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documentation

version 3.2 tutorial - Simulating pulverized coal combustion, coal/biomass co-combustion and slagging in a furnace using the Lagrangian approach in Code_Saturne

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FLUID MECHANICS, ENERGY AND ENVIRONMENT

FLUID DYNAMICS, POWER GENERATION AND ENVIRONMENT INDUSTRIAL REACTIVE AND MULTIPHASE FLOWS

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February 10 2014

Tutorial: Simulating pulverized coal combustion, coal/biomass co-combustion and slagging in a furnace using the Lagrangian approach in Code_Saturne

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H-I81-2013-04083-EN	**1.0**		

This tutorial is a continuation of the tutorial “Simulating Pulverized Coal Combustion with Code_Saturne”. It explains how to perform a Lagrangian simulation of pulverised coal combustion using Code_Saturne. This is an example of simulation of biomass slagging in a co-combustion (coal / biomass) case where most of the pulverized fuel remains coal (90% of injected mass). In that case, it is assumed that the biomass is almost insignificant so that the effects of biomass on the gaseous field can be ignored.

It will be suggested to:

1. Compute a carrier field (containing coal and flue gas) by taking into account only coal combustion
2. Use this carrier field to follow the behaviour of biomass particles and their slagging on a furnace wall. Using the assumption made before, the carrier field is considered frozen.

The purpose of this tutorial is to provide all the information needed to set up a Lagrangian (particle tracking module) pulverized coal combustion simulation using Code_Saturne's Graphical User Interface.

In detail, this tutorial demonstrates how to:

- Create a new “Pulverized Coal Combustion” case and launch Code_Saturne “Graphical User Interface”.
- Prepare a Eulerian frozen field to serve as an input for the particle tracking calculation.
- Set up (and explanation) of the appropriate computational parameters for the Lagrangian computation.

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MECANIQUE DES FLUIDES, ENERGIES ET ENVIRONNEMENT

ECOULEMENTS INDUSTRIELS REACTIFS ET POLYPHASIQUES

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10 février 2014

Tutoriel: Simulation de la combustion du charbon pulvérisé, de la co-combustion charbon/biomasse et de l'encrassement dans un four, en utilisant l'approche Lagrangienne de Code_Saturne

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H-I81-2013-04083-EN	**1.0**		

Ce tutoriel constitue la suite du tutoriel "Simulation de la Combustion du charbon pulvérisé avec Code_Saturne ". Il explique comment effectuer une simulation Lagrangienne de la combustion de charbon pulvérisé. Il s'agit d'un exemple de simulation d'encrassement dans un cas de co- combustion (charbon / biomasse) où la majeure partie du combustible pulvérisé est le charbon (90 % de la masse injectée). Dans ce cas , on suppose que les effets de la biomasse sur le mélange gazeux peuvent être négligés.

Les étapes suivantes sont réalisées :

1 . Calcul d'un champ Eulérien (contenant le charbon et les gaz de combustion) en ne prenant en compte que la combustion du charbon pulvérisé

2 . Utilisation de ce champ Eulérien pour suivre le comportement des particules de biomasse et leur encrassement sur les parois du four. D'après l'hypothèse faite plus tôt, le champ Eulérien est supposé figé.

Le but de ce tutoriel est de fournir toutes les informations nécessaires pour mettre en place un calcul Lagrangien (module de suivi de particules) de simulation de la combustion de charbon pulvérisé à l'aide de l'interface graphique utilisateur de Code_Saturne .

Dans le détail, ce tutoriel montre comment :

• Créer un nouveau cas " Combustion de charbon pulvérisé " et lancer l'interface graphique utilisateur de Code_Saturne .

• Préparer un champ Eulérien figé qui servira de base pour le calcul des trajectoires des particules .

• Mettre en place (avec explication) les paramètres de calcul appropriés pour le calcul Lagrangien.

Validation workflow

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AVERTISSEMENT / CAUTION

Executive Summary

This tutorial is a continuation of the tutorial "*Simulating Pulverized Coal Combustion with Code_Saturne".* It explains how to perform a Lagrangian simulation of pulverised coal combustion using *Code_Saturne.*

This tutorial will give an example of simulation of biomass slagging in a co-combustion (coal / biomass) case where most of the pulverized fuel remains coal (90% of injected mass). In that case, it is assumed that the biomass is almost insignificant so that the effects of biomass on the gaseous field can be ignored.

It will be suggested to:

1. Compute a carrier field (containing coal and flue gas) by taking into account only coal combustion

2. Use this carrier field to follow the behaviour of biomass particles and their slagging on a furnace wall. Using the assumption made before, the carrier field is considered frozen.

The purpose of this tutorial is to provide all the information needed to set up a Lagrangian (particle tracking module) pulverized coal combustion simulation using *Code_Saturne's* Graphical User Interface.

In detail, this tutorial demonstrates how to:

- Create a new "Pulverized Coal Combustion" case and launch *Code_Saturne* "Graphical User Interface".

- Prepare a Eulerian frozen field to serve as an input for the particle tracking calculation.

- Set up (and explanation) of the appropriate computational parameters for the Lagrangian computation.

Sommaire / Summary

1. Introduction

This tutorial is a continuation of the first tutorial "*Simulating Pulverized Coal Combustion with Code_Saturne".* It explains how to perform a Lagrangian simulation of pulverised coal combustion using *Code_Saturne.*

This tutorial will give an example of simulation of biomass slagging in a co-combustion (coal / biomass) case where most of the pulverized fuel remains coal (90% of injected mass). In that case, it is assumed that the biomass is almost insignificant so that the effects of biomass on the gaseous field can be ignored.

It will be suggested to:

- Compute a carrier field (containing coal and flue gas) by taking into account only coal combustion

- Use this carrier field to follow the behaviour of biomass particles and their slagging on a furnace wall. Using the assumption made before, the carrier field is considered frozen.

2. Objectives

The purpose of this tutorial is to provide all the information needed to set up a Lagrangian (particle tracking module) pulverized coal combustion simulation using *Code_Saturne's* Graphical User Interface.

In detail, this tutorial demonstrates how to:

- Create a new "Pulverized Coal Combustion" case and launch *Code_Saturne's* "Graphical User Interface".

- Prepare a Eulerian frozen field to serve as an input for the particle tracking calculation.

- Set up (and explanation) of the appropriate computational parameters for the Lagrangian computation.

3. Prerequisites

This tutorial is written assuming that the version of *Code_Saturne* which is installed on your computer is newer than revision 5331.

In this tutorial, the Lagrangian calculation will be run on a frozen carrier field. It means that there will be no coupling from the particles to the gaseous field. The Lagrangian computation will be a kind of postprocessing of a previous Eulerian computation.

In that case, a Lagrangian computation is performed in two steps:

1. Calculation of the gaseous field. An explanation on how to obtain such results is given in section 6. Thereafter, this step will be called as the *Eulerian calculation*.

2. A restart of the previous result is done with extra settings corresponding to the particle tracking module. This step is the *Lagrangian calculation* and is explained in section 7.

Although the computation is run on a frozen carrier field, *Code_Saturne* is very sensitive to the inputs parameters when restarting a computation (some fields -pressure, velocities, concentrations ...- are saved and changing one parameter may leads to discrepancies when loading the saved file as an input of a new computation).

The first precaution is the use of the same revision of *Code_Saturne* to run both Eulerian and Lagrangian calculation.

Other important recommendations are mentioned below in section 4.

4. Recommendations to ensure a proper restart

Keeping some parameters unchanged (between Eulerian and Lagrangian calculations) is strongly recommended to ensure a correct restart:

- Global settings:
    - Lagrangian calculation takes the drying of coal into account. That is why one should choose *homogeneous approach with moisture* from the pull down Menu *Pulverized fuel combustion* in the *Calculation features* subsection when setting the Eulerian calculation up (change compare to the first tutorial). See Figure 2.
    - The turbulence and radiative transfers model should not be changed (between Eulerian and Lagrangian calculations). See Figure 3 and Figure 10.
    - The NOx formation model must remain the same. See Figure 8.
- The coal types and composition:
    - The number of coals and of particle size classes should be the same even if it forces to set a type of coal injection flow rate equal to zero during either the Eulerian or the Lagrangian calculation. See Figure 4.
    - Do not change the diameter or the number of particle classes of the Eulerian coals when performing a Lagrangian restart. Please note that the diameter for Lagrangian and Eulerian calculations are independent so that you may configure your Lagrangian case as you wish without changing any coal parameters for Eulerian calculation. See Figure 4.
    - You may change coal properties (between first calculation and particle tracking restart) only if this type of coal has NOT been injected during the first calculation. See Figure 5, Figure 6 and Figure 7.
    - The oxidant should not be changed. See Figure 9.

5. Case description and mesh characteristics

The furnace and meshing of the first tutorial will be used. Please refer to the tutorial "*Simulating Pulverized Coal Combustion with Code_Saturne"*.in case of troubles.

6. Eulerian calculation

6.1. Preparation

- Open a new terminal window in order to execute the commands given in the following.
- Create a new *Code_Saturne* test case named *Tutorial* in your working directory (your working directory might be a directory anywhere on your local hard drive) by using the command **code_saturne create –s Tutorial**. This command automatically creates a folder hierarchy structured as follows:

```
- Tutorial
- CASE1
        - DATA
                -REFERENCE
        - RESU
        - SCRIPTS
        - SRC
                -EXAMPLES
                -REFERENCE
- MESH
- POST
```

- Copy the mesh file *Tutorial3D.cgns* to the folder */Tutorial/MESH*.
- Change to */Tutorial/CASE1/DATA* and launch the Graphical User Interface (GUI) by using the command **./SaturneGUI**

6.2. Setup

The simulation is set up into several consecutive steps. In the following, each step is entitled like the corresponding section shown in the most left window of the GUI. Keywords that can be found in the GUI itself are written in italic. The figure legends are always structured as follows: Step X – Section; Subsection; Rider A; Rider B; Rider …. .

6.2.1. Step1 – Verify the Computation Directories

- Create a new file from the *File* Menu. The GUI should look like it is shown in the following Figure 1.

- Verify that the *Directory of the case* and the *associated sub-directories* are well set (see also the directory structure given in section **Error! Reference source not found.**).

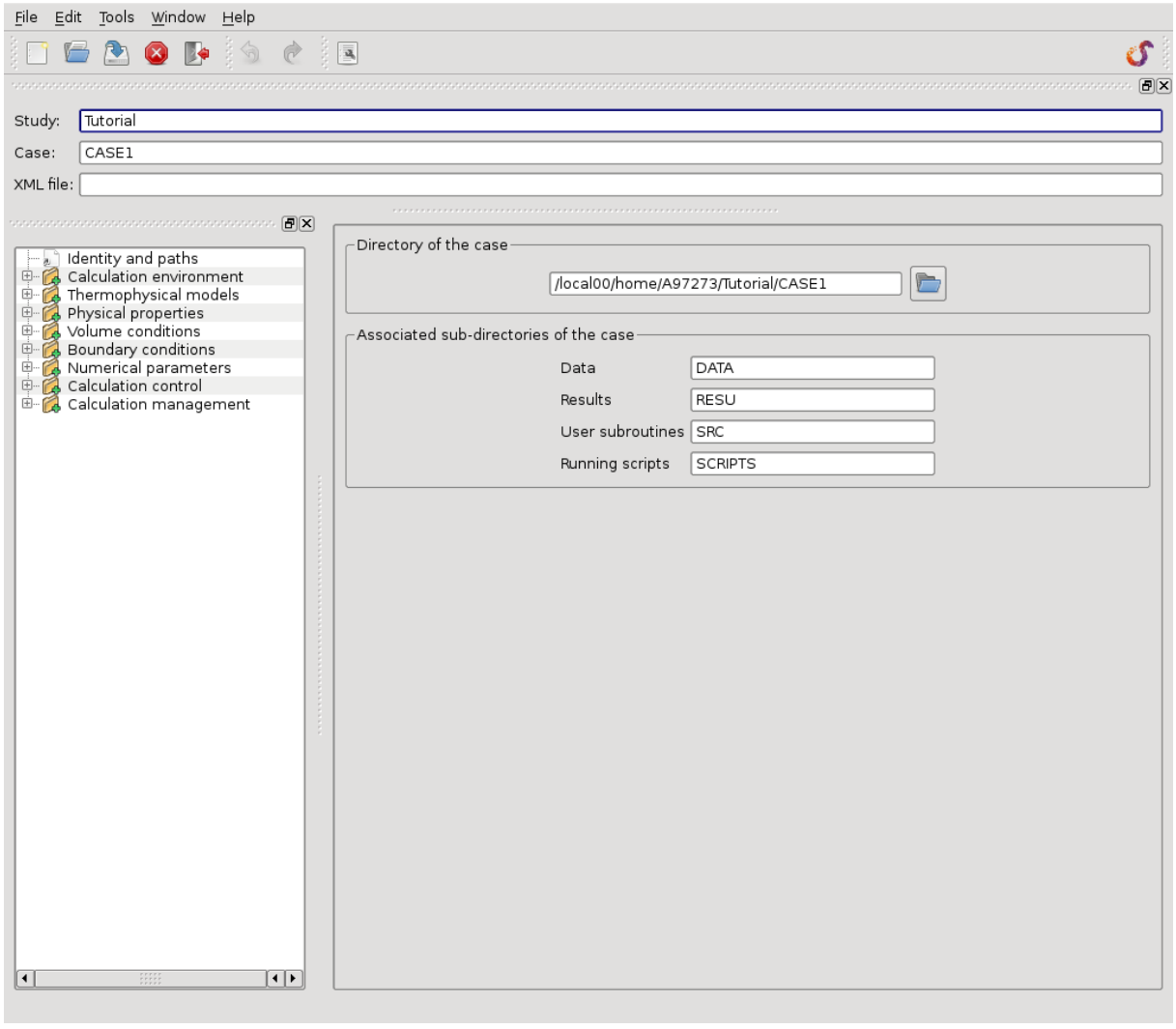

Figure 1: GUI Step 1 – Verification of the computation directories.

6.2.2. Step 2 – Calculation environment

- Change to the *Meshes selection* subsection.

- Select the *Import Mesh* option at the *Meshes* rider.

- Add the mesh *Tutorial3D.cgns* by clicking on the "+" – button.

- Change to the *Mesh quality criteria* subsection.

- Retain all default settings and click the *Check mesh* button.

  Code_Saturne's pre-processor should not have any trouble passing the *Mesh quality criteria* test. The corresponding results are stored in the automatically created folder */Tutorial/CASE1/RESU/check_mesh*. Use either Ensight or ParaView to visualize them.

- Click OK to close the pre-processor window.

- Save the case.

6.2.3. Step 3 – Thermophysical models

- In the *Calculation features* subsection, choose *steady flow* from the pull down Menu *Steady/Unsteady flow algorithm*. Select *homogeneous approach with moisture* from the pull down Menu *Pulverized fuel combustion* (Note that a new subsection called ***Pulverized fuel combustion*** should appear in the left window). Do not use *homogeneous approach (*explanation in section 4).

- Retain all other default settings.

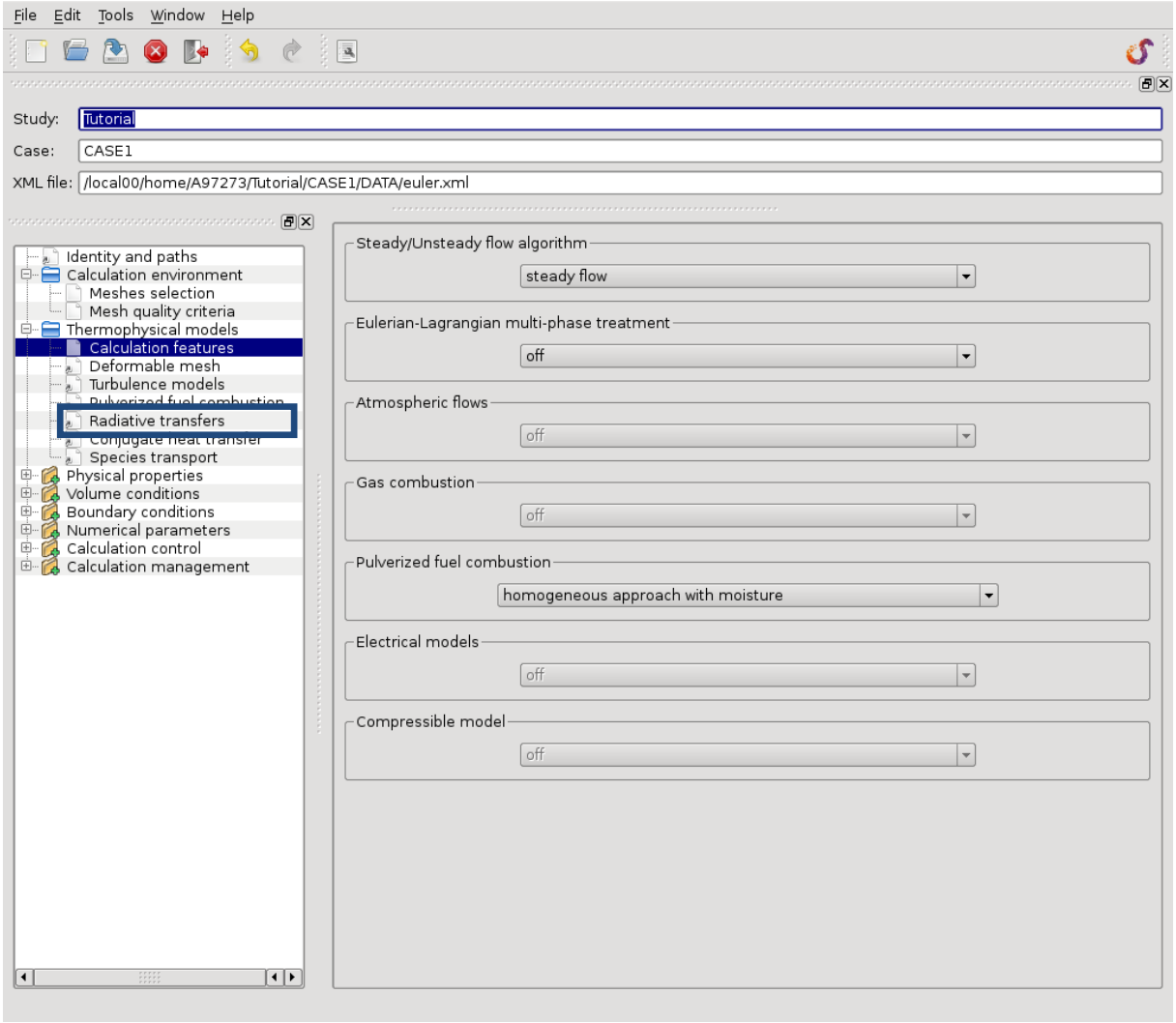

Figure 2: Step 3 - Thermophysical models; Calculation features subsection.

- Change to the *Turbulence models* subsection and select the *k-ε linear production* turbulence model. Don't modify any of the advanced options.

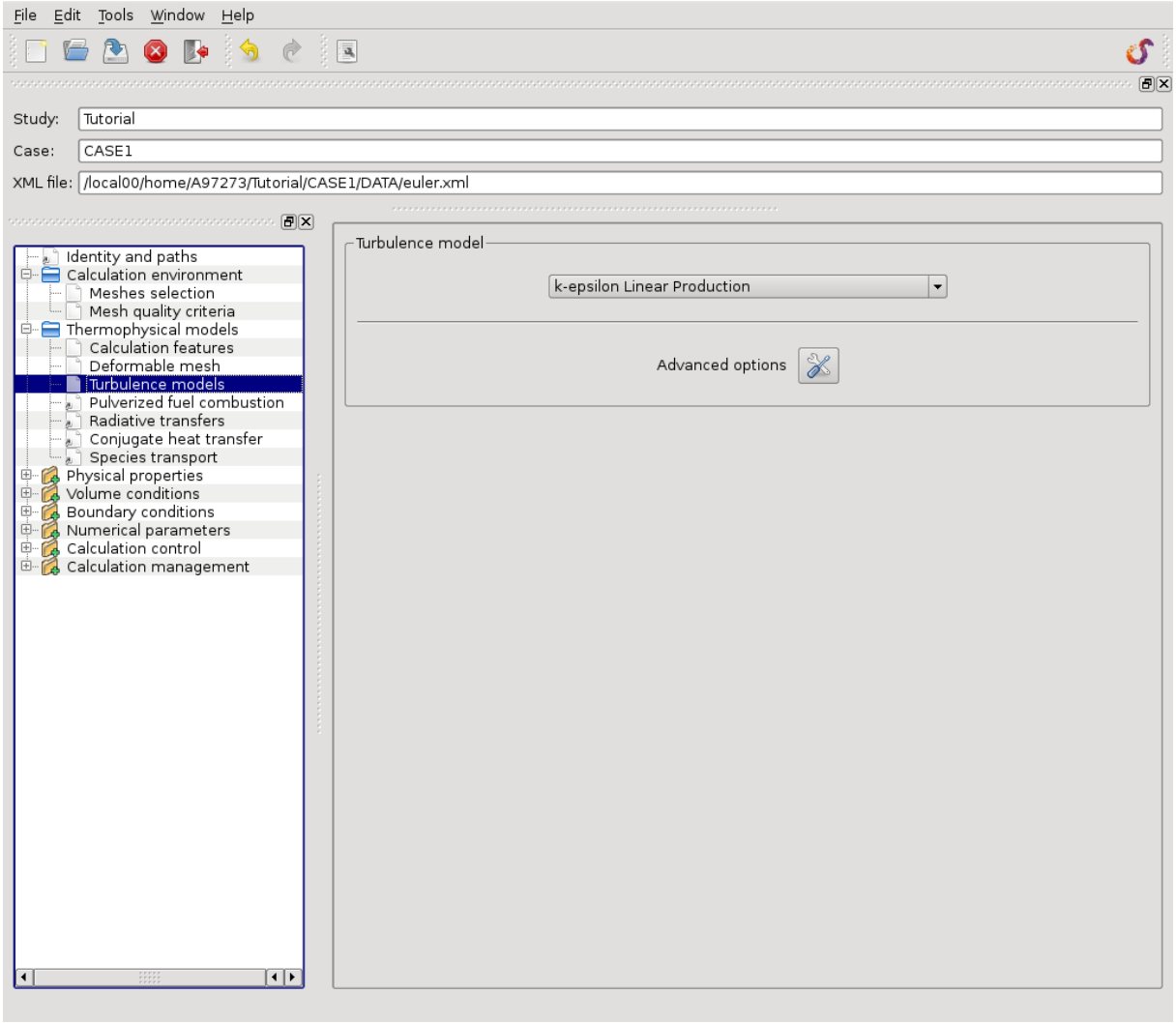

Figure 3 : Step 3 - Thermophysical models; Selection of the turbulence model.

