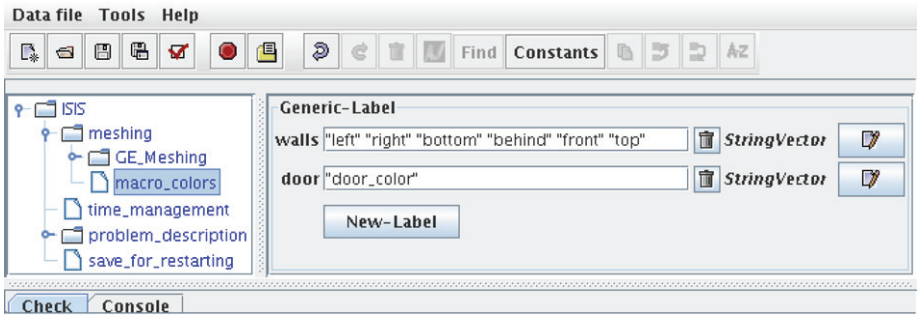



**Figure D.11 — Defining macrocolours**

For the various macrocolours, the type of boundary condition that applies (macroboundary conditions) is to be defined and for each unknown, the selected boundary condition.

The first macroboundary condition applies to the "walls" macrocolour and is of the "wall" type.

— The boundary condition for velocity is a slip condition given by the turbulence wall laws.

— An "adiabatic" condition for enthalpy is also selected.

Fluid can enter or exit at the door; therefore, the "inlet_outlet" macroboundary condition is used. For each field, the potential incoming value shall be set:

— for enthalpy, "inlet_value" is 0 (fluid enters at $T$ = 300 K);

— for $k$, the incoming value is a fraction of the turbulent kinetic energy:

$k_{in}$ = 1,5 $(\alpha v)^2$, with the "turbulent_intensity" parameter, $\alpha$, set at 0,01 % in this example;

— for $\varepsilon$, the incoming value is given by a mixing length law:

$\varepsilon_{in} = C_{\mu}^{0,75} k_{in}^{1,5} / l_m$, with the "mixing_length_scale" parameter, $l_m$, set at 0,001 m in this example.

## D.10 Turbulence model

In the "turbulence" section, the standard $k$-$\varepsilon$ model is chosen (RNG variants are also available). Two "numerical" parameters are necessary:

— length characteristic of the largest turbulence scales, which serves to limit turbulent viscosity (here, "maximal_mixing_length" is set at 3 m, representing the characteristic size of the room);

— the distance to the wall where the wall laws are assessed: this distance shall be small compared to mesh cell size (here, "delta_for_wall_law" is set to 0,01 m).

For more details on these two parameters, see Reference [15].

The various constants of the $k$-$\varepsilon$ model have default values. These values can be changed by opening an optional "problem_description/turbulence/parameters" section (right mouse click" problem_description/turbulence").