- Change to the *Pulverized fuel combustion* subsection.
- Name the fuel as *Tutorial_Coal* and make sure the type of fuel is well set to *coal*.
- Add a second type of call *Tutorial_Biomass* and make sure the type of fuel is well set to *biomass*.
- Select the *user define* option at the *size distribution* rider and set the *initial diameter* of *Class 1* to $2.5e^{-5}$ m for *Tutorial_Coal* and $8.0e^{-4}$ m for *Tutorial_Biomass.*

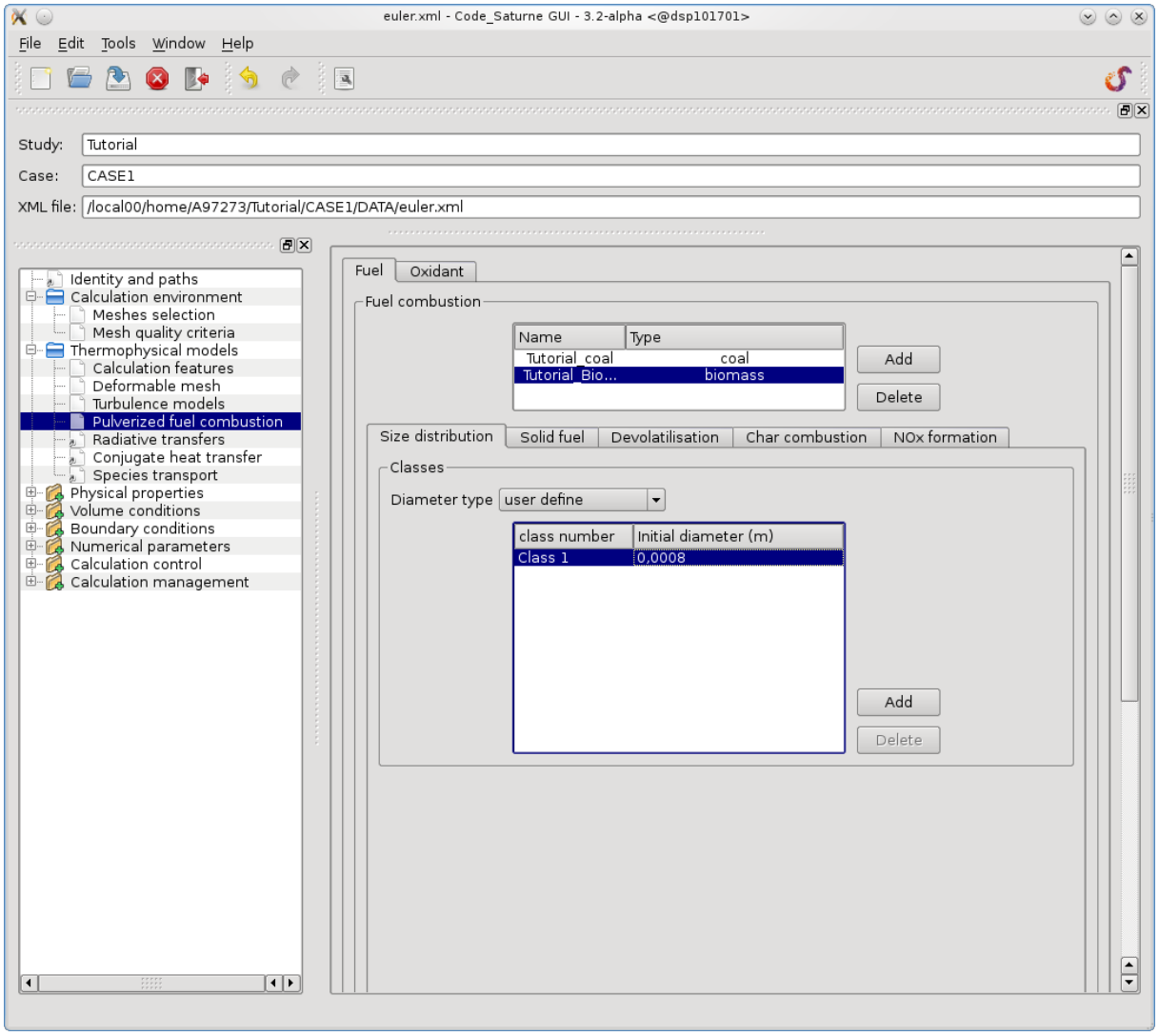

Figure 4 : Step 3 - Thermophysical models; Pulverized fuel combustion; Fuel; Size distribution.

- Change to the *Solid fuel* rider and modify the *Elementary analysis,* the *Immediate analysis,* the *Solid fuel physical properties,* the *Ashes physical properties,* and the *Coke elementary analysis* settings as shown in the following in the table below and in the Figure 5. **Note:** At a first glance it might be confusing that the V*olatile matter* content is left to zero. This is done because the stoichiometric coefficients of the two competitive reactions of the Kobayashi devolatisation model, Y_1 and Y_2, are known (see next point). If these coefficients are unknown, they have to be calculated from the user provided volatile matter content.

Label	*Zone*	*Tutorial_Coal*	*Tutorial_Biomass*
Elementary analysis (refers to dry coal)	Mass content of C	76.65 %	53 %
	Mass content of H	5.16 %	5.8 %
	Mass content of O	9.9 %	37.62 %
	Mass content of N	0 %	0 %
	Mass content of S	0 %	0 %
Immediate analysis	Heating model LHV	30000000.0 J/kg (dry basis)	18614000.0 J/kg (dry basis)
	Volatile matter	0 %	0 %
	Ash content	6.21 %	2.74 %
	Moisture	0 %	8.88 %
Solid fuel physical properties	Cp	1800 J/kg/K	1500 J/kg/K
	ρ	1200 kg/m^3	549.8 kg/m^3
Ashes physical properties	Enthalpy	0 J/kg	0 J/kg
	Cp	1800 J/kg/K	1500 J/kg/K
Coke elementary analysis (refers to dry)	Mass content of C	100 %	100 %
	Mass content of H	0 %	0 %
	Mass content of O	0 %	0 %
	Mass content of N	0 %	0 %
	Mass content of S	0 %	0 %

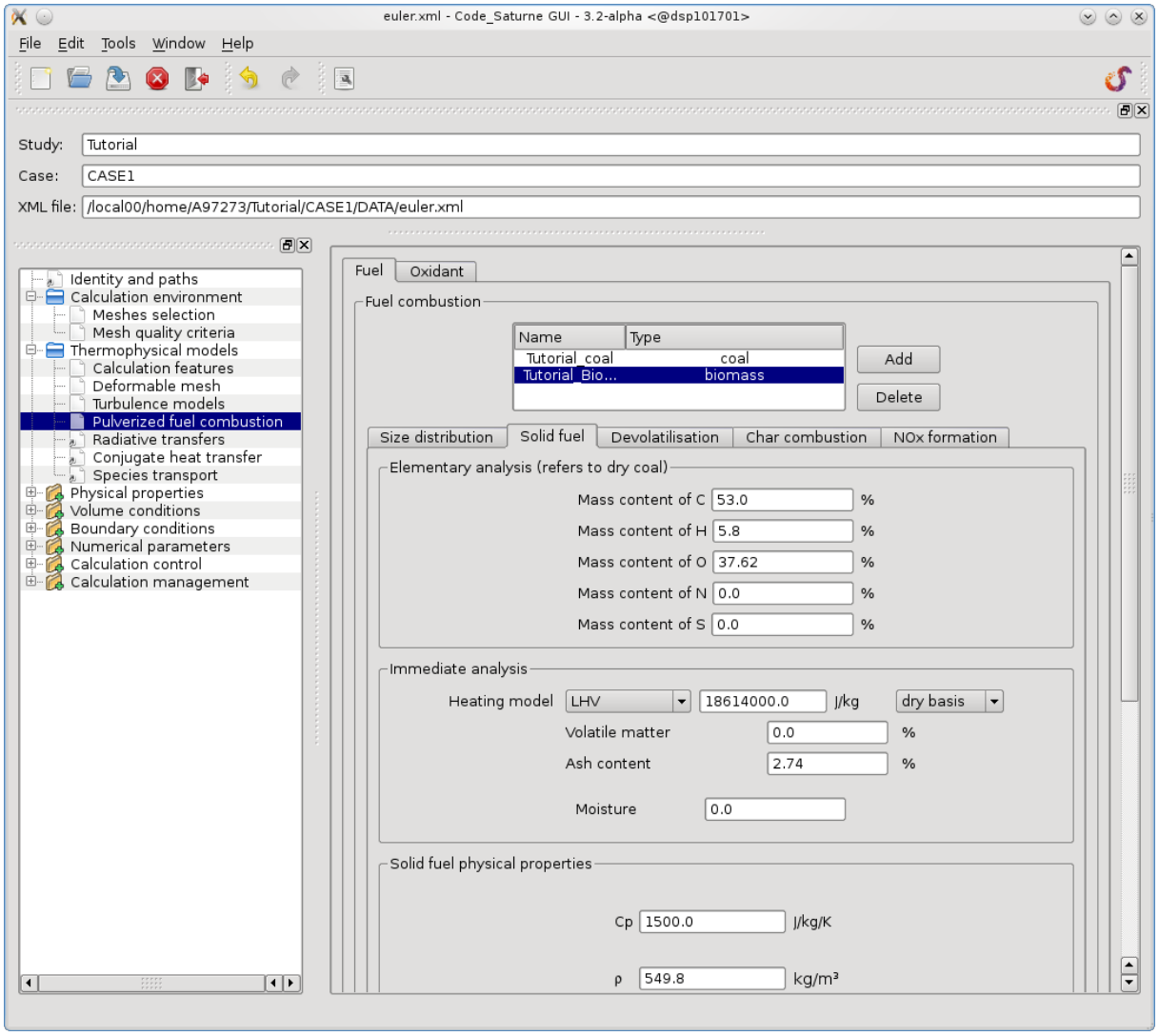

Figure 5: Step 3 - Thermophysical models; Pulverized fuel combustion; Fuel; Solid fuel.

- Change to the *Devolatisation* rider and set the *Stoichiometric coefficients* to *user define*.

- For *Tutorial_Coal* set Y_1 = 0.37 and Y_2 = 0.74 and for *Tutorial_Biomass* set Y_1 = 0.7507 and Y_2 = 0.7508. Don't modify the *Pre-exponential constants* and the *activation energies*.

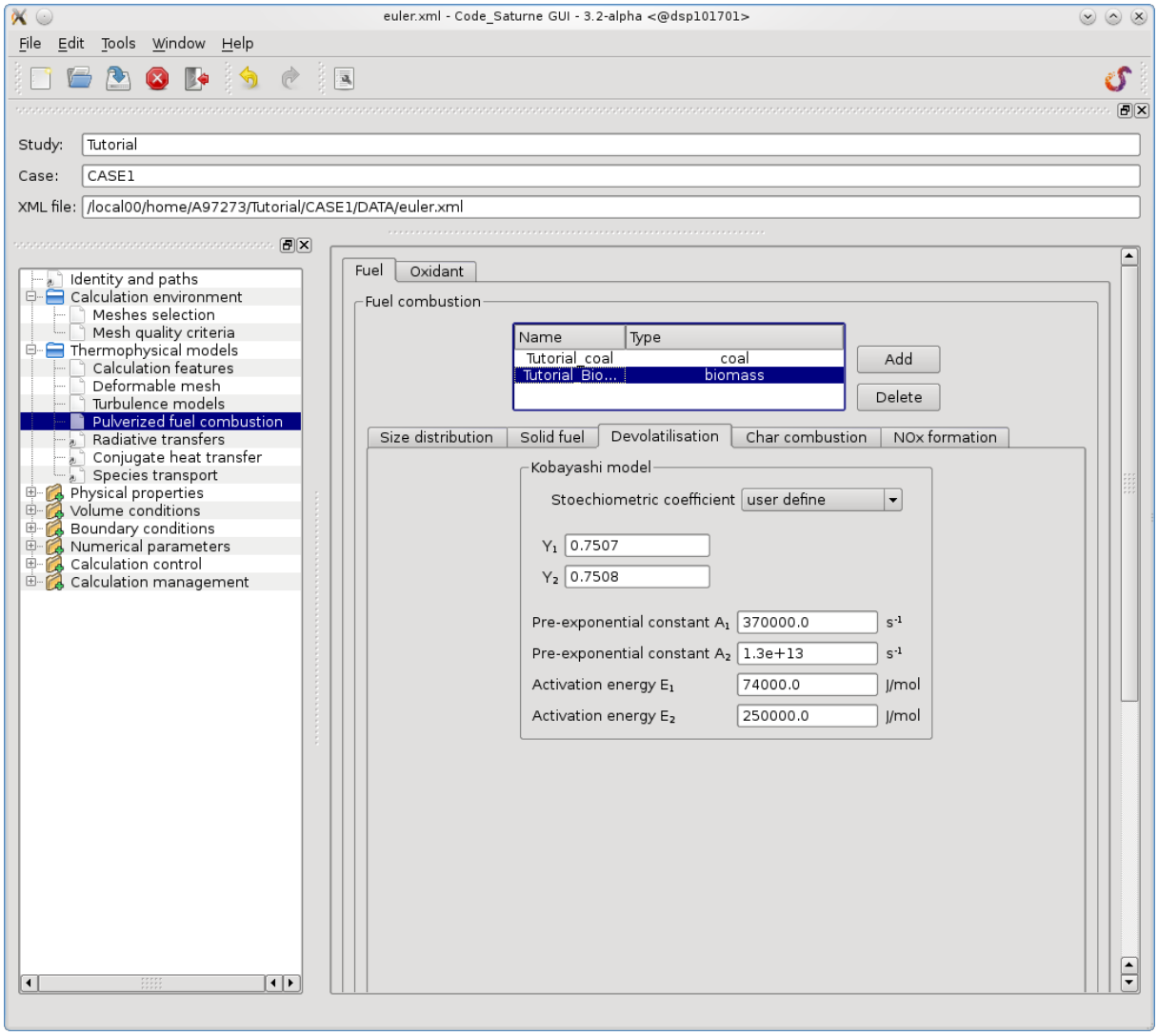

Figure 6: Step 3 - Thermophysical models; Pulverized fuel combustion; Fuel; Devolatisation.

- Change to the *Char combustion* rider and set *the pre-exponential factor* to 17.88, the *activation energy* to 16.55, and the *reaction order* to 1 (for both *Tutorial_Coal* and *Tutorial_Biomass*). Don't activate the gasification of char by CO_2 and H_2O.

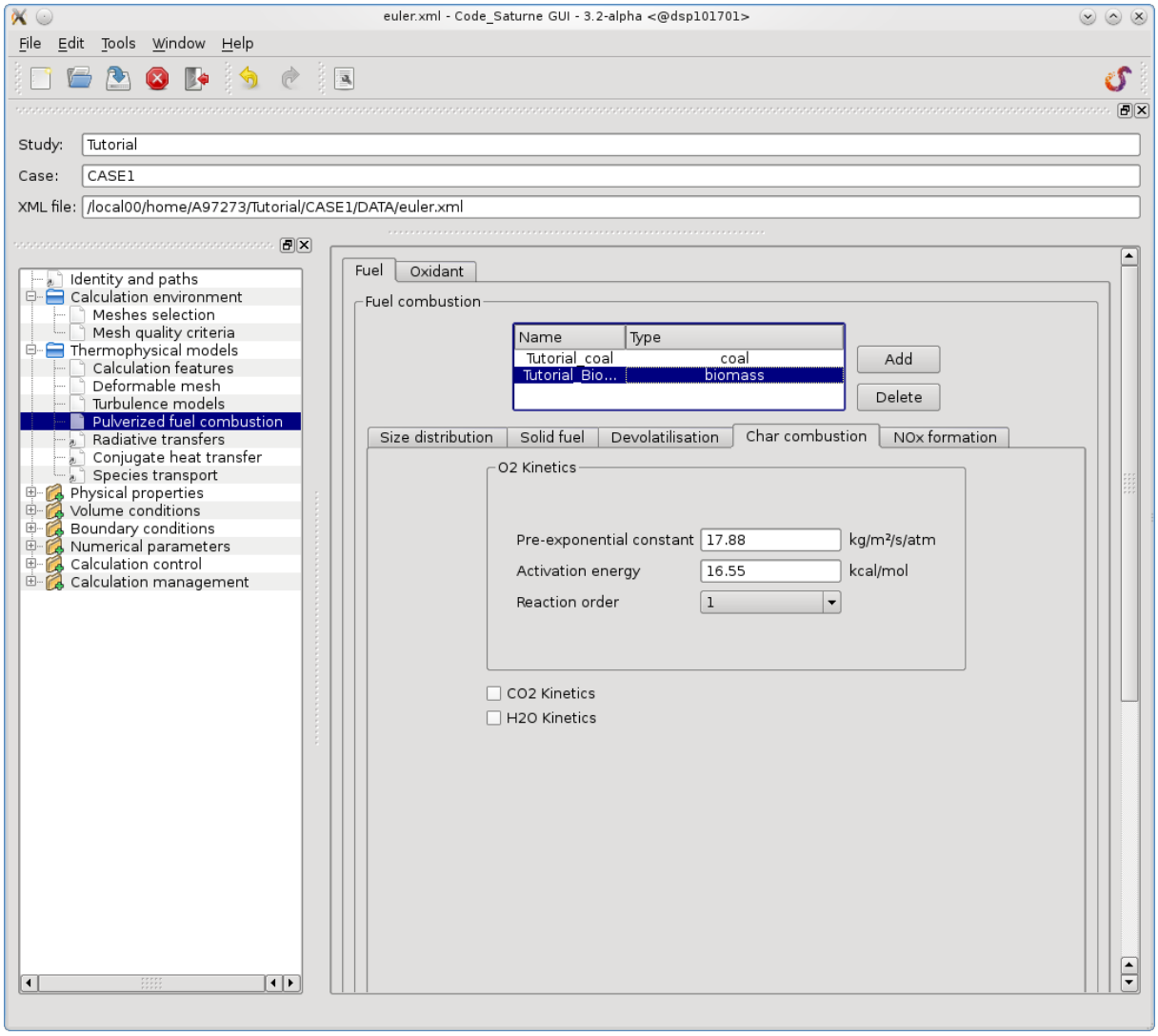

Figure 7: Step 3 - Thermophysical models; Pulverized fuel combustion; Fuel; Char combustion.

- Change to the *NOx formation* rider and deactivate *NOx formation*.

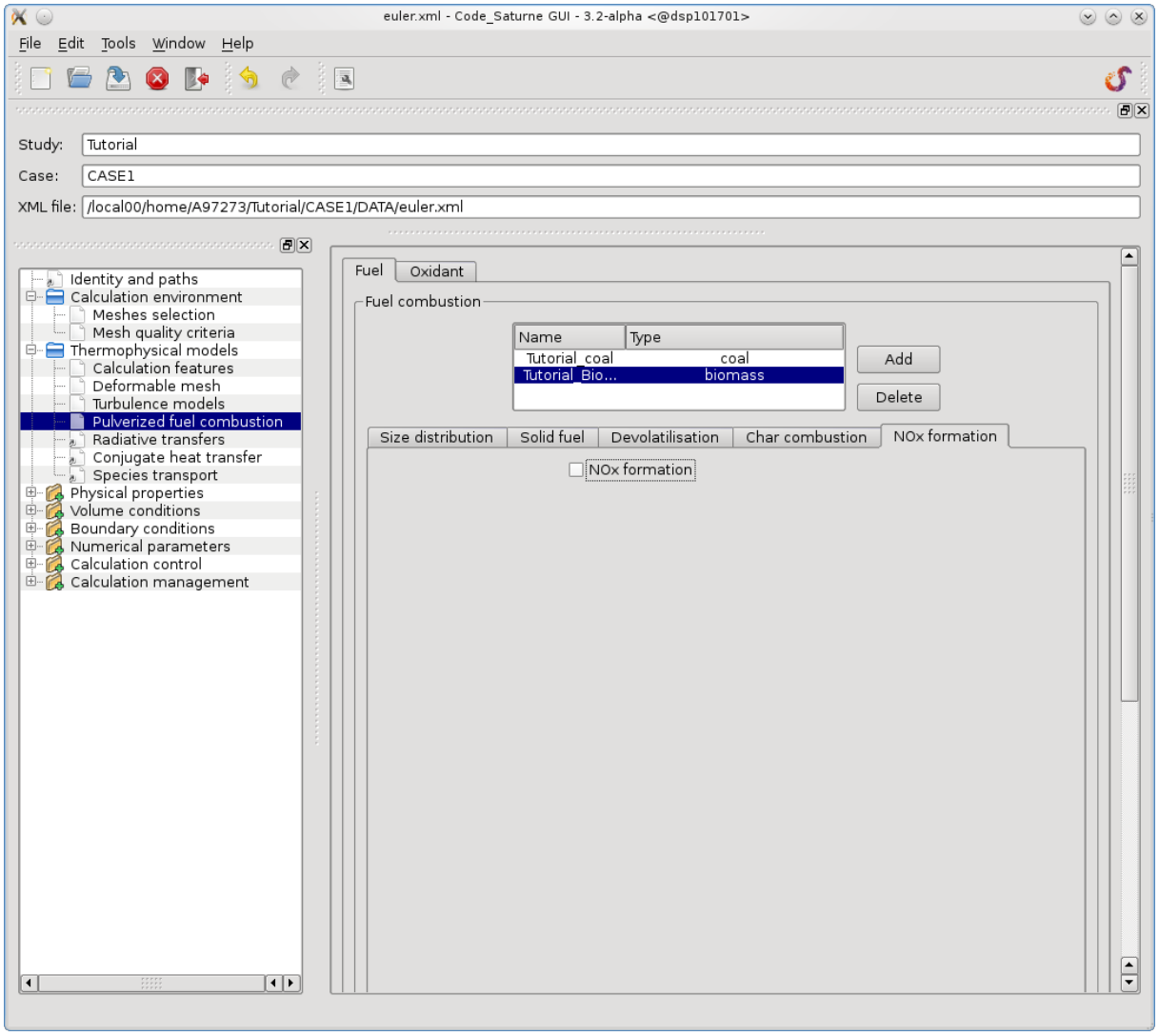

Figure 8: Step 3 - Thermophysical models; Pulverized fuel combustion; Fuel; NOx formation.

- In order to conclude the *Pulverized fuel combustion* subsection, it is necessary to characterize the composition of the gaseous oxidizer (most of the time air is used for this purpose). In doing so you have to change from the *Fuel* rider to the *Oxidant* rider. Make sure the composition of the oxidizer is given in *molar* units. Set the number of moles for *Oxidant number 1* to 1 mol for O_2, 3.76 mol for N_2, and 0 mol for both CO_2 and H_2O.

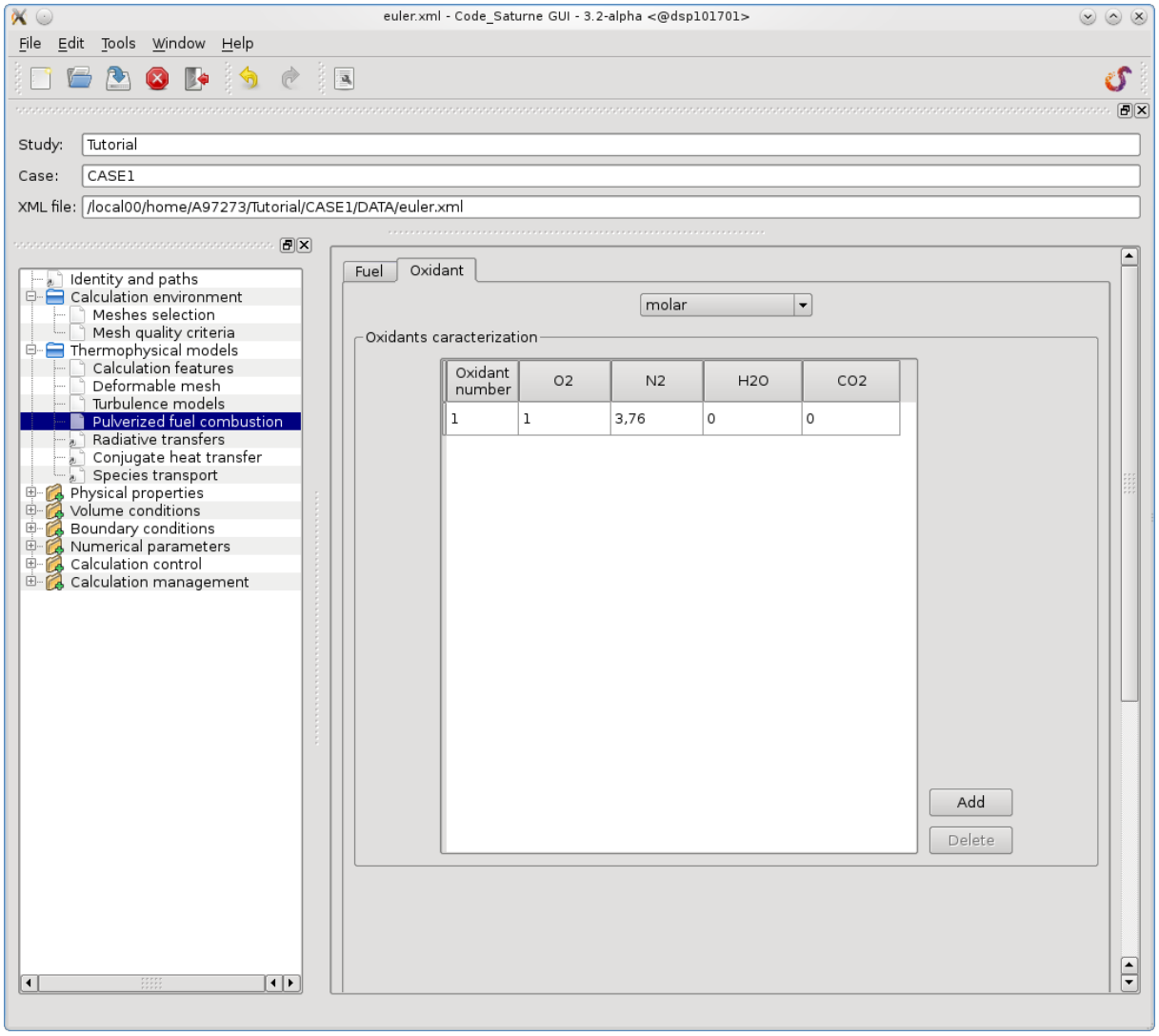

Figure 9: Step 3 - Thermophysical models; Pulverized fuel combustion; Oxidant.

- Changing to the *Radiative transfer* subsection and selecting the *P-1 Model* activates the radiative heat transfer. The absorption coefficient is set to be *constant* and its value is 0.85 m^{-1}. Modify neither the restart calculation options nor the advanced options.

- Save the case.

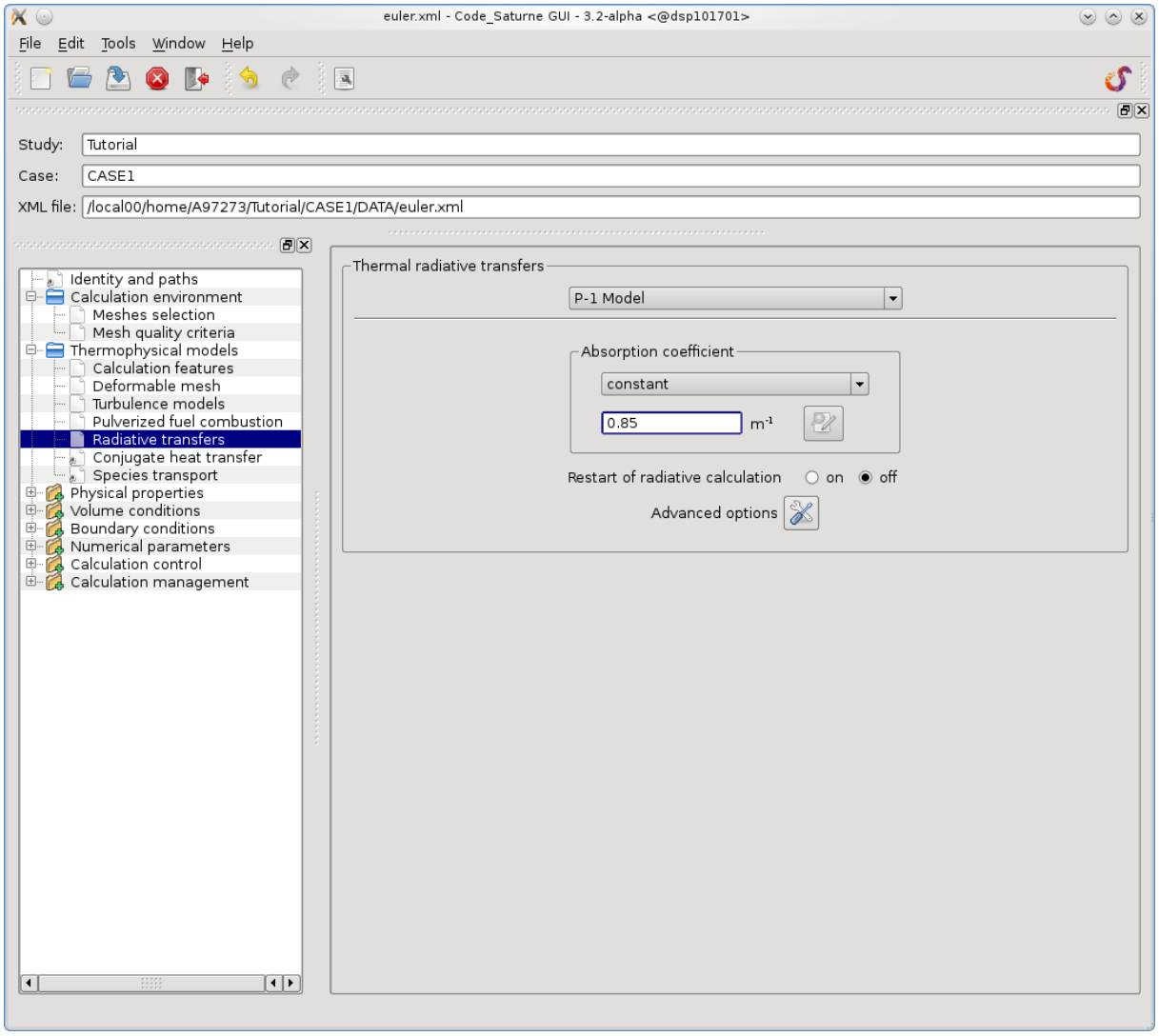

Figure 10: Step 3 - Thermophysical models; Radiative transfer

6.2.4. Step 4 – Physical properties

- Make sure that the *Reference pressure* is set to 101325Pa in the *Reference values* subsection. The Reference velocity must be set to 1 m/s. Keep the default values for all other reference values (see the following Figure 11).

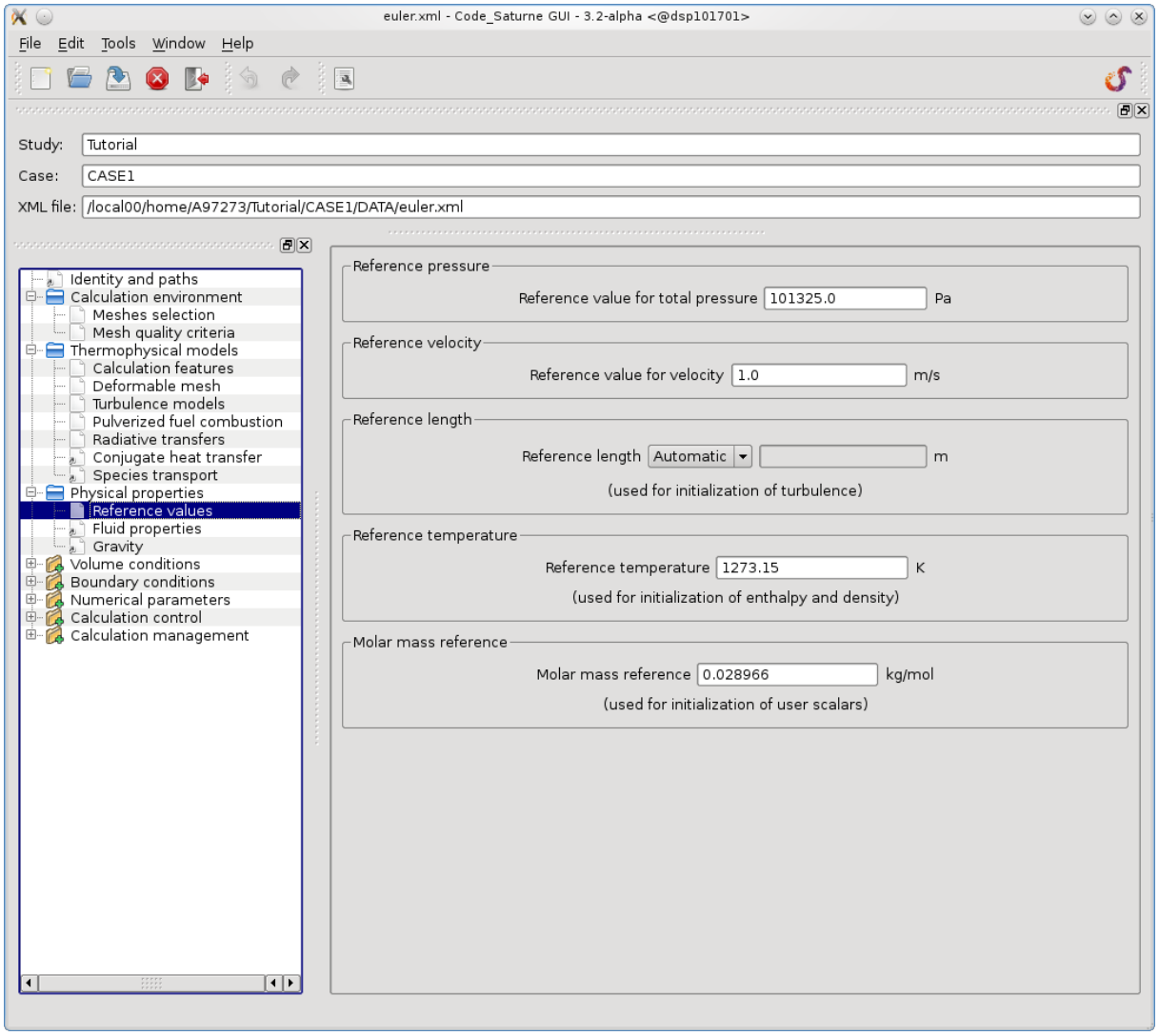

Figure 11: Step 4 – Physical properties; Reference values.

- Don't modify the default values of the *Fluid properties*.
- Set the gravity vector in the *Gravity* subsection as shown in Figure 12.
- Save the case.

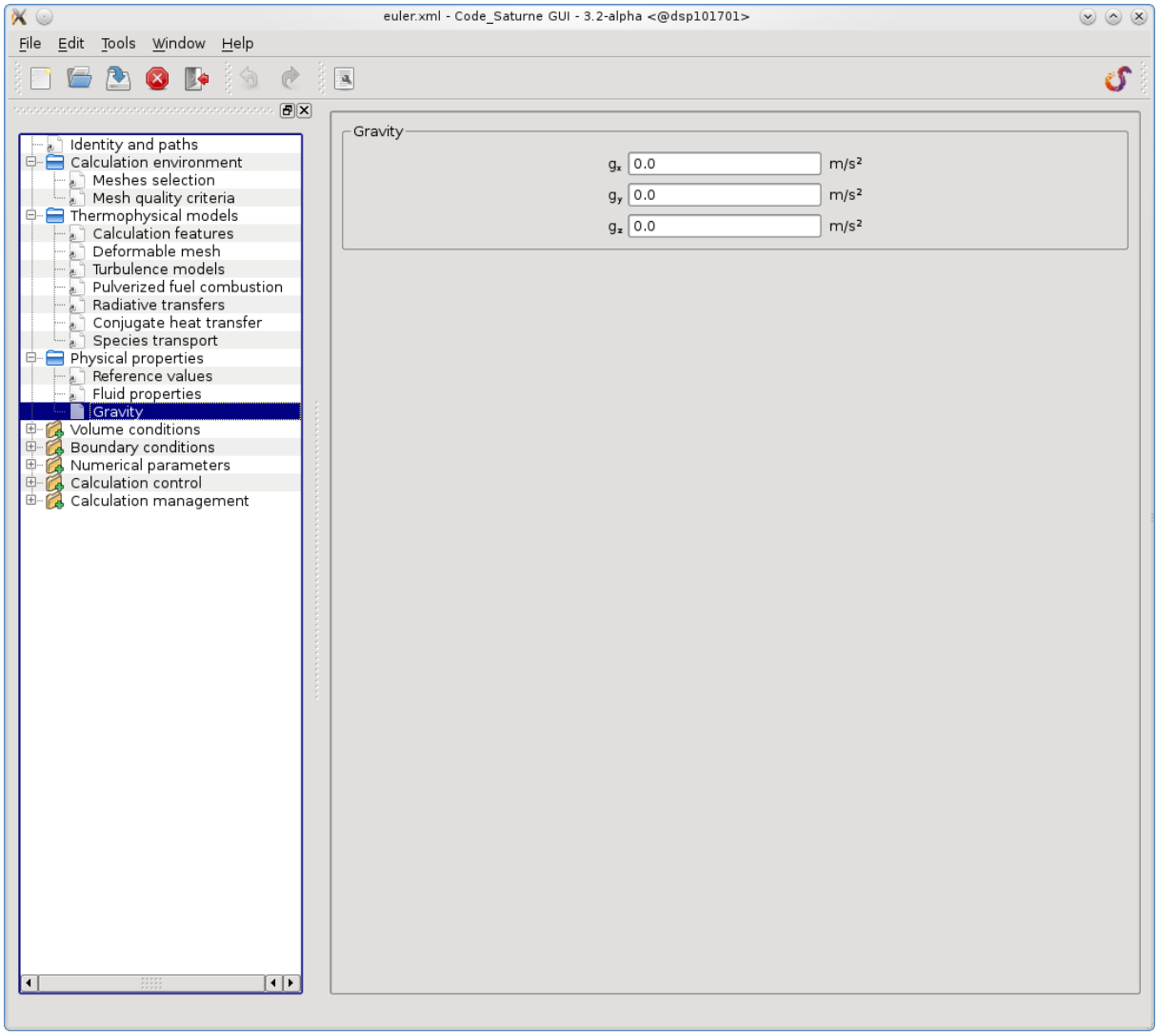

Figure 12: Step 4 – Physical properties; Gravity.

6.2.5. Step 5 – Boundary Conditions

- At first, the boundary regions and their corresponding boundary faces have to be defined. In doing so, change to the *Definition of boundary regions* subsection. In the *Add from Preprocessor listing*, click the icon corresponding to *Import groups and references from Preprocessor listing* and select the file *check_mesh.log* generated by the preprocessor. In the menu *Definition of boundary regions*, 5 lines should have appeared (*Label* from BC_1 to BC_5).

- Change *BC_1 Nature* to *Inlet*. Repeat this procedure for the remaining boundary regions like it is shown in the following table:

Label	*Zone*	*Nature*	*Selection criteria*
BC_1	1	Inlet	AIRPRIM
BC_2	2	Inlet	AIRSEC
BC_3	3	Inlet	AIRTER
BC_4	4	Outlet	OUTLET
BC_5	5	Wall	WALL

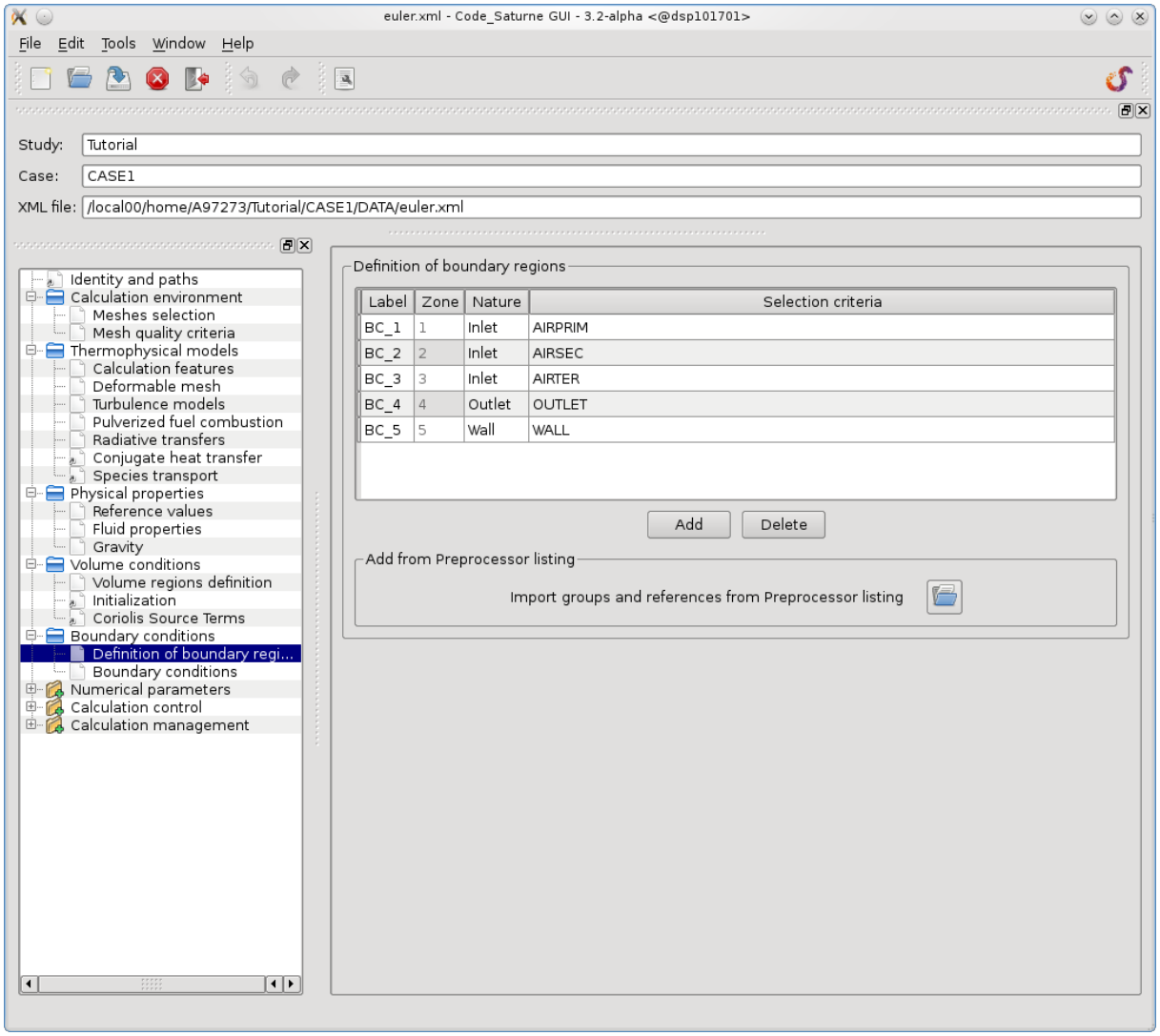

Figure 13: Step 5 – Boundary conditions; Definition of boundary regions.

- Change to the *Boundary conditions* subsection.

- Click on BC_1 (AIRPRIM) in the list of *Boundary conditions* and set the following options and values:

Criteria	Option	Value
Flows and temperatures	Oxydant and coal	
Mass flow rate and temperature for oxydant	Massflowrate	0.194 kg/s
	Oxydant number	1
	Temperature	310 K
Direction	Normal to the inlet	
Mass flow rate and temperatures of coals	Coal Number	Coal 1
	Flow	0.125 Kg/s
	Temperature	310 K
Mass flow rate and temperatures of coals	Coal Number	Coal 2
	Flow	0 Kg/s
	Temperature	310 K
Ratio of mass distribution for each class of coal	Class 1 - Coal 1	100
	Class 1 - Coal 2	100
Turbulence	Calculation by hydraulic diameter	0.0758 m

- Click on BC_2 (AIRSEC) in the list of *Boundary conditions* and set the following options and values:

Criteria	Option	Value
Flows and temperatures	Only oxydant	
Mass flow rate and temperature for oxydant	Massflowrate	0.639 kg/s
	Oxydant number	1
	Temperature	623 K
Direction	User profile	
Turbulence	Calculation by hydraulic diameter	0.0774 m

- The User profile of the inlet velocity vectors should look like it is shown in the following Figure 14. It can be edited using the *Mathematical expression editor*, which pops by pushing the button next to *User profile*.

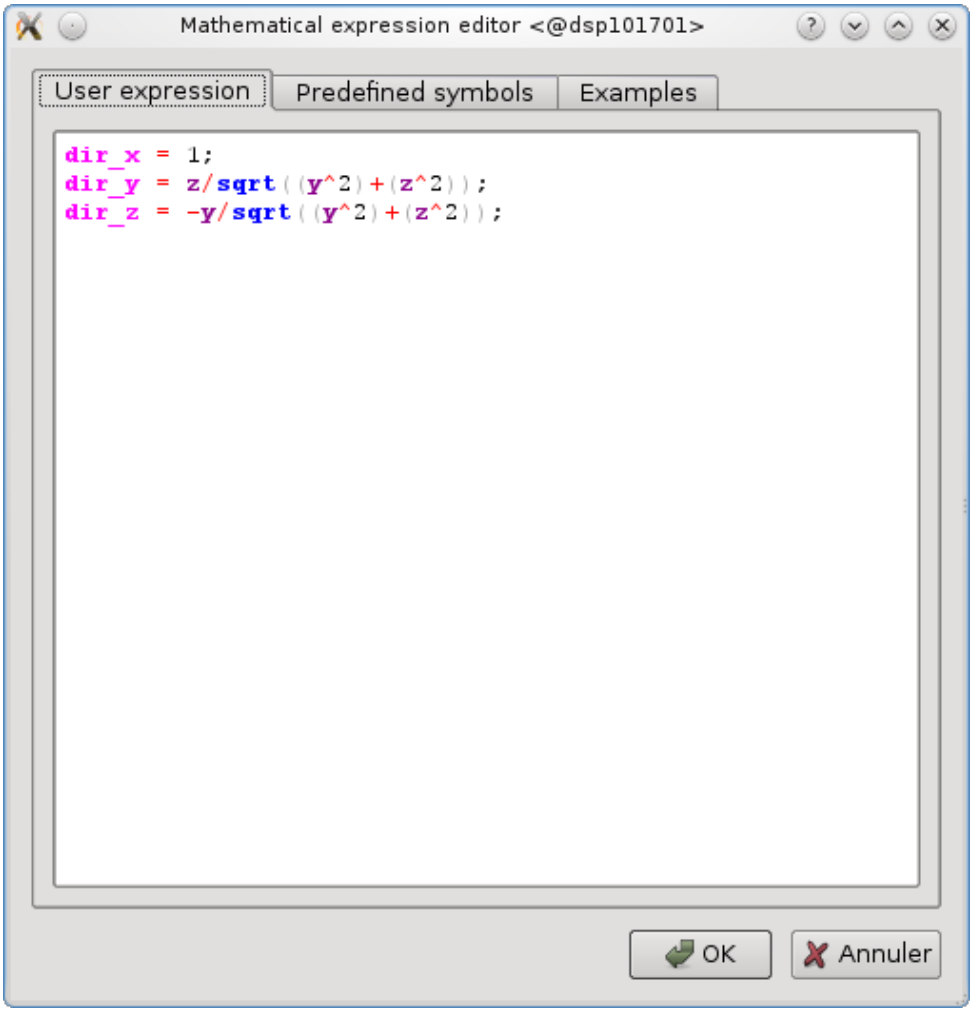

Figure 14: Step 5 – Boundary conditions; Boundary conditions; User profile of the inlet velocity vectors of BC_2 (AIRSEC).

- Click on BC_3 (AIRTER) in the list of *Boundary conditions* and set the following options and values:

Criteria	Option	Value
Flows and temperatures	Only oxydant	
Mass flow rate and temperature for oxydant	Massflowrate	0.583 kg/s
	Oxydant number	1
	Temperature	310 K
Direction	Normal to inlet	
Turbulence	Calculation by hydraulic diameter	0.048 m

- No additional information is needed with respect to the outlet boundary condition (BC_4).