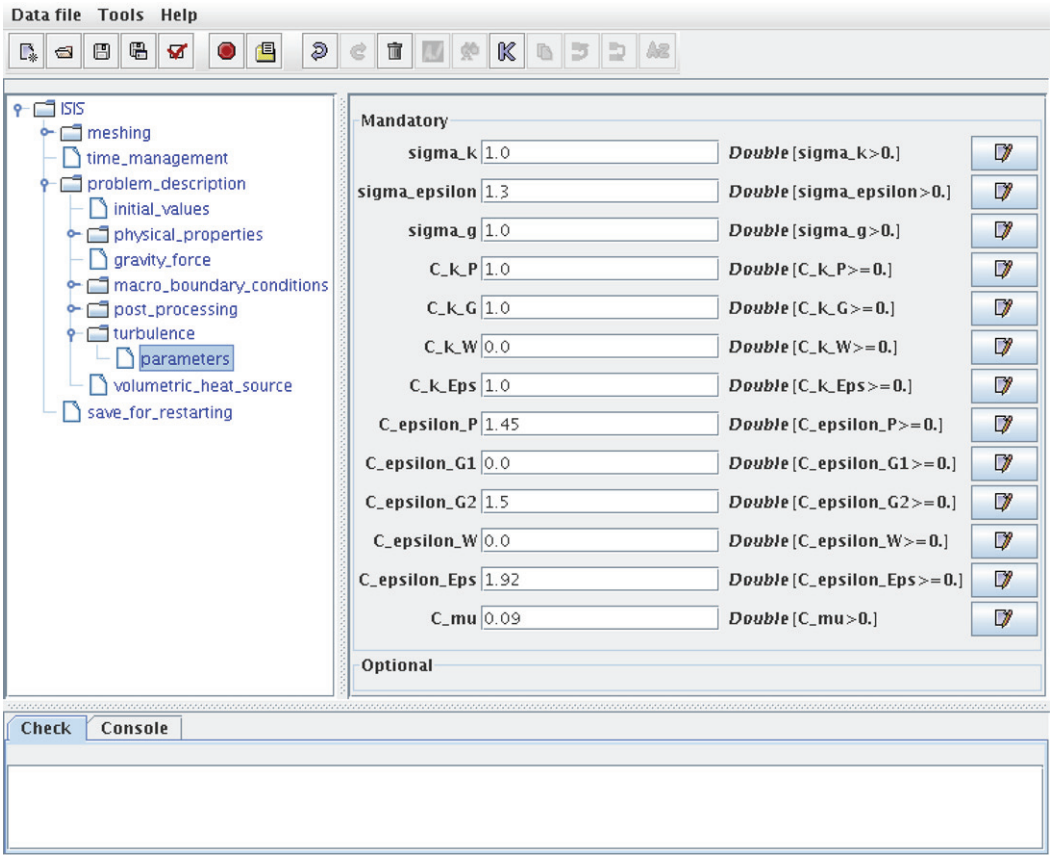



**Figure D.12 — Constants for the *k-ε* model**

## D.11 Fire modelling: volumetric heat source

The combustion module is not activated in this example and the fire is modelled by a volumetric heat source at the level of the fire.

In the “constantes” menu, a constant as a function of the position in space, “$DV_X”, is defined, which is “true” in the fire and “false” outside it:

```
(in_box($DV_X,
       vector(1.25, 1.25, 0.00),
       vector(1.55, 1.55, 0.30)))
```

The expression above returns true if all the following properties are simultaneously verified:

— component 0 of $DV_X (*x* coordinate) is between 1,25 and 1,55;

— component 1 of $DV_X (*y* coordinate) is between 1,25 and 1,55;

— component 2 of $DV_X (*z* coordinate) is between 0,00 and 0,30.

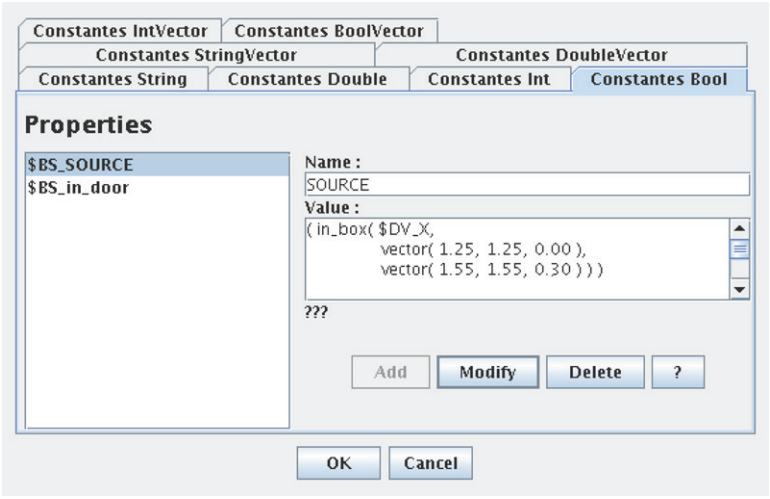



**Figure D.13 — Defining the Boolean variable "SOURCE"**

Using the "SOURCE" variable, the heat source term is defined with the following expression:

```
(($BS_SOURCE ? 2.3E6: 0.))
```

The expression returns 2.3E6 if $BS_SOURCE (function of $DS_X, coordinates for the centre of the current mesh cell) is true and 0. otherwise.