- Click on BC_5 (WALL) in the list of *Boundary conditions* and set the following options and values:

Criteria	Option	Value
Smooth or rough wall	Smooth wall	On
Sliding wall		Off
Thermal radiative transfer	Gray or black wall and profile of fixed internal temperature	On
	Emissivity	0.7
	Initial temperature	773 K
	Post-processing zone: no.	1

- Save the case.

6.2.6. Step 6 – Numerical parameters

- In the *Global parameters* subsection, set the *Gradient calculation method* to *Least squares method over partial extended cell neighbourhood*. Keep the default settings for all other options and parameters.

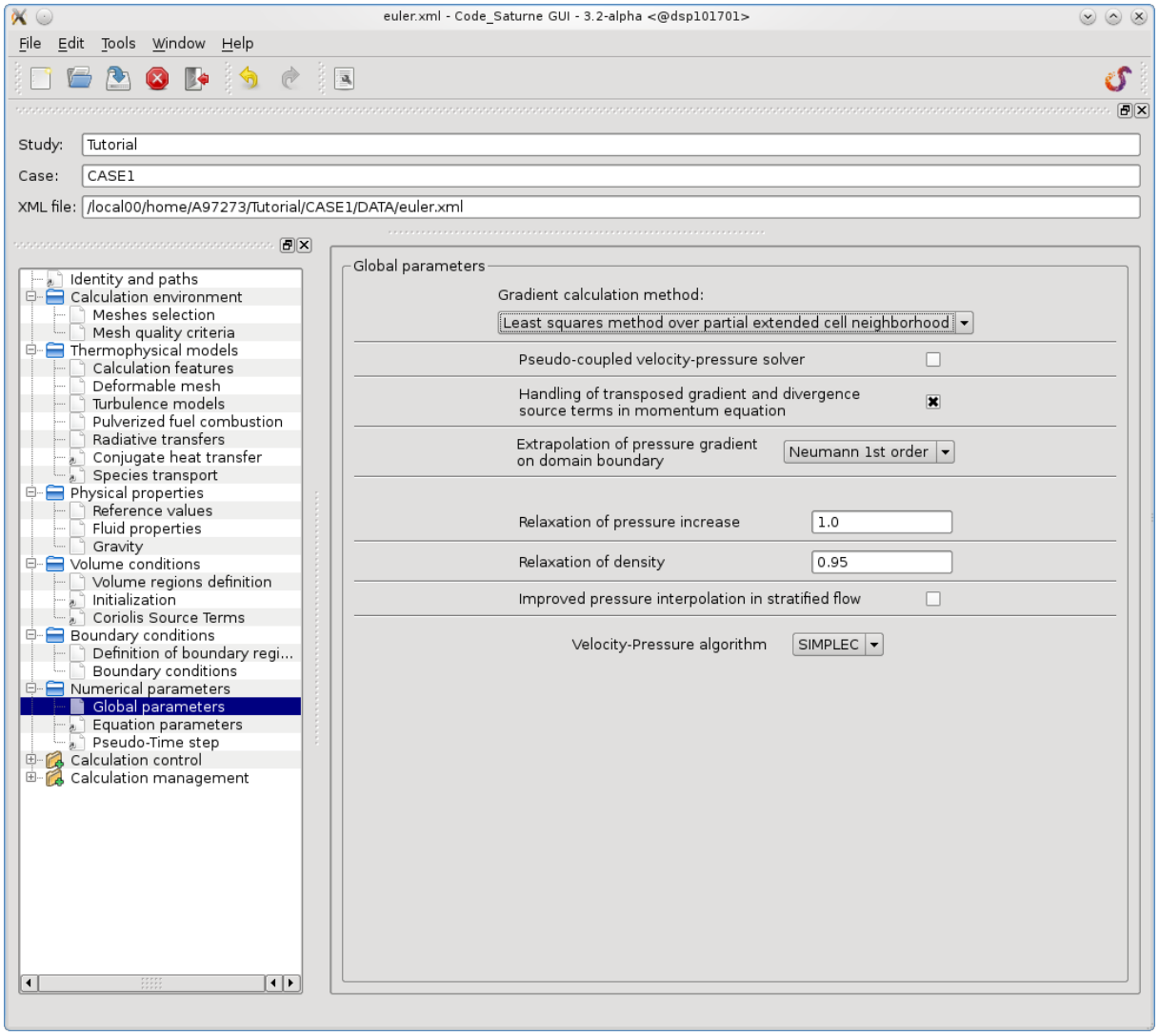

Figure 15: Step 6 – Numerical Parameters; Global parameters.

- In the Pseudo-*Time step* subsection, enter 0.001s for the *Reference time* step. The *Number of iterations* should be 3000. Enter 1 for the *Maximal CFL number* and 10 for the *Maximal Fourier number*. The *Minimal time step factor* must be set to 0.001; the *Maximal time step factor* to 1000. Retain the default value 0.1 of the *Time step maximal variation*. Activate neither the *Time step limitation* option nor the *Zero time step* option.

- Save the case.

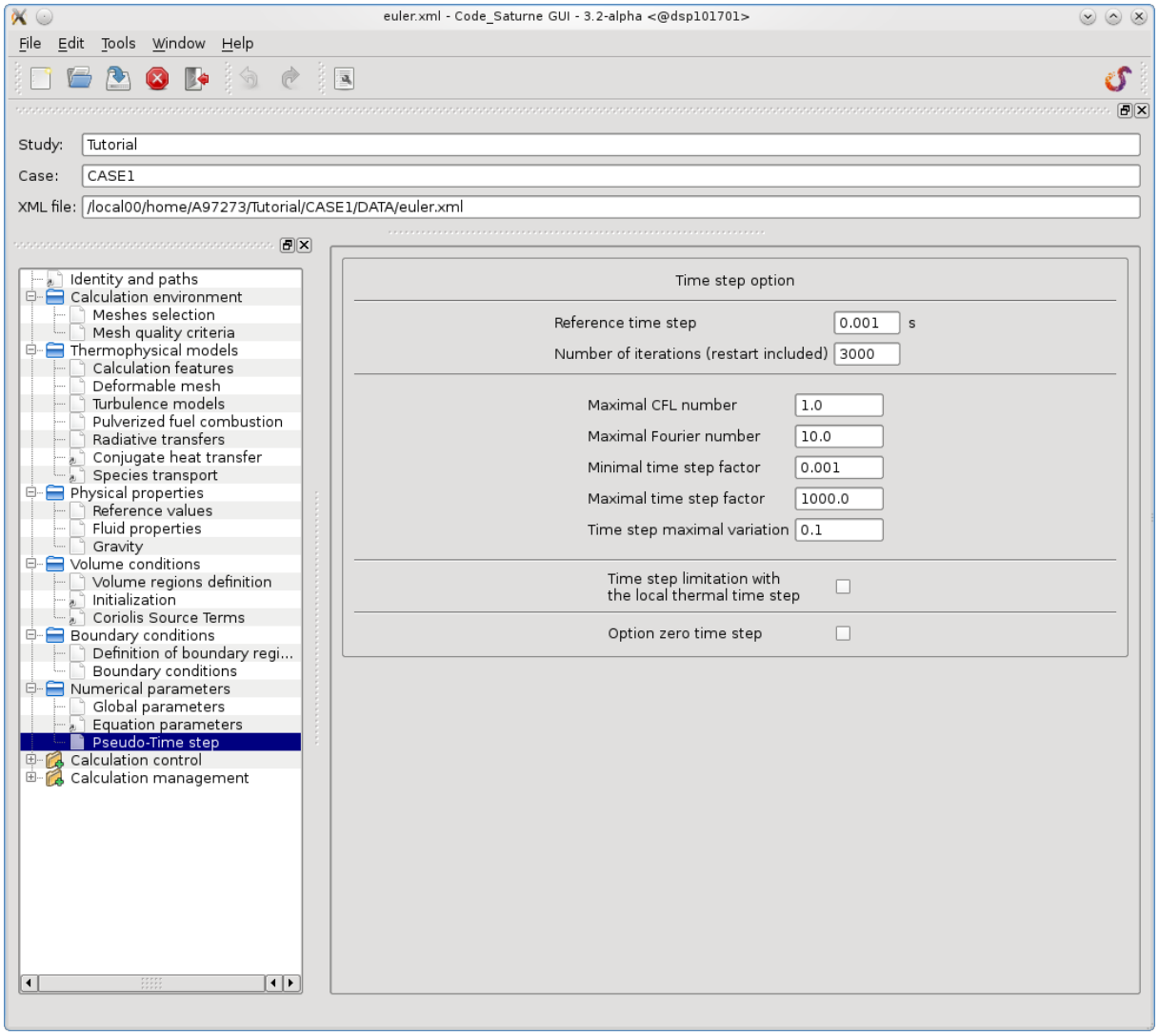

Figure 16: Step 6 – Numerical parameters; Time step.

6.2.7. Step 7 – Calculation control

- In order to create intermediate results files you have to change to the *Writer* rider in the *Output control* subsection. Click on the first line appearing in the main window and change the *Frequency* output from *No periodic output* to *Output every 'n' time steps*. Set the value to 100 and leave the *Output at the end of calculation* option activated.

- Save the case.

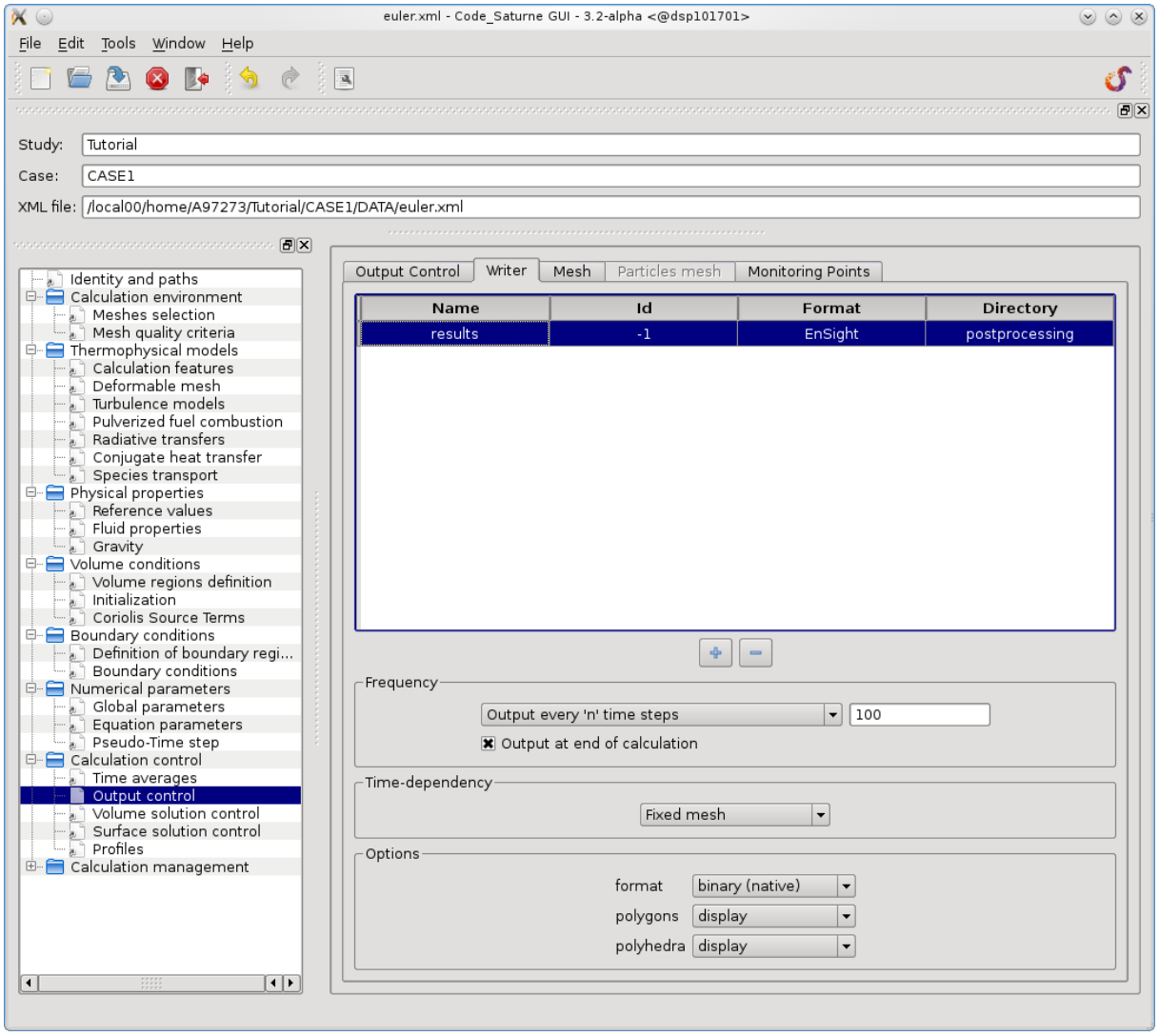

Figure 17: Step 7 – Calculation control; Output control.

6.2.8. Step 8 – Calculation management

- Make sure the *Calculation restart* option is set to *off* in the *Start/Restart* subsection.
- Select the *Standard* option from the *Prepare batch calculation* subsection as *Run type* and increase the *Number of processors* up to 6.
- Save the case.
- Start the calculation

6.3. Post – processing

According to the settings made, the intermediate post – process files are written every 100th iteration. These intermediate files as well as the final result files are stored in the

/Tutorial/CASE1/RESU/YYYYMMDD-HHMM folder (where YYYY is standing for the year, MM for the month, DD for the day, HH for the hour and MM for the minutes). They can be opened using either Ensight or ParaView (both viewers should be accessible on your computer). Once you have opened these files using the viewer of your choice, you can compare the obtained results with those shown on the following pages.

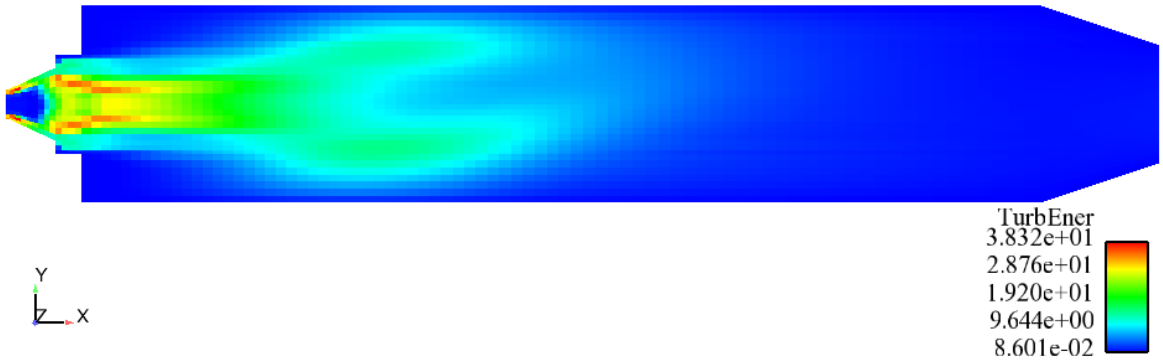

Figure 18 : Turbulent kinetic energy.

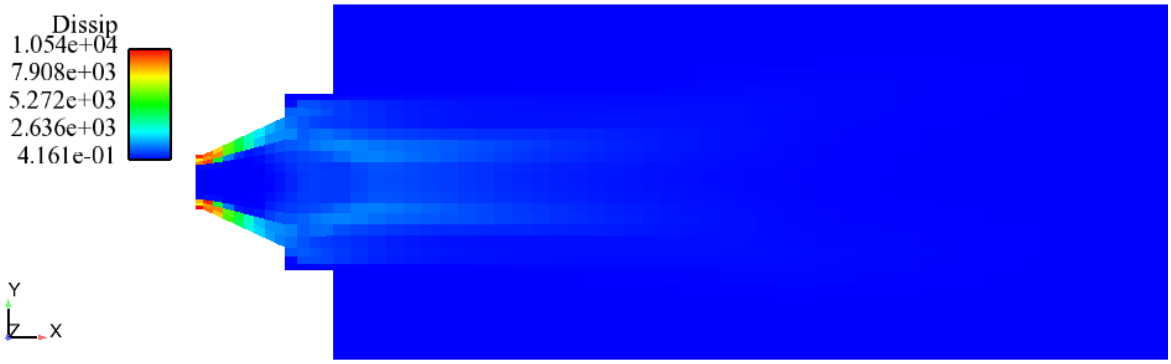

Figure 19 : Turbulent dissipation.

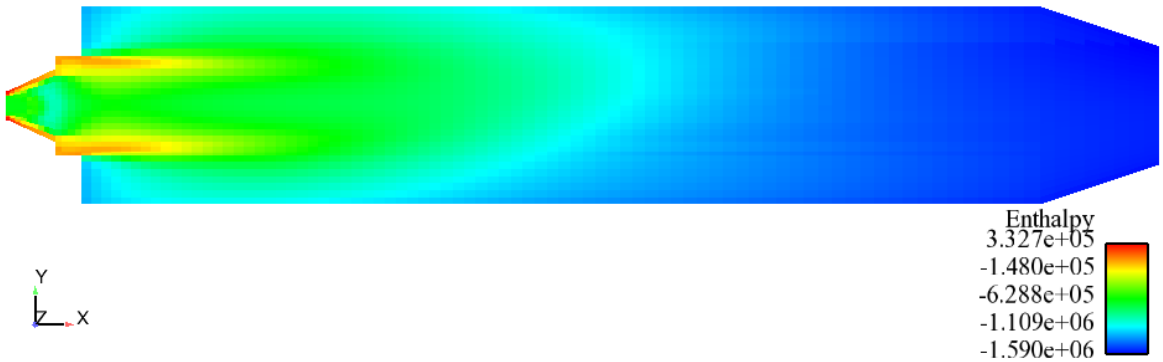

Figure 20 : Spatial enthalpy distribution.

Figure 21 : Number of particles.

Figure 22 : Mass fraction of reactive coal.

Figure 23 : Mass fraction of char.

Figure 24 : Mass fraction of the light volatile matter.

Figure 25 : Mass fraction of the heavy volatile matter.

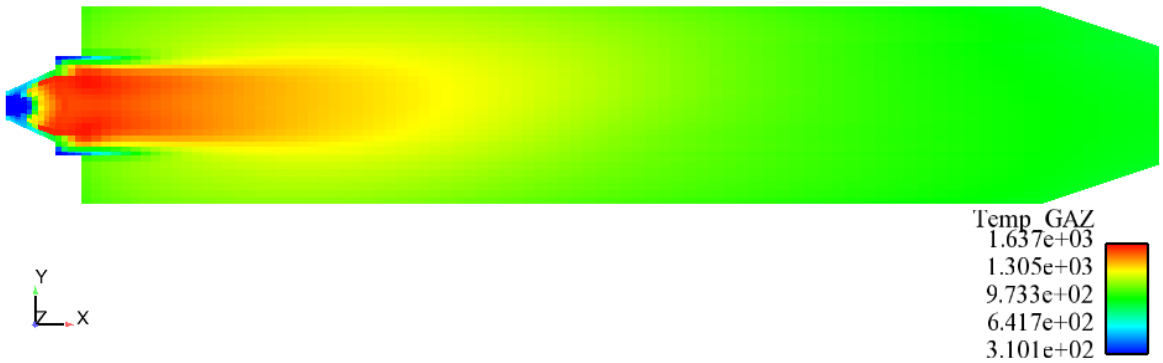

Figure 26 : Temperature of the gas phase in K.

7. Lagrangian calculation

7.1. Checking the Eulerian calculation and creating new case

- Before running the Lagrangian calculation, Eulerian results should be checked.
- Create a new *Code_Saturne* case named *CASE2* in the *Tutorial* study folder. Return to the Tutorial folder: **cd ../..** and create a new case by using the command **code_saturne create –c CASE2**. This command automatically adds a folder called CASE2.
- Change to */Tutorial/CASE2/DATA* and launch the Graphical User Interface (GUI) by using the command **./SaturneGUI**

7.2. Setup

The simulation is set up in several consecutive steps. In the following, each step is entitled like the corresponding section shown in the most left window of the GUI. Keywords that can be found in the GUI itself are written in italic. The figure legends are always structured as follows: Step X – Section; Subsection; Rider A; Rider B; Rider …

7.2.1. Step1 – Verify the Computation Directories

Create a new file from the *File* Menu. Check that the setting are correct (please refer to paragraph 6.2.1).

7.2.2. Step 2 – Calculation environment

- Load the mesh (*Tutorial3D.cgns*) and make sure that the pre-processor is running well (the procedure is explained in details in paragraph 6.2.2).
- Save the case.

7.2.3. Step 3 – Thermophysical models

- In the *Calculation features* subsection, choose *particles and droplets tracking* from the pull down Menu *Eulerian-Lagrangian multi-phase treatment* (Note that a new subsection called ***Particles and droplets tracking*** should appear in the left window).
- Choose *homogeneous approach with moisture with Lagrangian transport* from the pull down Menu *Pulverized fuel combustion* (Note that a new subsection called ***Pulverized fuel combustion*** should appear in the left window).
- Retain all other default settings.
- Save the case.

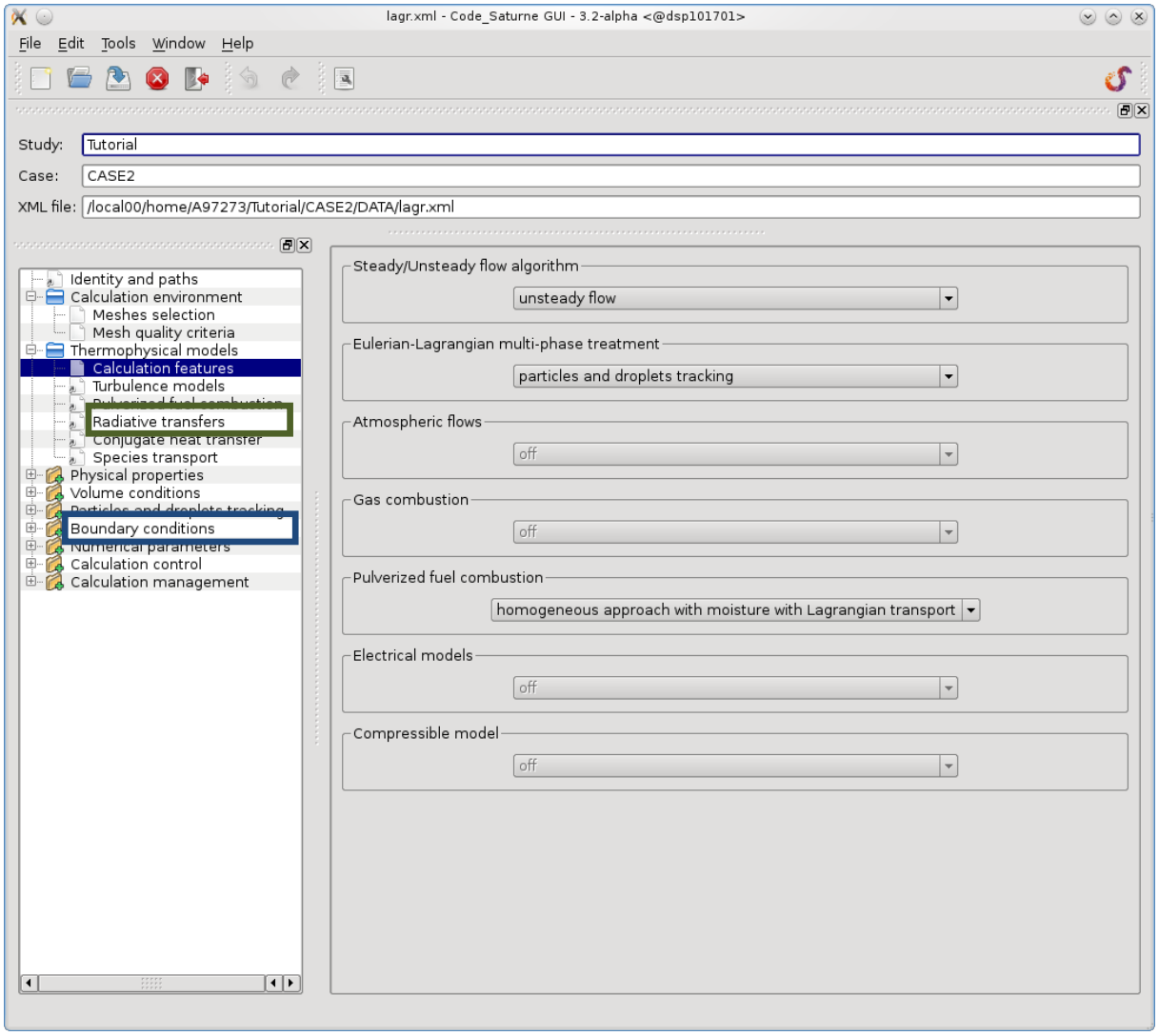

Figure 27: Step 3 - Thermophysical models; Calculation features subsection.

- Change to the *Turbulence models* subsection and select the *k-ε linear production* turbulence model. Don't modify any of the advanced options. Note that the Lagrangian calculation will be run on a frozen carrier field so that the setting of this parameter should not have any influence. Nevertheless the *k-ε linear production* model should be selected to ensure a troublefree Lagrangian restart (refer to section 4 for more details).

- Save the case.

- Change to the *Pulverized fuel combustion* subsection.

- Name the fuel as *Tutorial_Coal* and make sure the type of fuel is well set to *coal*.

- Add a second type of call *Tutorial_Biomass* and make sure the type of fuel is well set to *biomass*.

- Select the *user define* option at the *size distribution* rider and set the *initial diameter* of *Class 1* to 2.5e^{-5} m for *Tutorial_Coal* and 8.0e^{-4} m for *Tutorial_Biomass.*

- **Note:** the total number of class, coal and the diameter should not be changed to ensure a troublefree Lagrangian restart (refer to section 4 for more details). Anyway, the diameters that are given at this point will not be taken into account by the Particle and droplet tracking module.

- Change to the *Solid fuel* rider and modify the *Elementary analysis,* the *Immediate analysis,* the *Solid fuel physical properties,* the *Ashes physical properties,* and the *Coke elementary analysis* settings as shown in the following in the table below and in the Figure 5.

- Do not forget to fill the thermal conductivity which is required to compute thermal gradient inside particles.

- **Note:** as explained in the section 4, the properties of the *Tutorial_Coal*, which was previously injected in the furnace, should not be changed. On the other hand, you may change the properties of the biomass as it was not previously injected.

Label	*Zone*	*Tutorial_Coal*	*Tutorial_Biomass*
Elementary analysis (refers to dry coal)	Mass content of C	76.65 %	53 %
	Mass content of H	5.16 %	5.8 %
	Mass content of O	9.9 %	37.62 %
	Mass content of N	0 %	0 %
	Mass content of S	0 %	0 %
Immediate analysis	Heating model LHV	3.0 e^7 J/kg (dry basis)	1.8614 e^7 J/kg (dry basis)
	Volatile matter	0 %	0 %
	Ash content	6.21 %	2.74 %
	Moisture	0 %	8.88 %
Solid fuel physical properties	Cp	1800 J/kg/K	1500 J/kg/K
	ρ	1200 kg/m^3	549.8 kg/m^3
	λ	0.045 W/m/K	0.12 W/m/K
Ashes physical properties	Enthalpy	0 J/kg	0 J/kg
	Cp	1800 J/kg/K	1500 J/kg/K
Coke elementary analysis (refers to dry)	Mass content of C	100 %	100 %
	Mass content of H	0 %	0 %
	Mass content of O	0 %	0 %
	Mass content of N	0 %	0 %
	Mass content of S	0 %	0 %

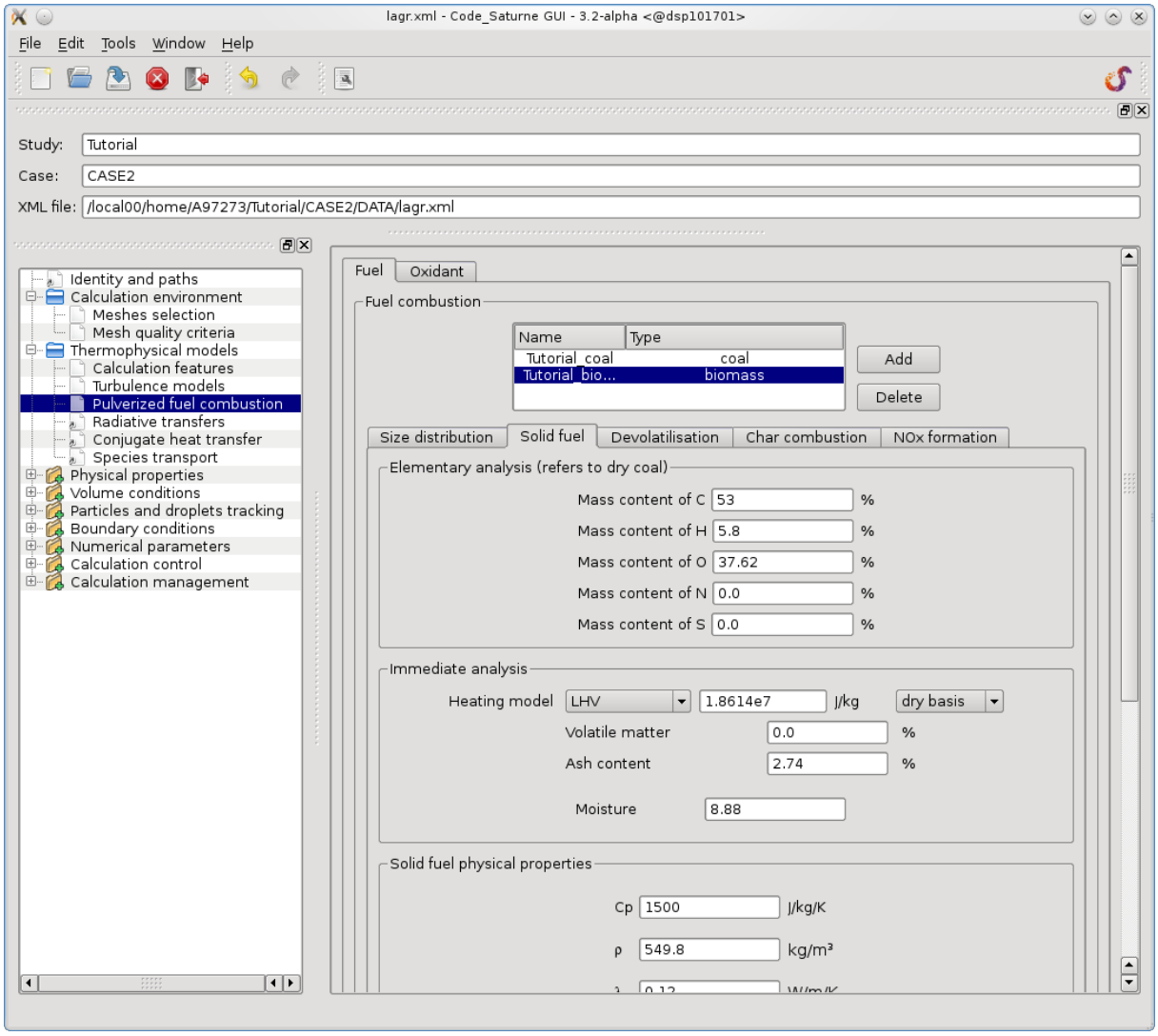

Figure 28: Step 3 - Thermophysical models; Pulverized fuel combustion; Fuel; Solid fuel.

- Change to the *Devolatisation* rider and set the *Stoichiometric coefficients* to *user define*.
- For *Tutorial_Coal* set Y_1 = 0.37 and Y_2 = 0.74 and for *Tutorial_Biomass* set Y_1 = 0.7507 and Y_2 = 0.7508. Don't modify the *Pre-exponential constants* and the *activation energies*.
- Change to the *Char combustion* rider and set *the pre-exponential factor* to 17.88, the *activation energy* to 16.55, and the *reaction order* to 1 (for both *Tutorial_Coal* and *Tutorial_Biomass*). Don't activate the gasification of char by CO_2 and H_2O.
- Change to the *NOx formation* rider and deactivate *NOx formation*.
- This option will not have any impact on the Lagrangian computation as it will be run on a frozen carrier field. Nevertheless changing this parameter form Eulerian calculation to

Lagrangian calculation may cause trouble during the Lagrangian restart (refer to section 4 for more details).

- In order to conclude the *Pulverized fuel combustion* subsection, you have to characterize the composition of the gaseous oxidizer (most of times air is used for this purpose). In doing so you have to change from the *Fuel* rider to the *Oxidant* rider. Make sure the composition of the oxidizer is given in *molar* units. Set the number of moles for *Oxidant number 1* to 1 mol for O_2, 3.76 mol for N_2, and 0 mol for both CO_2 and H_2O.

- This option will not have any impact on the Lagrangian computation as it will be run on a frozen carrier field. Nevertheless changing this parameter form Eulerian calculation to Lagrangian calculation may cause trouble during the Lagrangian restart (refer to section 4 for more details).

- Save the case.

- Changing to the *Radiative transfer* subsection and selecting the *P-1 Model* activates the radiative heat transfer. The absorption coefficient is set to be *constant* and its value is 0.85 m^{-1}. Set the restart calculation options to *on*.

- Enabling the restart calculation will force *Code_Saturne* to reuse the radiative calculation made before. It is a good way to spare calculation time.

- Changing the radiative transfers model from Eulerian calculation to Lagrangian calculation may cause trouble during the Lagrangian restart (refer to section 4 for more details).

- Save the case.

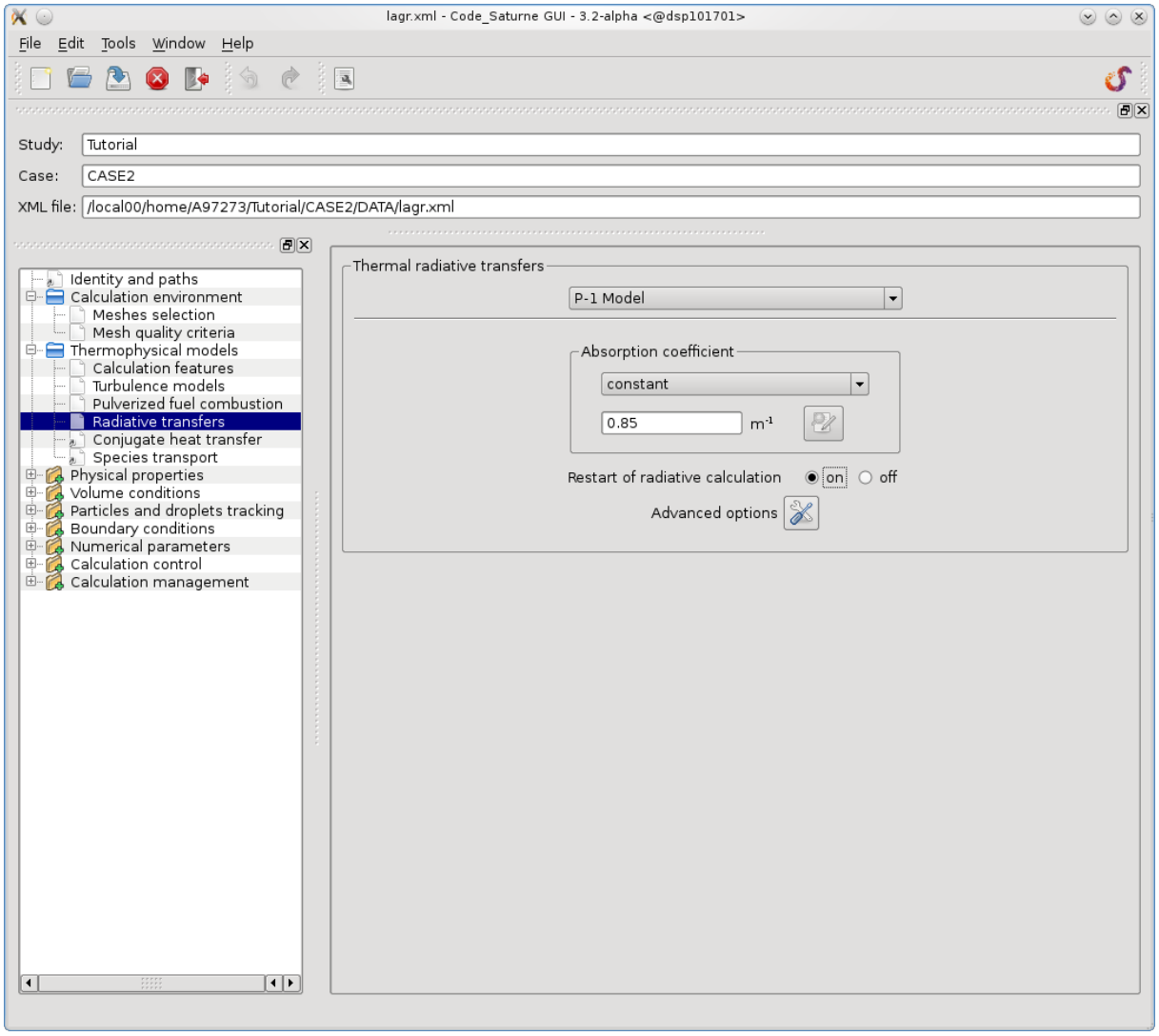

Figure 29: Step 3 - Thermophysical models; Radiative transfer.

7.2.4. Step 4 – Physical properties

- Refer to the paragraph 6.2.4
- Note that a change of gravity between Eulerian and Lagrangian computation may lead to physical discrepancies.
- Save the case.

7.2.5. Step 5 – Particles and droplets tracking

- In the *Global settings* subsection, make sure that the *Frozen carrier flow* option is selected in the pull down Menu *Eulerian-Lagrangian multi-phase Treatment*. As of 16 October 2013, other Eulerian/Lagrangian Multi-phase Treatment are not available with coal combustion.

- In the *Main parameters* menu, set the *Maximum number of particles at each time step* to 500000. Note that this number should be adapted depending on the quantity of RAM available on your computer. Reducing maximum number of particle will decrease the memory load.

- Select *Pulverised coal model* in the pull down Menu *Additional models associated with the particles* and enable *Coal particle fouling (Watt & Fereday's model).* Set the fouling parameters like it is shown in the following table:

Name	*Limit temperature of fouling (deg C)*	*Ash critical viscosity (Pa.s)*	*Coefficient 1*	*Coefficient 2*
Tutorial_Coal	1 000	1.0e4	0.5415	-0.489122
Tutorial_Biomass	900	1.0e25	0.5415	-0.489122

- Make sure that no *Particle deposition sub-model* is activated and check the *Advanced options* of the *Numerical scheme*. Select the *first-order scheme* for *Integration for the stochastic differential equations* (*second-order scheme* is not available with coal combustion at the moment). Do not change the other options.

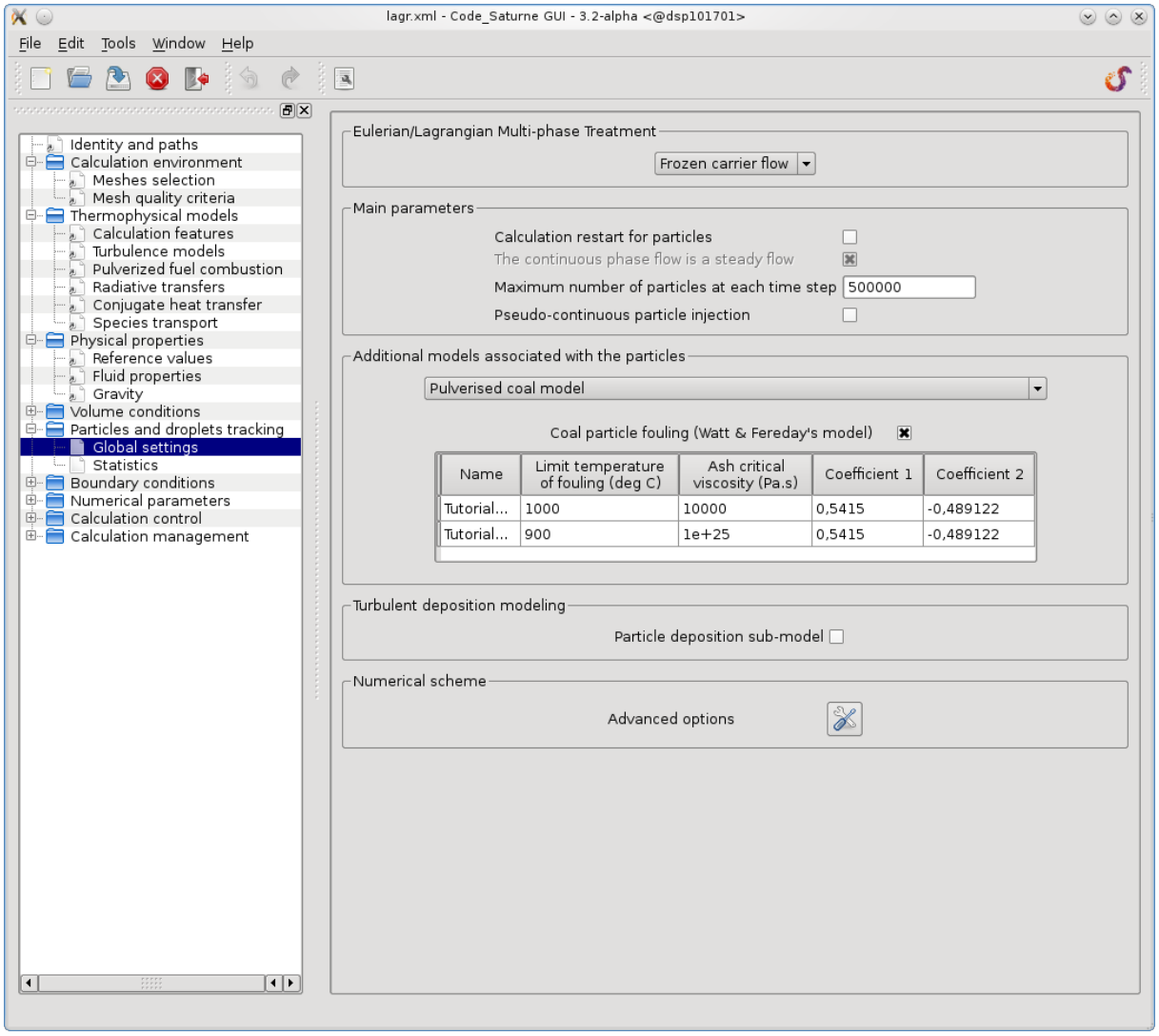

Figure 30: Step 5 – Particles and droplets tracking; Global settings.

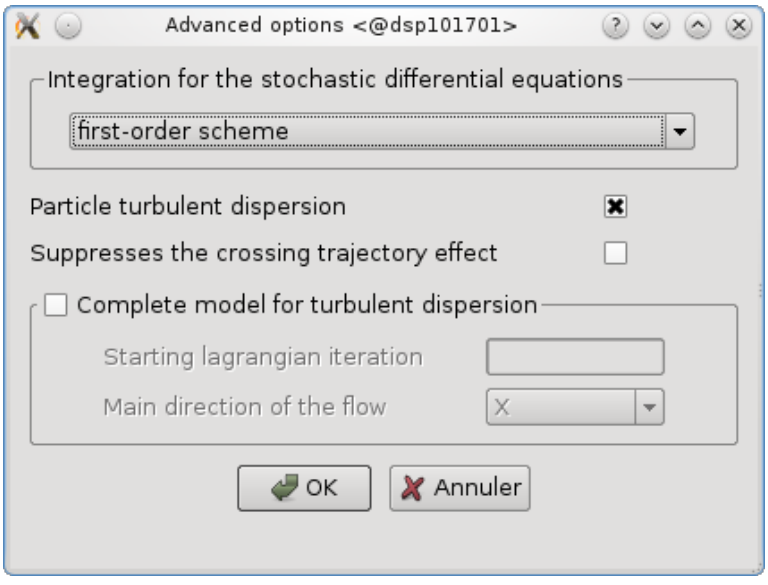

Figure 31: Step 5 – Particles and droplets tracking; Global settings; Advanced options.

Change to the *Statistics* subsection, activate *Calculation of volume statistics.* To ensure that statistics have a good quality, it's better to calculate the statistics from the steady state (which means that the number of particle in the furnace is steady). Set *Calculation start from Lagrangian iteration n° (restart(s) included)* at 2000. Make sure that the *Start of steady-state statistics from Lagrangian iteration n° (restart(s) included)* is at 2000. The *Threshold for statistical weight* should be 0.0 and all *Post-processing* options in the table should be selected.

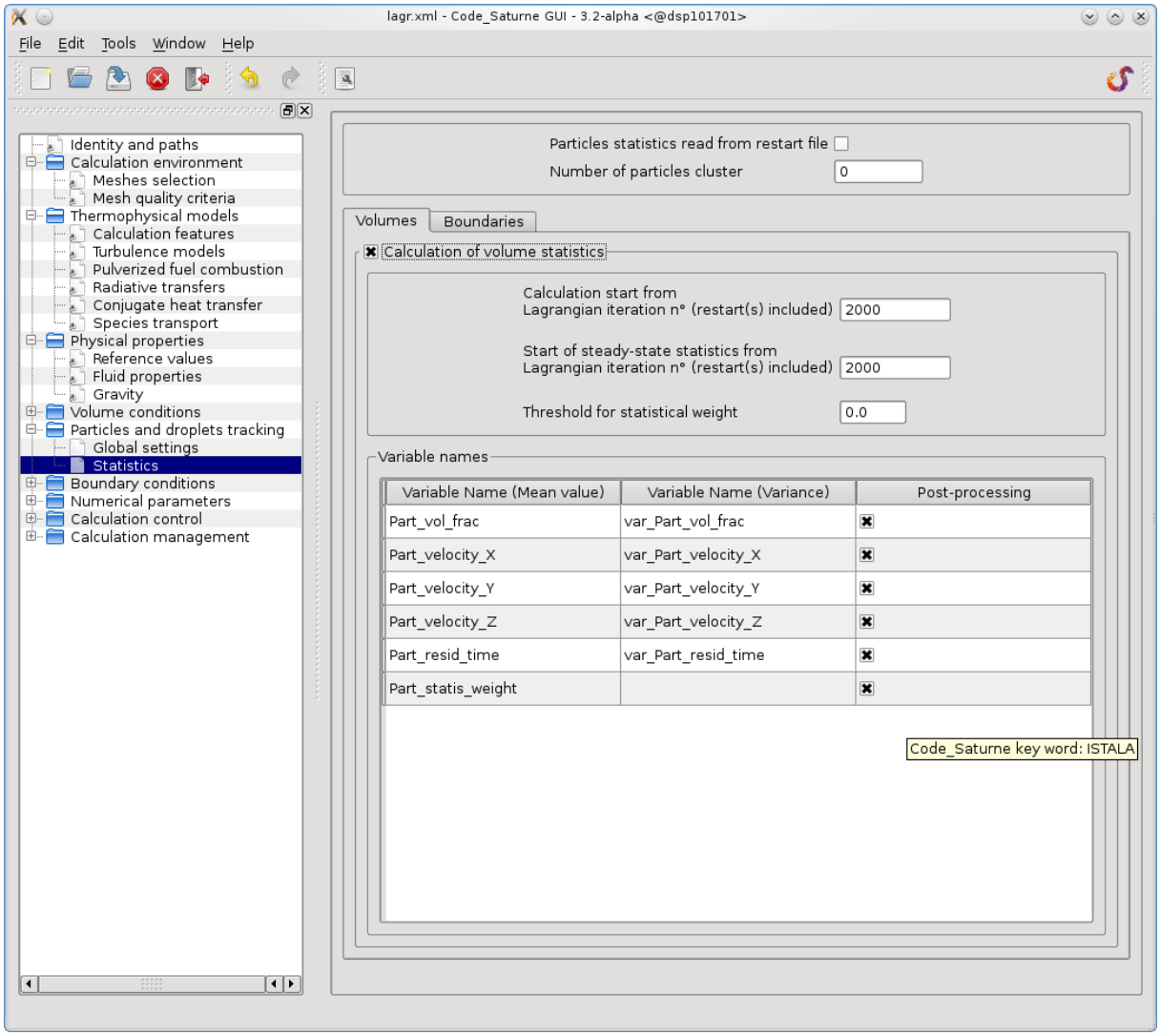

Figure 32: Step 5 – Particles and droplets tracking; Statistics; Volumes.