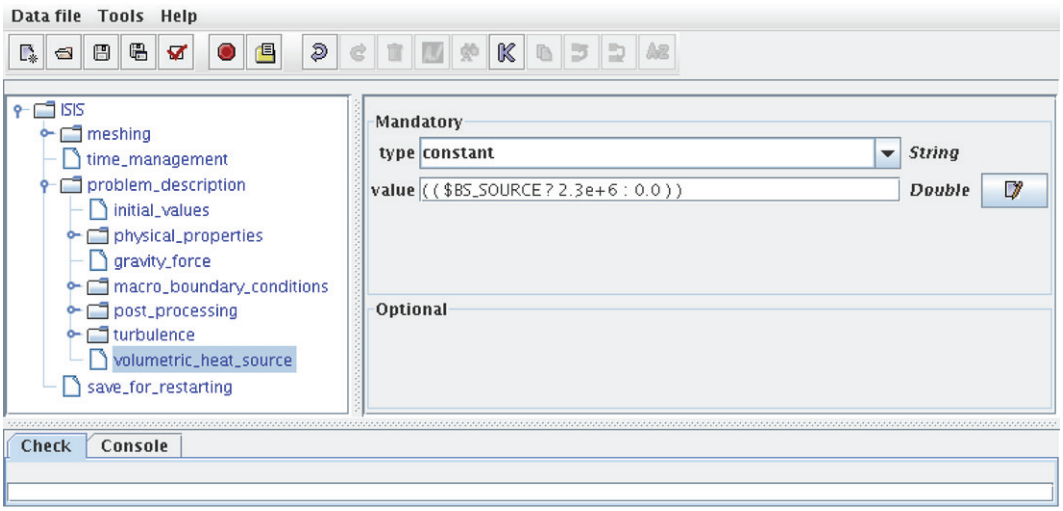



**Figure D.14 — Defining the volumetric heat source**

## D.12 Running the calculation

The calculation can be run directly from the user-system interface ("Data file/run"), and then be tracked in the window that opens up.

Below is the temperature map for the centre of the room at the end of the calculation; the flame modelled by the volumetric heat source can be seen, supplied with fresh air from the door (to the left).

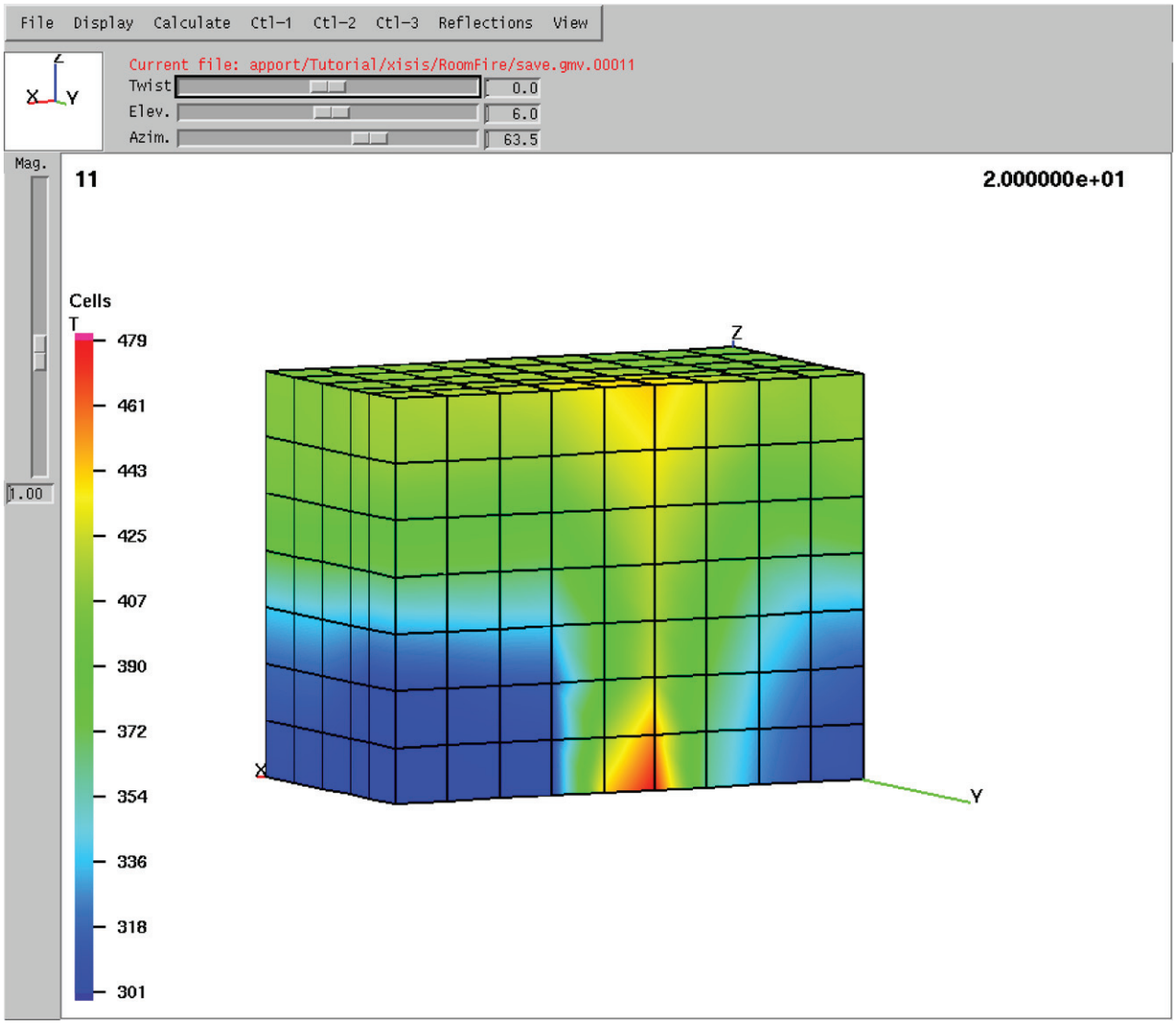



**Figure D.15 — Temperature profile,** $y$ = 1,4

The mesh selected for this example is intentionally coarse (567 cells). Below is the same temperature map for a calculation in which the number of cells has been multiplied by 3 in each direction (15,309 cells).