- Change from the *Volumes* rider to the *Boundaries* rider. Activate *Calculation of boundary statistics.* For the same reason, set *Iteration starting* at 2000. Make sure that the *Threshold for statistical weight* should be 0.0 and all *Post-processing* options in the table should be selected.

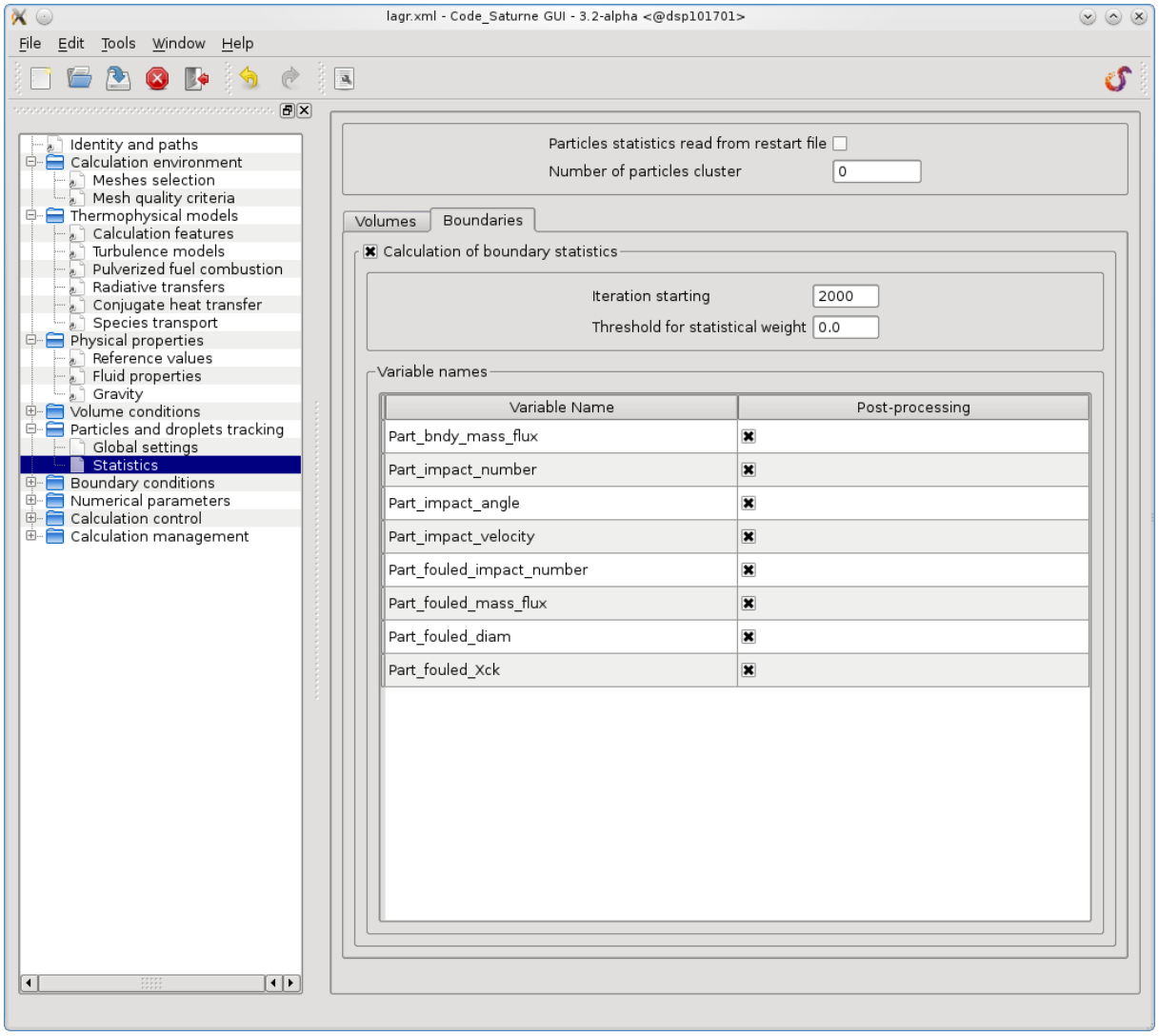

Figure 33: Step 5 – Particles and droplets tracking; Statistics; Boundaries.

7.2.6. Step 6 – Boundary Conditions

- Set *Definition of boundary region* and *Boundary conditions* subsections as explained in 6.2.5
- Change to the *Particles boundary conditions* subsection. Set the options and values as shown in the following in the table below and in the Figure 34.

Label	Nature	Particle-boundary interaction	Number of classes
BC_1	inlet	Particles inlet	1
BC_2	inlet	Particles inlet	0
BC_3	inlet	Particles inlet	0
BC_4	outlet	Particles outlet	0
BC_5	wall	Fouling	0

- Click on BC_1 in the list of *Lagrangian boundary conditions* and set the following options and values:

Criteria	Option	Value
Class number		1
Number of particles in class		25
Frequency of injection		1
Statistical weight set by values		
Statistical weight		18.21 [1]
Velocity	Fluid velocity	
Diameter	Diameter set by values	
	Mean value	0.0008 m
	Standard deviation	0.0 m
Coal	Coal number	2
	Coal composition	Raw coal
	Temperature	310.0 K

- No additional information is needed with respect to the other Lagrangian boundary conditions.

- Save the case.

[1] With the following parameters, the Lagrangian flow rate is 7.37 10^{-4} kg/s where as the biomass flow rate should be 1.34 10^{-2} kg/s. The statistical weight is the ratio between both figures and is used to calculate a consistent fouling flow rate (in kg/s/m^2).

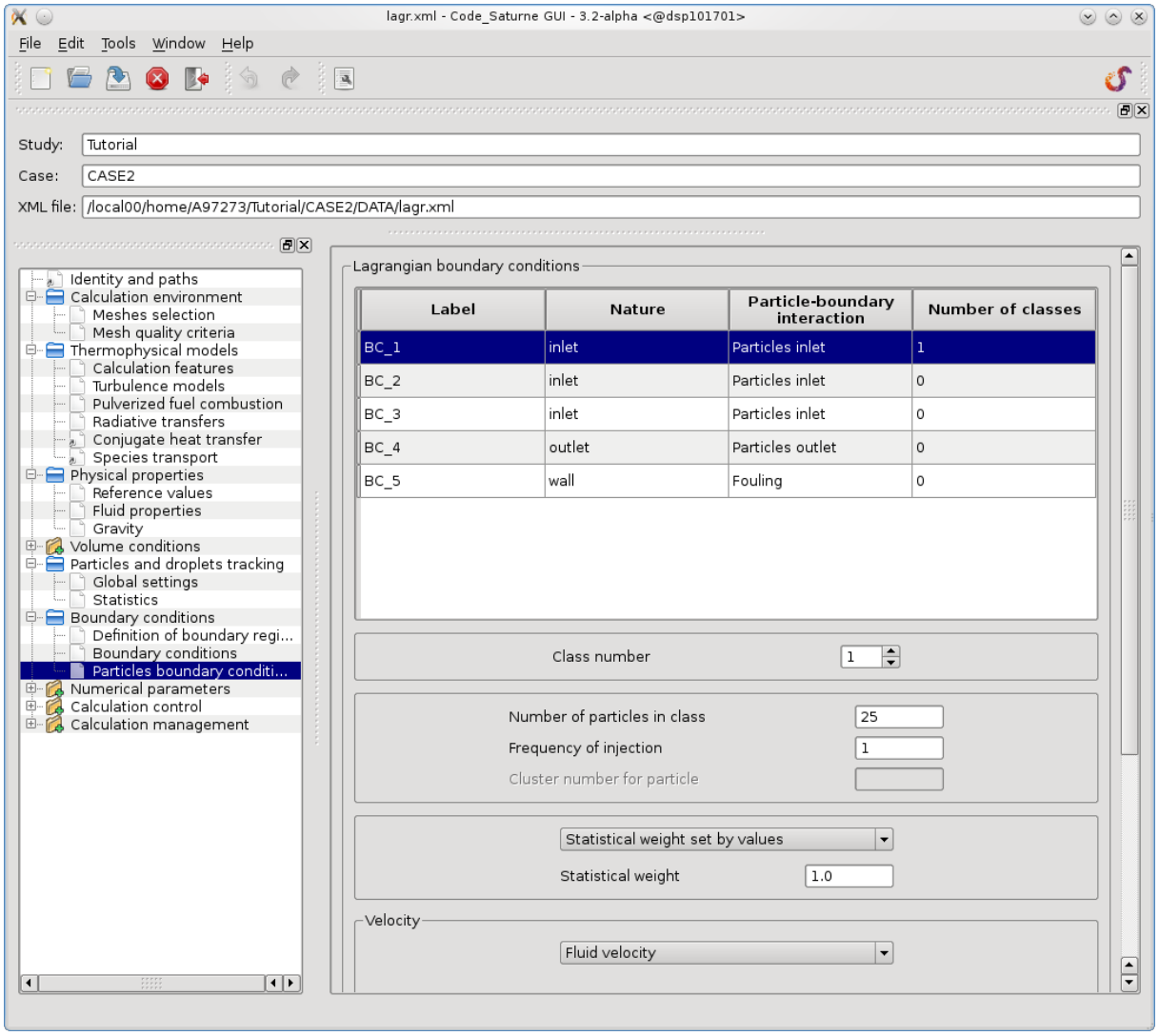

Figure 34: Step 6 – Boundary Conditions; Particles boundary conditions.

7.2.7. Step 7 – Numerical parameters

- Configure the *Global parameters* subsection as in paragraph 6.2.6
- Set the *Time step option* to *Constant* in the *Time step* subsection. Enter 0.005s for the *Reference time* step. The *Number of iterations* should be at least 10 000. Check that the *Zero time step* option is not activated.
- Save the case.

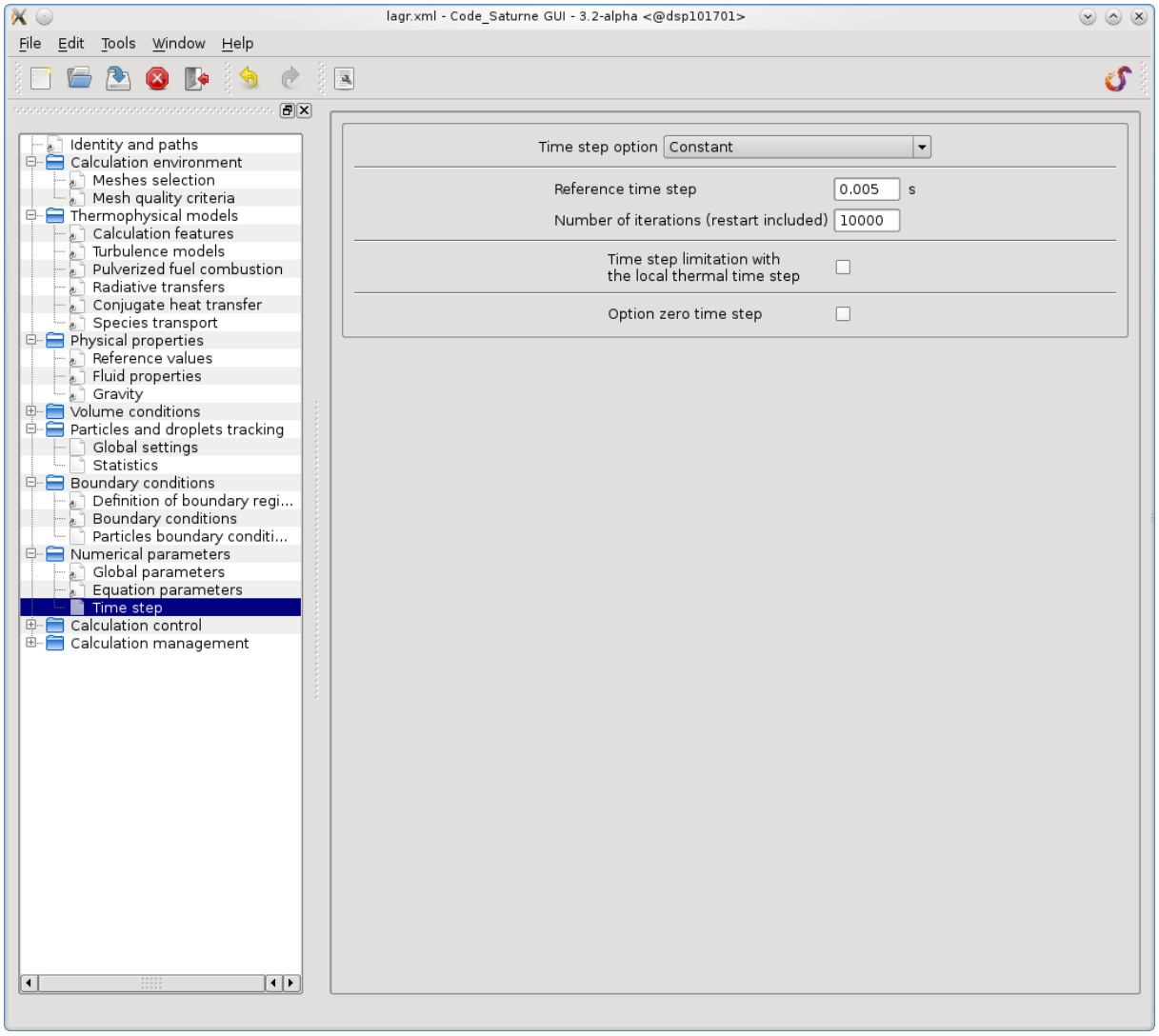

Figure 35: Step 7 – Numerical parameters; Time step.

7.2.8. Step 8 – Calculation control

- In order to create intermediate results files you have to change to the *Writer* rider in the *Output control* subsection. Click on *results* (first line appearing in the main window) and change the *Frequency* output from *No periodic output* to *Output every 'n' time steps*. Set the value to 100 and leave the *Output at the end of calculation* option activated.

- Click on *particles* (second line appearing in the main window) and deactivate the *Output at the end of calculation* option.

- Click on *trajectories* (third line appearing in the main window) and deactivate the *Output at the end of calculation* option.

- Save the case.

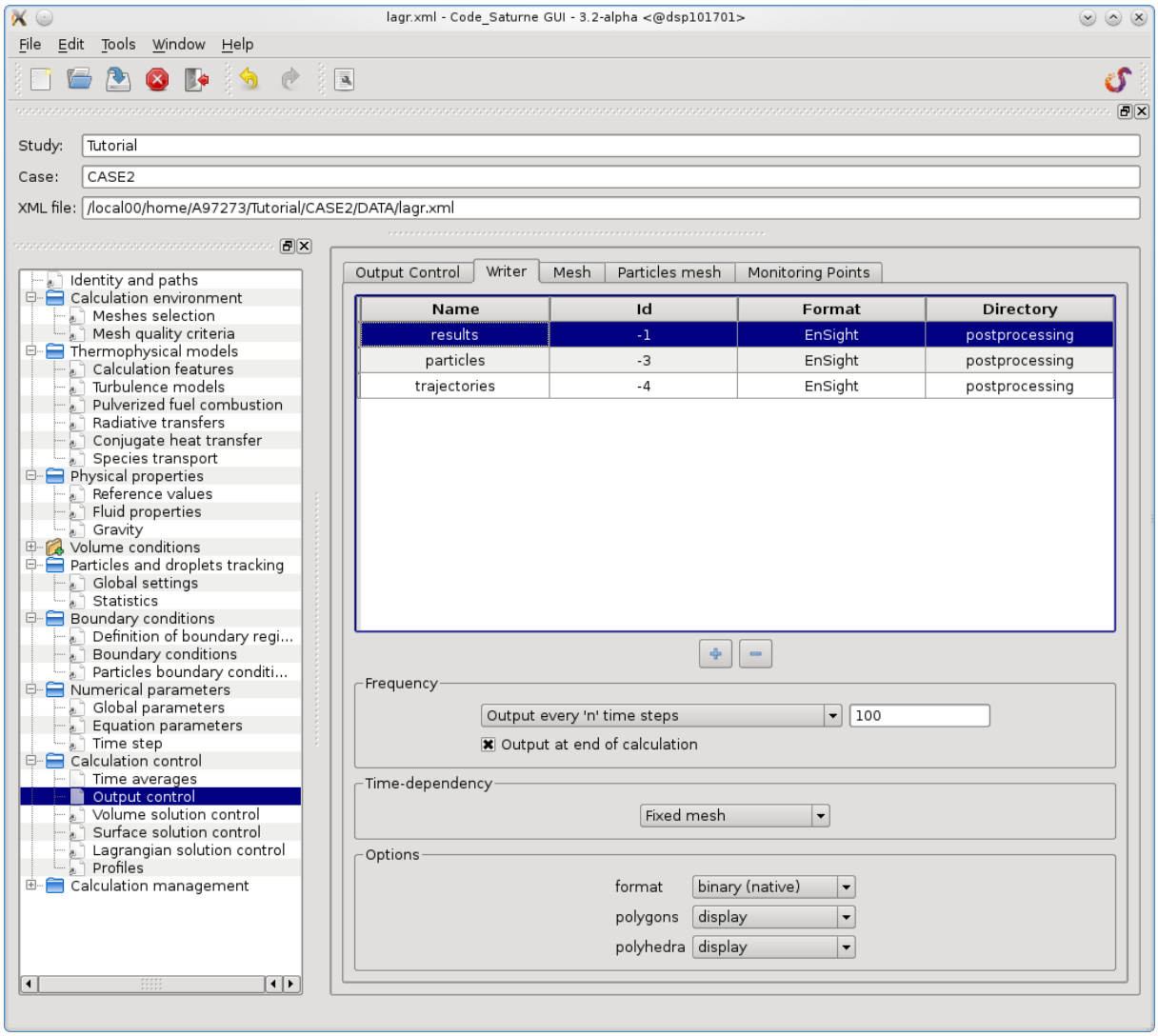

Figure 36: Step 8 – Calculation control; Output control.

7.2.9. Step 9 – Calculation management

- Make sure the *Calculation restart* option is set to *on* in the *Start/Restart* subsection and indicate the checkpoint folder corresponding to the Eulerian calculation (/Tutorial/CASE1/RESU/YYYYMMDD-HHMM/checkpoint -where YYYY is standing for the year, MM for the month, DD for the day, HH for the hour and MM for the minutes-). Select the *Calculation on frozen velocity and pressure fields* option.

- Select the *Standard* option from the *Prepare batch calculation* subsection as *Run type* and increase the *Number of processors* up to 6.

- Save the case.

- Start the calculation

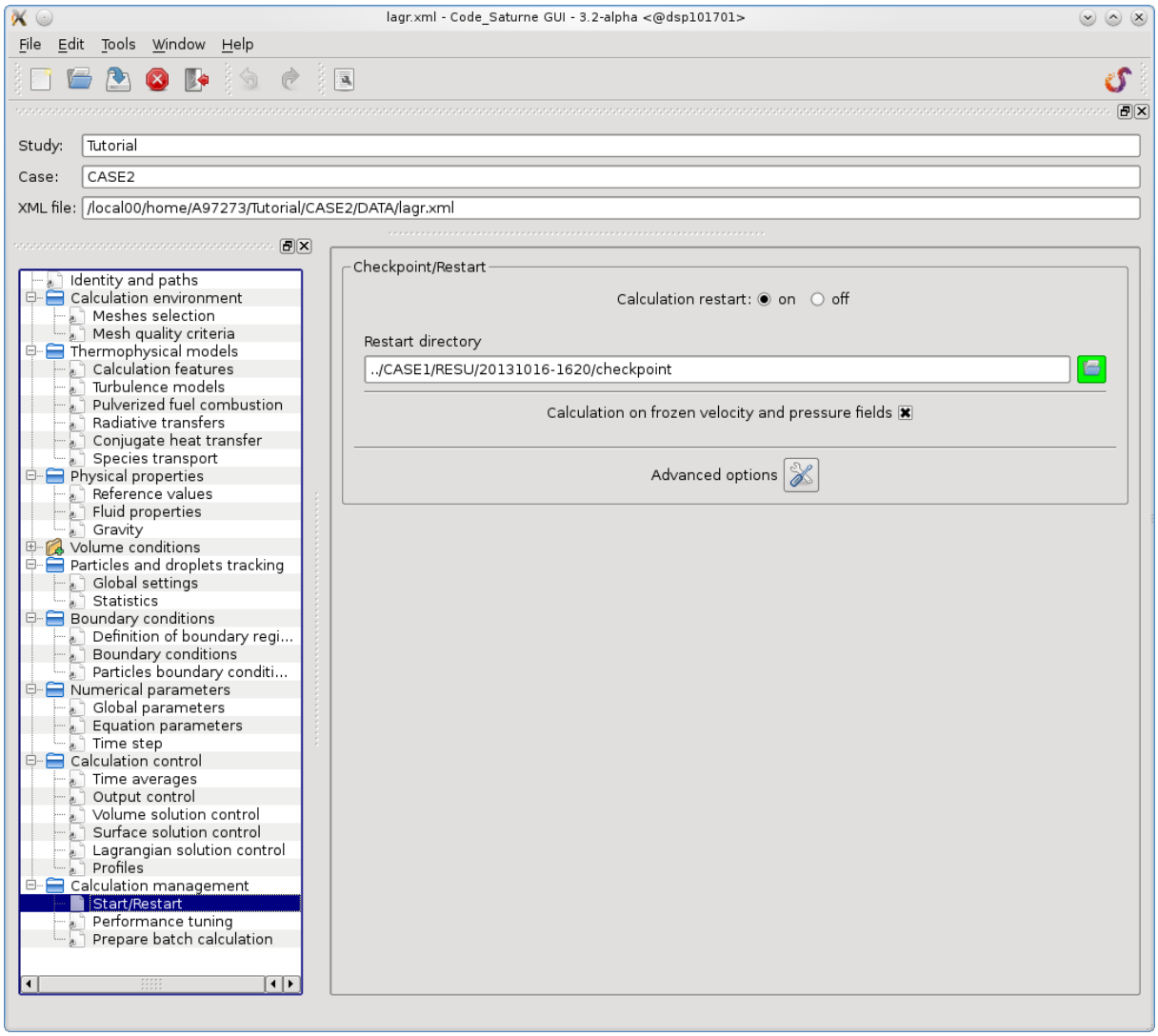

Figure 37: Step 9 – Calculation management; Start/Restart.

8. Other features

8.1. Output of trajectories

The aim of this paragraph is to introduce alternative settings to configure the output of particles trajectories.

Open the file Tuto_Lagr.xml saved at the end of the paragraph 7.2: **./SaturneGUI Tuto_Lagr.xml**

8.1.1. Step 1 – Particles and droplets tracking:

- In the *Statistics* subsection, deactivate *Calculation of volume statistics*. Change from the *Volumes* rider to the *Boundaries* rider. Deactivate *Calculation of boundary statistics*.
- Save the case.

8.1.2. Step 2 – Boundary Conditions:

- In the *Particles boundary conditions* subsection, click on *BC_1* (AIRPRIM) in the list of *Lagrangian boundary conditions* and set *the Number of particles in class* to 25, *Frequency of injection* to 0. With these settings, 25 particles will be initially injected, then nothing. Do not change anything else.
- Save the case.

8.1.3. Step 3 – Numerical parameters

- In the *Time step* subsection, set the *Number of iterations* to 3500.
- Save the case.

8.1.4. Step 4 – Calculation control

- Change to the *Writer* rider in the *Output control* subsection. Click on *results* (first line appearing in the main window) and change the *Frequency* output from *Output every 'n' time steps* to *No periodic output*.
- Click on *trajectories* (third line appearing in the main window) and change the *Frequency* output from *No periodic output* to *Output every 'n' time steps.* Set the value to 1 and leave the *Output at the end of calculation* option activated.

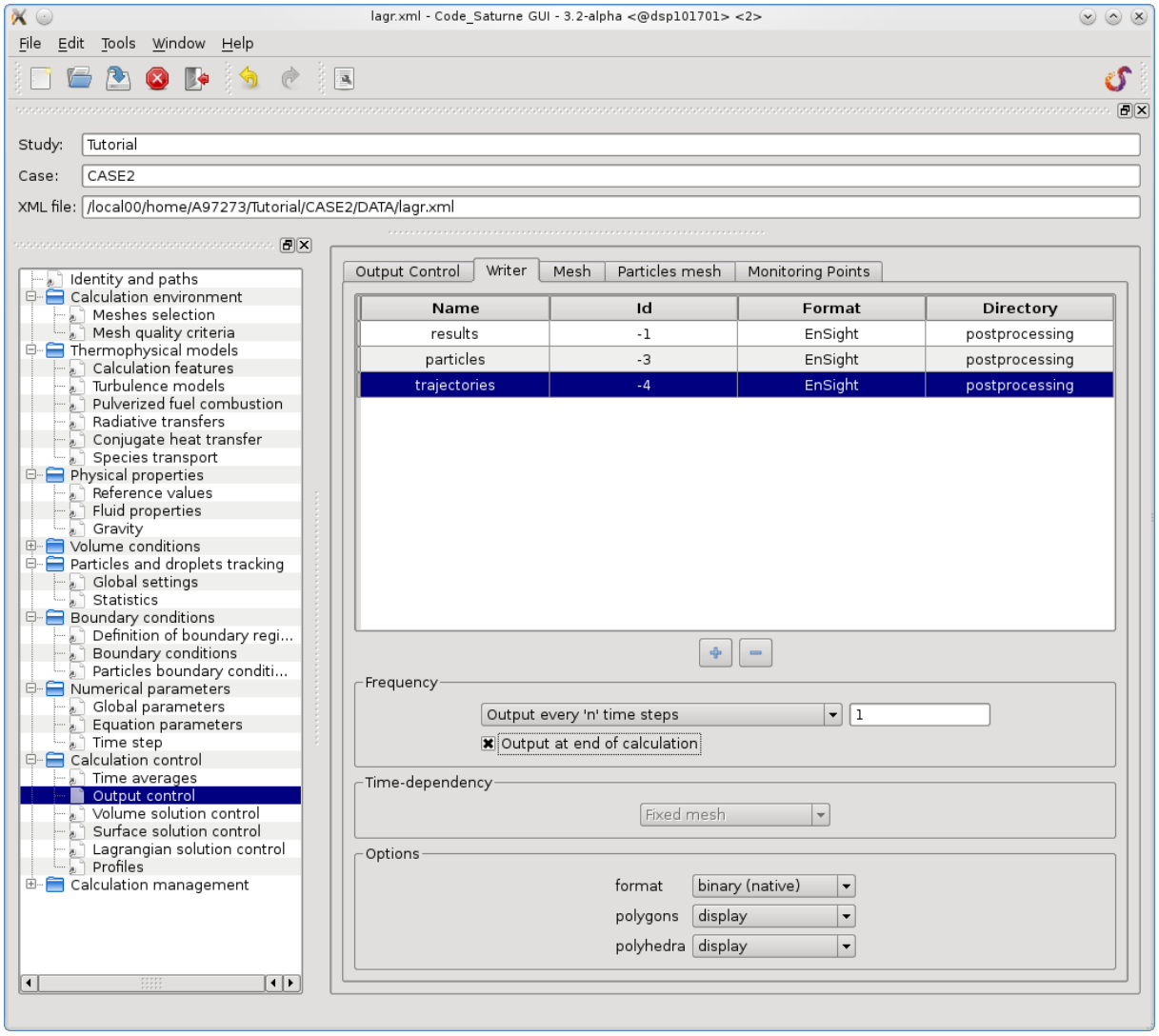

Figure 38: Step 4 – Calculation control; Output control; Writer.

- Change to the *Particles mesh* rider. Click on the "+" – button at the bottom of the page. A second line should appear in the table. Click on it and rename the mesh *Trajectories*. Click on the *trajectories* line. At the bottom of the page, in the *Associated writers* menu, click on the "+" – button. A line with *particles* should appear. Double-click on it and choose *trajectories.*

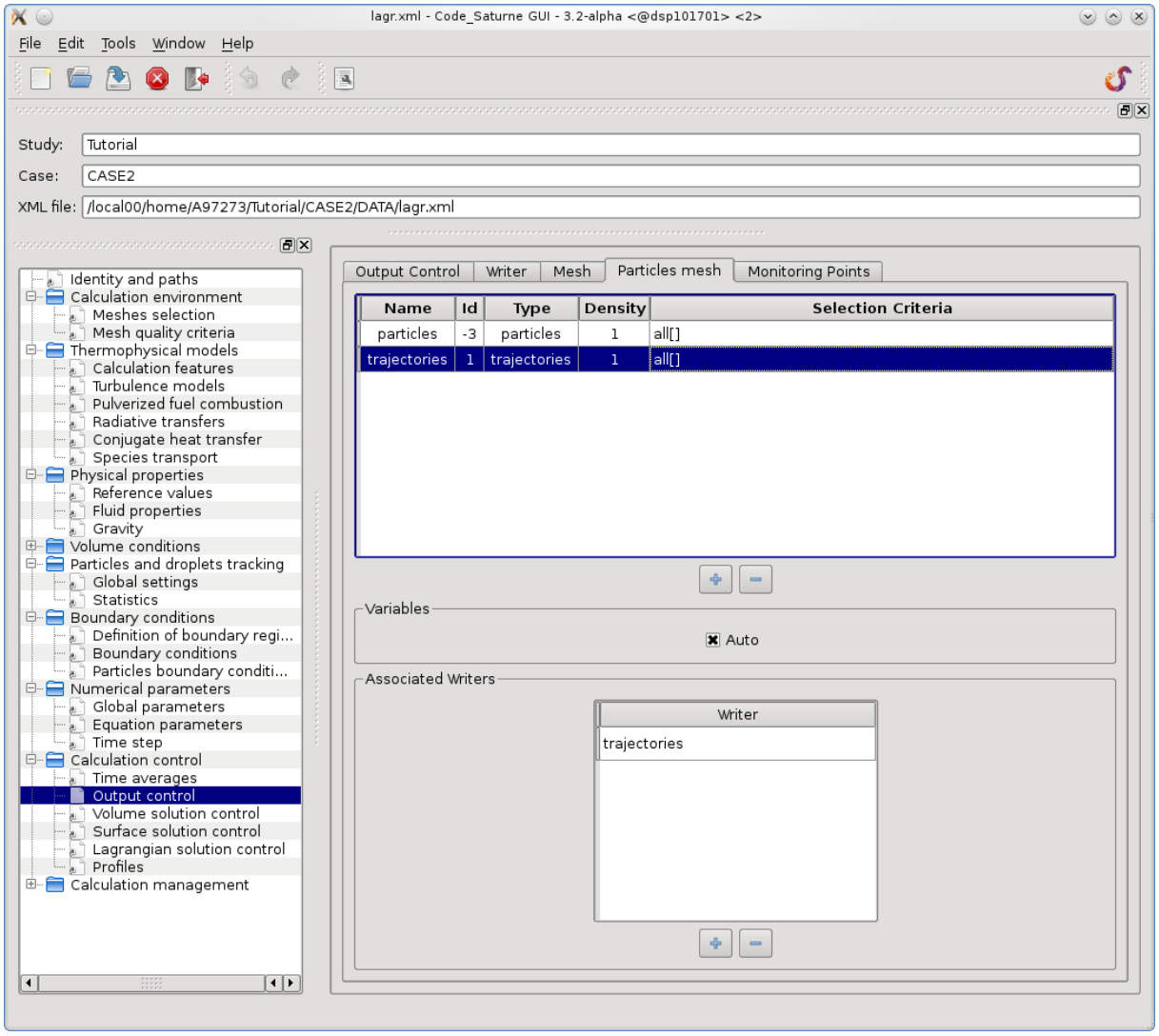

Figure 39: Step 4 – Calculation control; Output control; Particles mesh.

- Change to the *Lagrangian solution control* subsection. Select the variables you wish to output.

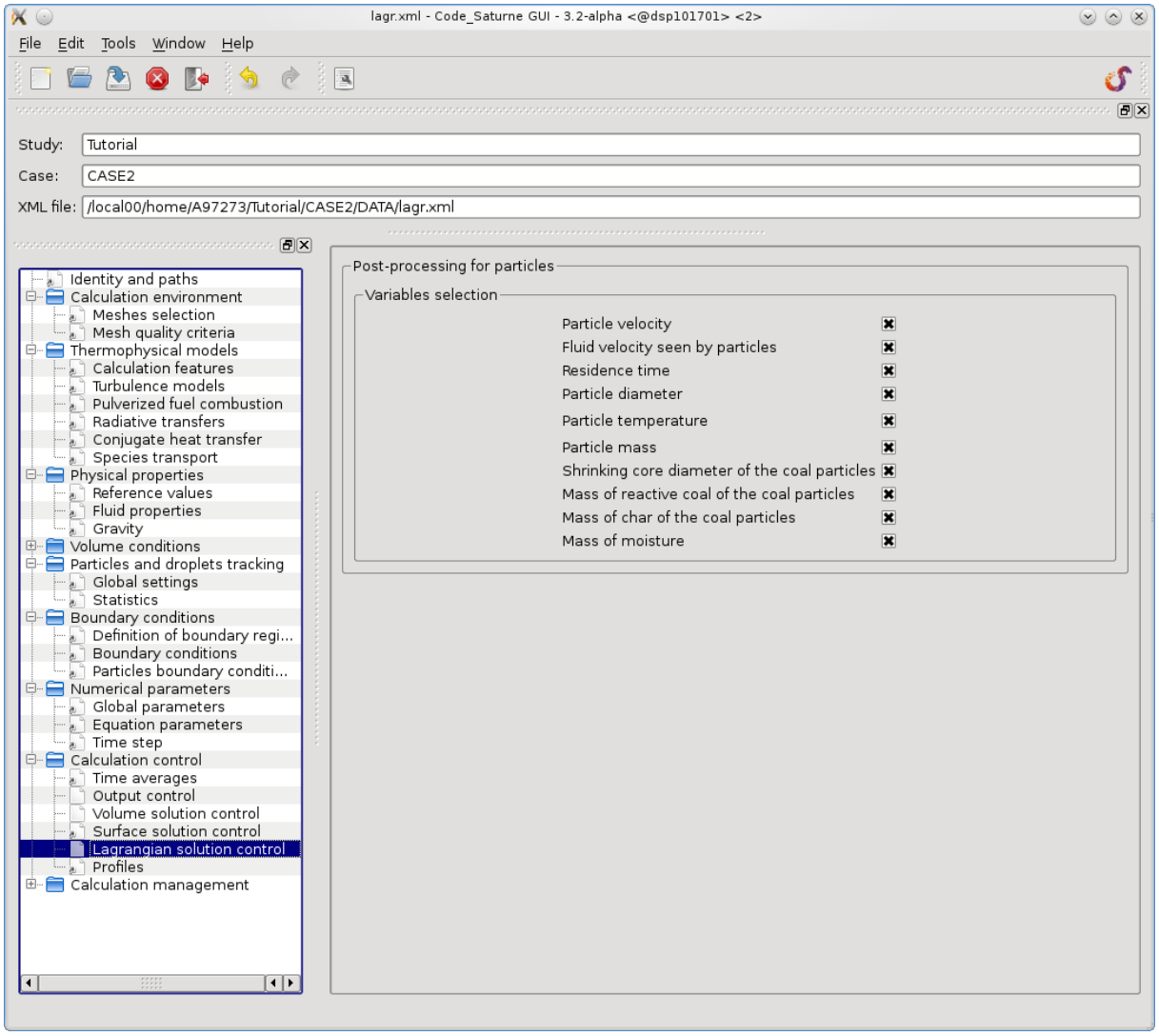

Figure 40: Step 4 – Calculation control; Langrangian solution control.

- Save the case.

8.1.5. Step 5 – Calculation management

- Go to the *Prepare batch calculation* subsection.
- Save the case.
- Start the calculation

8.2. Output of movies

The aim of this paragraph is to introduce alternative settings to configure the output of a movie.

Open the file Tuto_Lagr.xml saved at the end of the paragraph 7.2: **./SaturneGUI Tuto_Lagr.xml**

8.2.1. Step 1 – Particles and droplets tracking:

- In the *Statistics* subsection, deactivate *Calculation of volume statistics*. Change from the *Volumes* rider to the *Boundaries* rider. Deactivate *Calculation of boundary statistics*.
- Save the case.

8.2.2. Step 2 – Boundary Conditions:

- In the *Particles boundary conditions* subsection, click on *BC_1* (AIRPRIM) in the list of *Lagrangian boundary conditions* and set *the Number of particles in class* at 1000, *Frequency of injection* at 0. With these settings, 1000 particles will be initially injected then nothing. Do not change anything else.
- Save the case.

8.2.3. Step 3 – Numerical parameters

- In the *Time step* subsection, set the *Number of iterations* to 3500.
- Save the case.

8.2.4. Step 4 – Calculation control

- Change to the *Writer* rider in the *Output control* subsection. Click on *results* (first line appearing in the main window) and change the *Frequency* output from *Output every 'n' time steps* to *No periodic output* and deactivate the *Output at the end of calculation* option.
- Click on *particles* (second line appearing in the main window) and change the *Frequency* output from *No periodic output* to *Output every 'n' time steps.* Set the value to 1 and leave the *Output at the end of calculation* option activated.

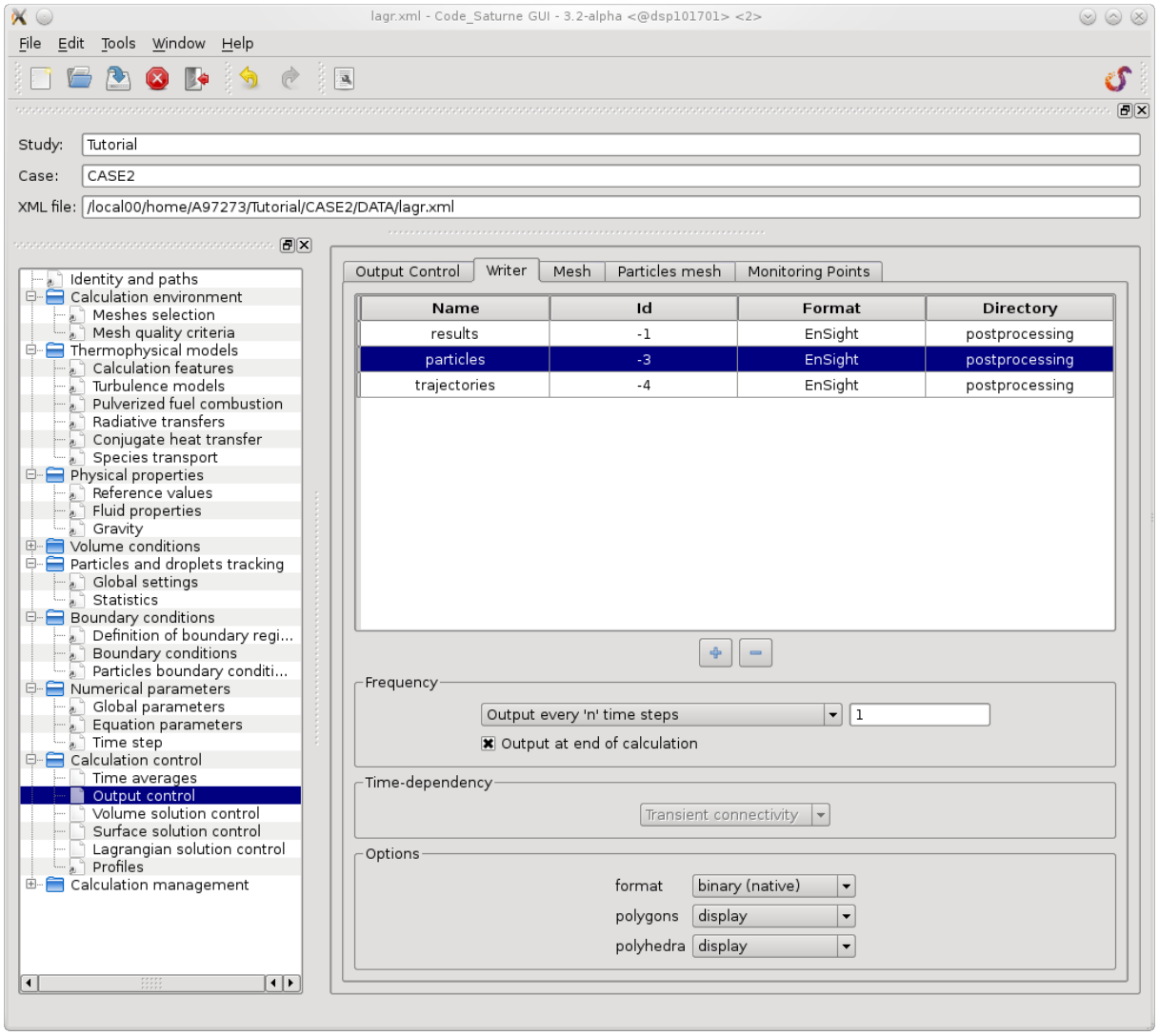

Figure 41: Step 8 – Calculation control; Output control; Writer.

- Change to the *Lagrangian solution control* subsection. Select the variables you wish to output.

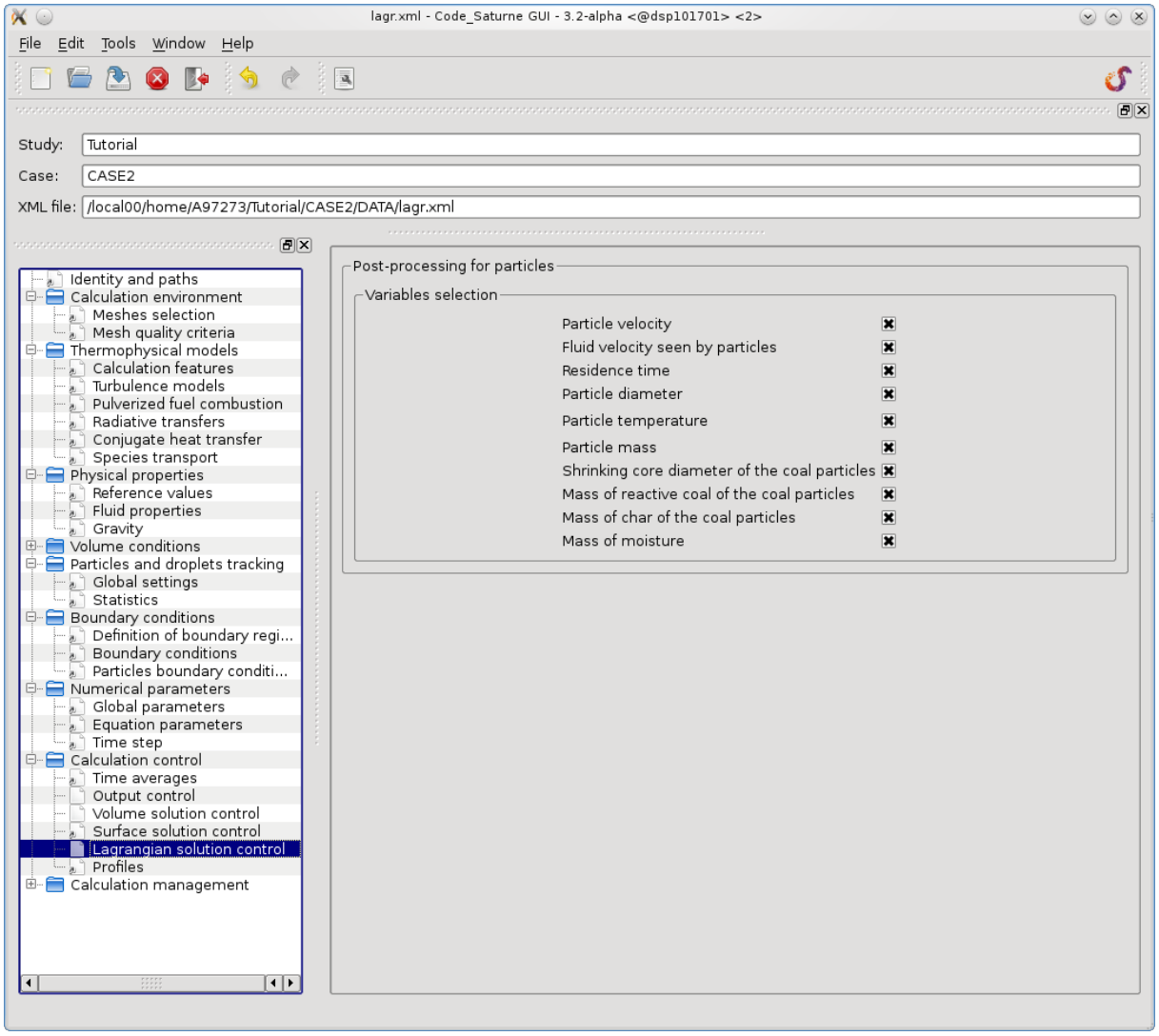

Figure 42: Step 4 – Calculation control; Langrangian solution control.

- Save the case.

8.2.5. Step 5 – Calculation management

- Go to the *Prepare batch calculation* subsection.
- Save the case.
- Start the calculation

8.3. Changing the number of layers (advanced user only)

A discretisation of the coal particles is proposed in *Code_Saturne*. This discretisation enables the computation of intra-particle thermal gradient and heterogeneous composition. By default, the number

of layers is set at 5. It is possible to change this parameter.

Go in the directory containing the source code of *Code_Saturne*. Change to src/lagr. Open *cs_lagr_tracking.h* and change the value of *CS_LAGR_N_LAYER*. Open *lagpar.f90* and change *nlayer*. Make sure that the values of *CS_LAGR_N_LAYER* and *nlayer* are the same.

If this version has already been installed, go in the "build" directory. Clean the previous installation by using **make clean**. Then compile as usual: **make –j16 && make install**. Otherwise, compile as usual: **make –j16 && make install**.

Note: it is not enough to modify these two files in the SRC directory of the CASE. Indeed, Code_Saturne would not be fully re-compiled which could lead to some troubles (as the size of some structure is changed).

8.4. Changing the drag coefficient (advanced user only)

The particles of biomass seem to be more cylindrical than spherical. It could be useful to change the drag coefficient to take the change of geometrical properties into account.