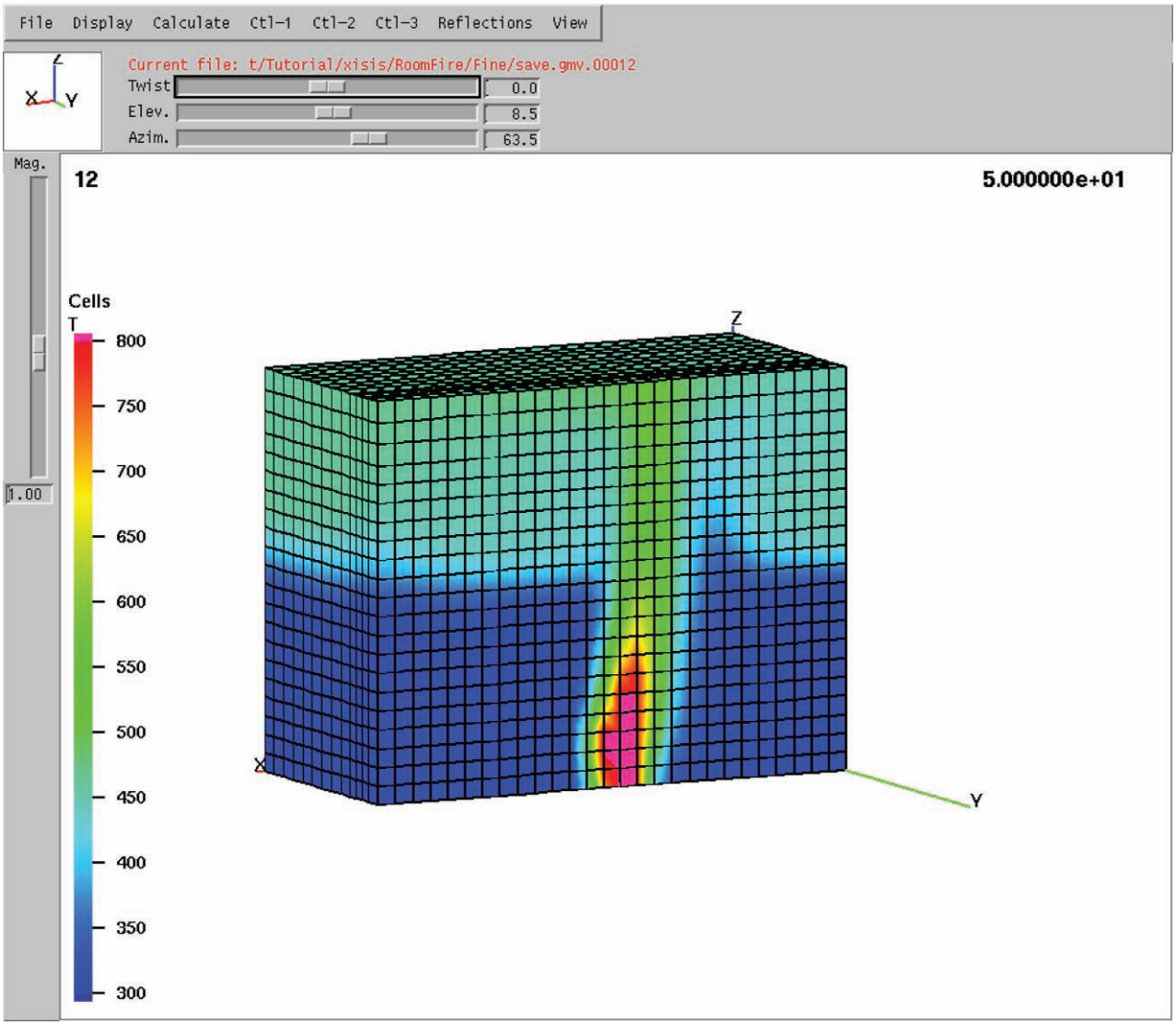



**Figure D.16 — Temperature profile, refined mesh,** $y = 1{,}4$

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