- Edit the user-subroutine: *uslatp* in the file *cs_user_particle_tracking.f90*

- Make sure that no other operation is performed and add the following code:

```
!===============================================================================
! 1. Initializations
!===============================================================================

ip = numpt


!===============================================================================
! 2. Relaxation time with Haider and Levenspiel drag coefficient
!    (Drag coefficient and terminal velocity of spherical and nonspherical
particles,
!     Powder technology 58 (1989))
!===============================================================================

! Sphericity parameter
phi = 0.9

! Intermediate calculation
cte1 = exp(2.3288-6.4581*phi+2.4486*phi**2)
cte2 = 0.0964+0.5565*phi
cte3 = exp(4.9050-13.8944*phi+18.4222*phi**2-10.2599*phi**3)
cte4 = exp(1.4681+12.2584*phi-20.7322*phi**2+15.8855*phi**3)

! Drag coefficient (Haider and Levenspiel)
cd = 24.0/rep*(1+cte1*rep**cte2)+cte3*rep/(cte4+rep)

! Intermediate calculation 2
fdr = 3.0*cd*uvwr/(4.0*ettp(ip,jdp))

! Caracteristic time
taup = romp / romf / fdr
```

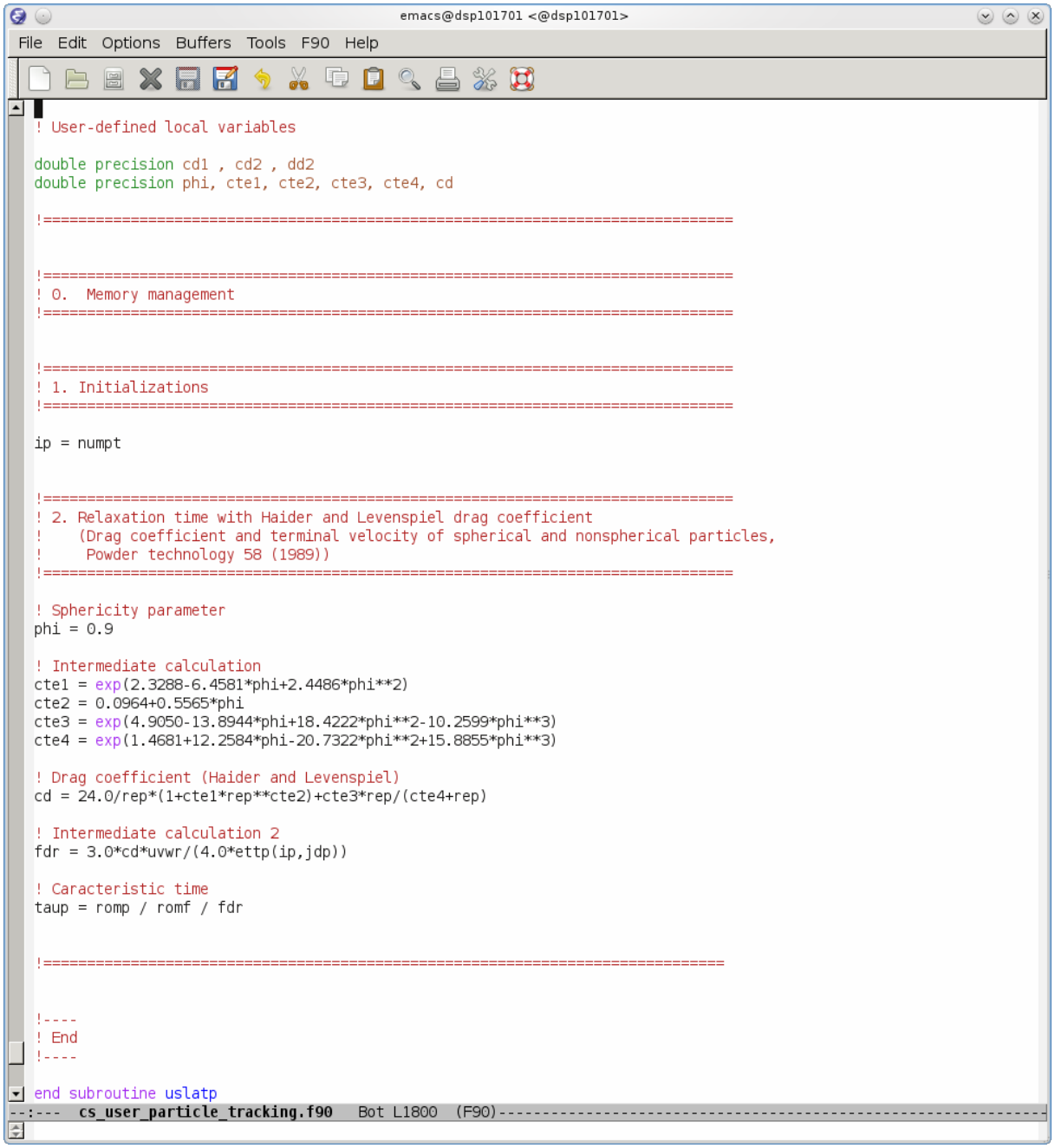

Figure 43: Edition of the subroutine *uslatp* in *cs_user_particle_tracking*.f90.

8.5. Suppressing the particles that are stucked in the corner (advanced user only)

The biomass particles are circulating in the furnace and have a high probability to be stucked in the corner near the entrance of the furnace. As they are not leaving this area, a lot of particles will be concentrated close to the corner and the computer is losing a lot of CPU time to update their trajectories although they are not very interesting to get statistical results. It could be useful to check the presence of “old” particle in the corner and to suppress them. The code proposed bellow suppress the particle on a test depending on the position of a particle (close enough to the corner) and his

residence time (more than 5s corresponding to twice the average age of the particles leaving the furnace).

- Edit the user-subroutine: *uslast* in the file *cs_user_particle_tracking.f90*

- Make sure that no other operation is performed and add the following code:

```
!===============================================================================
! 1. Suppress particles stucked in the corner
!===============================================================================

! Loop on the particles
do npt = 1,nbpart

  ! Position criteria
  if (ettp(npt,jxp)                              .lt. 8.7d-1  .and. &
      (sqrt(ettp(npt,jyp)**2+ettp(npt,jzp)**2)) .gt. 6.5d-1) then

    ! Residence time criteria
    if (tepa(npt,jrtsp) .gt. 5.d0) then

      ! Suppression of the particle
      itepa(npt,jisor)=0

    endif

  endif

enddo
```

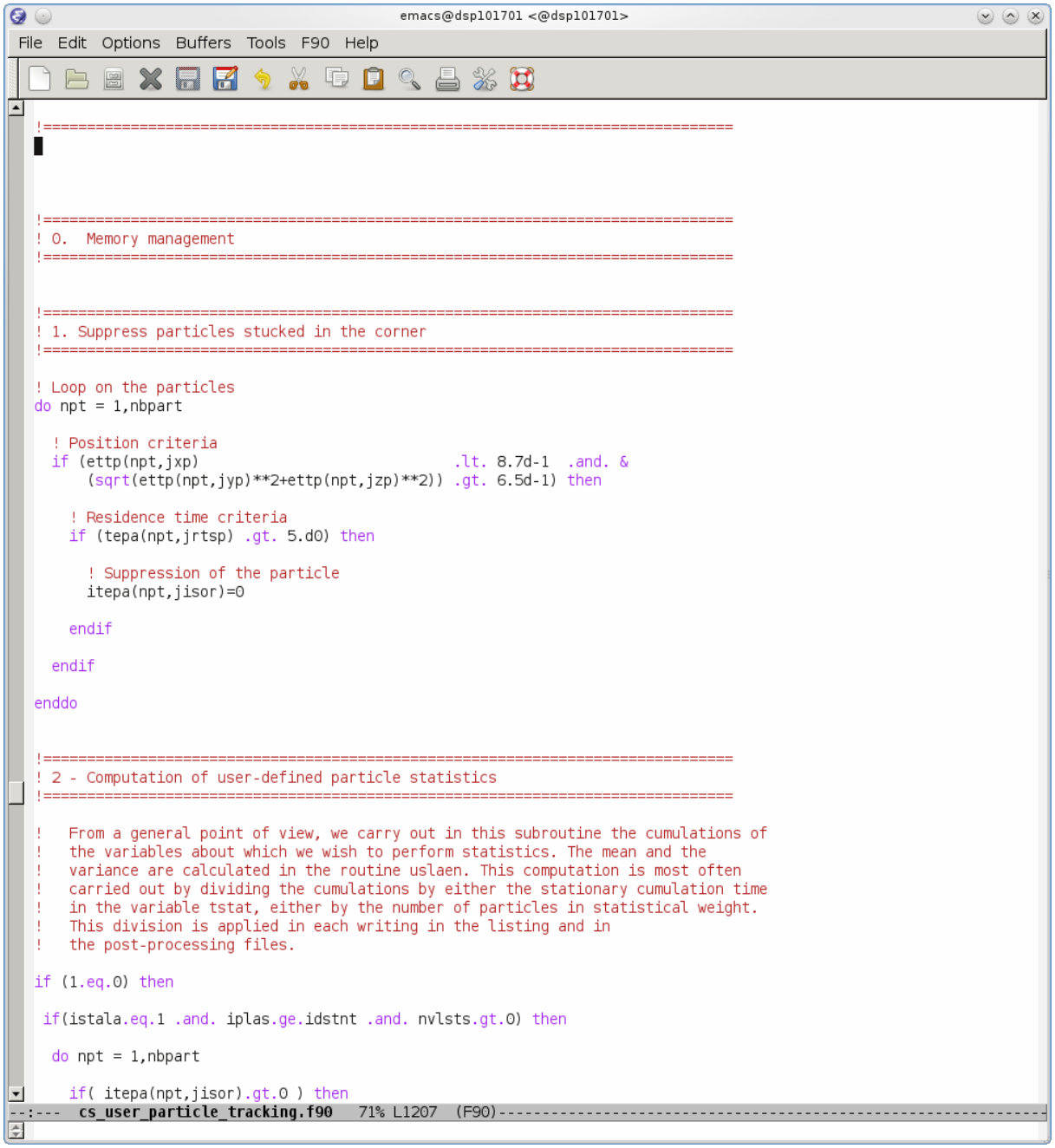

Figure 44: Edition of the subroutine *uslast* in *cs_user_particle_tracking.f90*.

8.6. Using time average to enhance data quality (advanced user only)

To enhance the quality of the results, time average for some Eulerian variables could be computed and used as the Frozen Field for the Lagrangian computation. The variables that should be averaged are:

- Gas temperature (*Temp_GAZ*)

- Velocities (*VelocityX*, *VelocityY*, *VelocityZ*)
- Turbulent kinetic energy and dissipation (*TurbEner*, *Dissip*)
- 0_2 and H_20 concentrations (*YM_O2*, *YM_H2O*)
- Radiative luminance (*IntLuminance_4PI*)

There is no easy solution to reuse a time-average on *Code_Saturne, t*hat's why this section should be reserved for advanced users of *Code_Saturne*. The aim of this section is to explain how to compute a time average and how to overwrite a temporal average on top of an instantaneous variable.

8.6.1. Computing a time-average

- Set up the scenario as usual (see section 6.2).
- We will define the time average in the section *Calculation control* and the subsection *Time averages* (this example is written for the temperature of the gaz: *Temp_GAZ*):
    - Write the name of the variable (for exemple Average_Temp_GAZ) in the *Label of time average*
    - Set up the *Start iteration number for time average calculation* at 3001
    - Click on the variable in the table at the bottom left of the page (e.g. *Temp_Gaz*) and click on the arrow to right to copy the variable in the table at the bottom right of the page

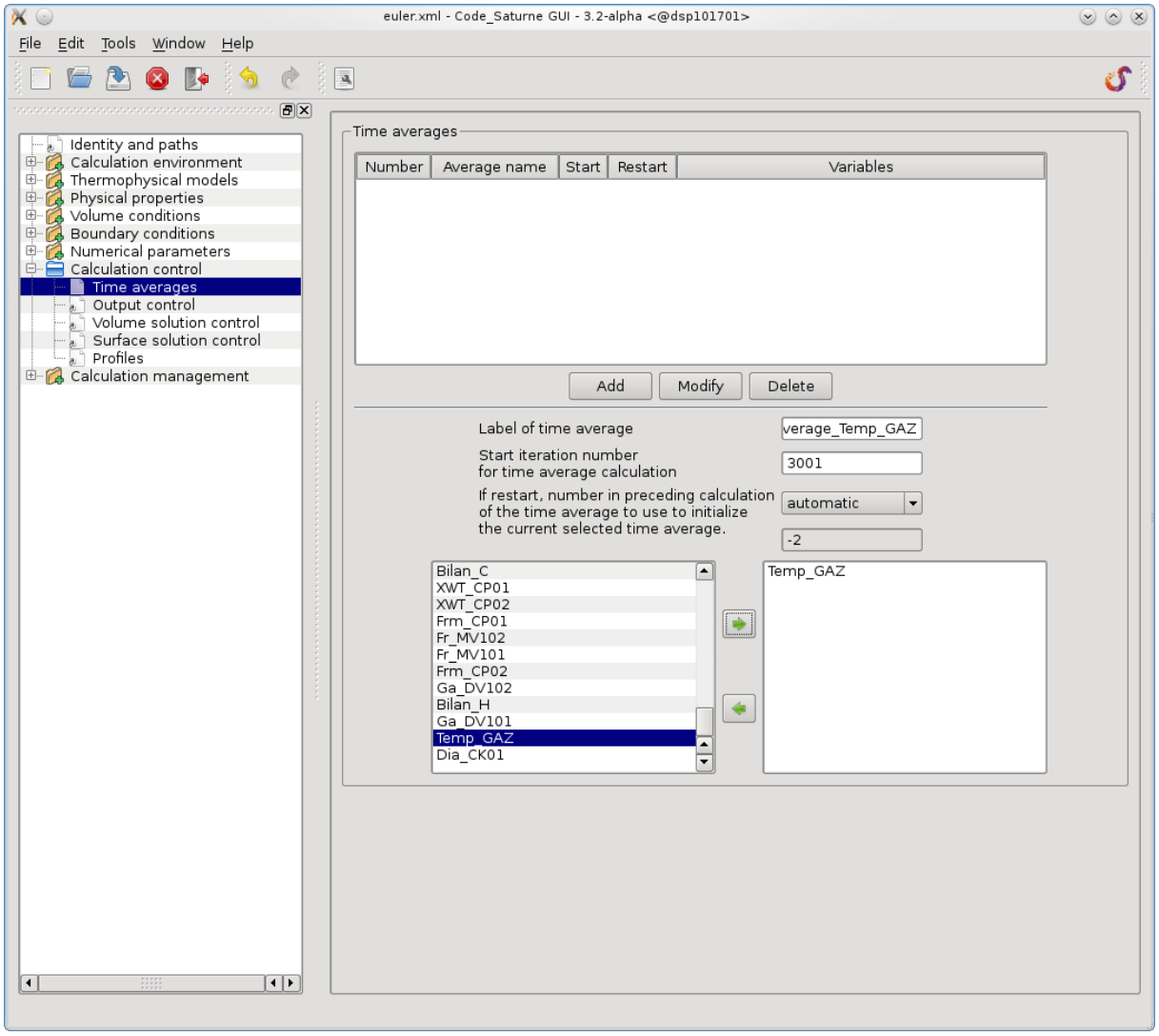

Figure 45: Calculation control; Time average.

- Click on Add button. The average should appear in the *Time averages* table at the top of the page.

- Repeat this operation for all the variables you would like to compute.

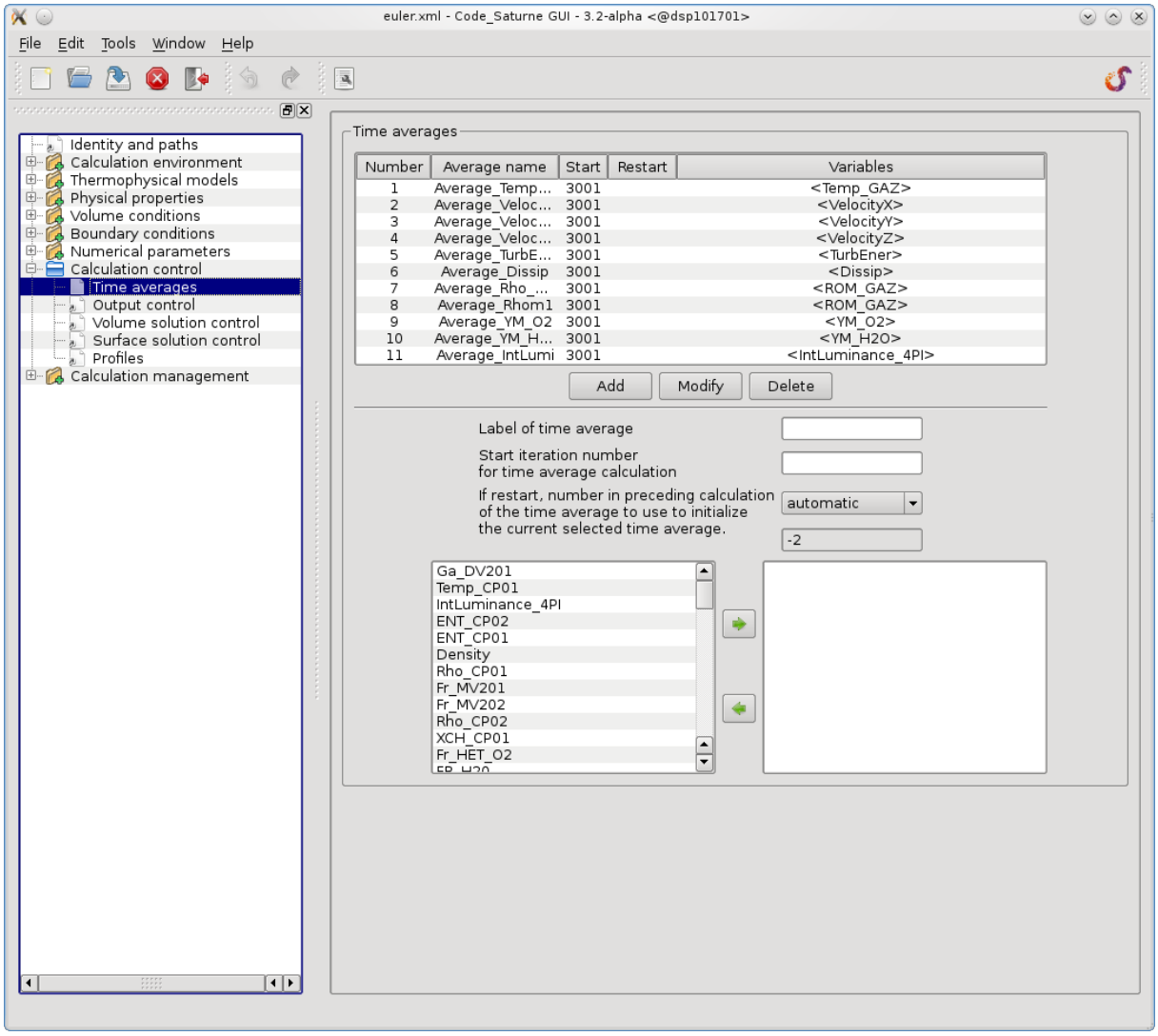

Figure 46: Calculation control; Time average.

- Save the case.

- Change to the *Numerical parameters* section. In the Pseudo-*Time step* subsection, increase the *Number of iterations*. Choosing 4000 iterations is recommended (3000 iterations to converge plus 1000 iterations to compute a steady time average).

- **Note:** as of today, it is not possible to set up the computation of time averages for some variables (*YM_O2*, *YM_H2O* or *IntLuminance_4PI*) with the GUI. I recommend to configure these variables manually in addition to the graphical initialisation presented before:

    - Run the case a first time and print the values of *ilumin*.

    - Edit the user-subroutine: *usipsu* in the file *cs_user_parameter.f90* by initialising the value *idfmom(1,7)*, *idfmom(1,8)* and *idfmom(1,9)* as on Figure 47.

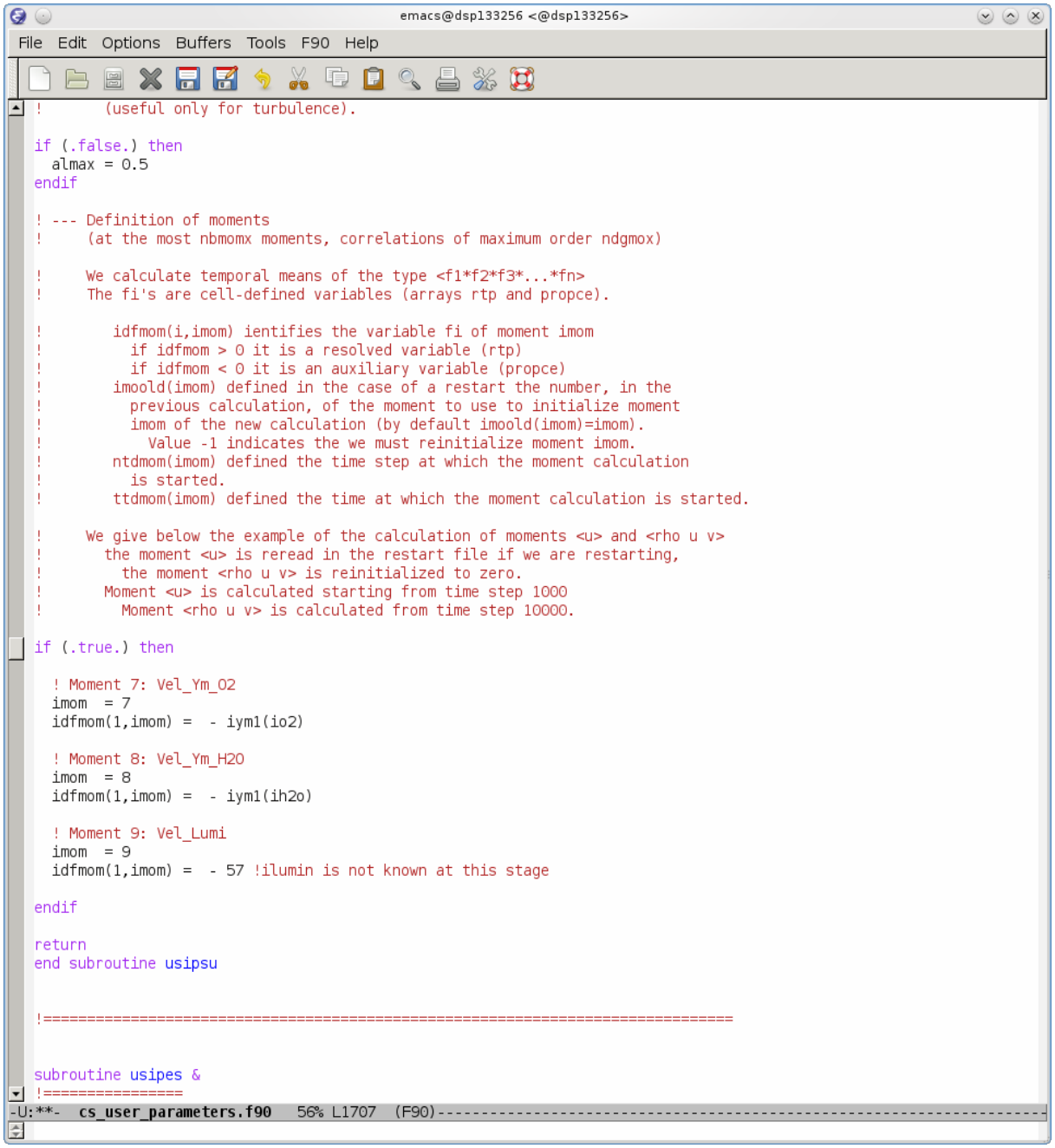

Figure 47: Edition of the subroutine *usipsu* in *cs_user_parameters.f90*.

- To avoid a security stop, modify the file *varpos.f90* and comment the instruction *iok = iok + 1* just between the test *idfmji.lt.-nprmax* and *write(nfecra,8210) ...*

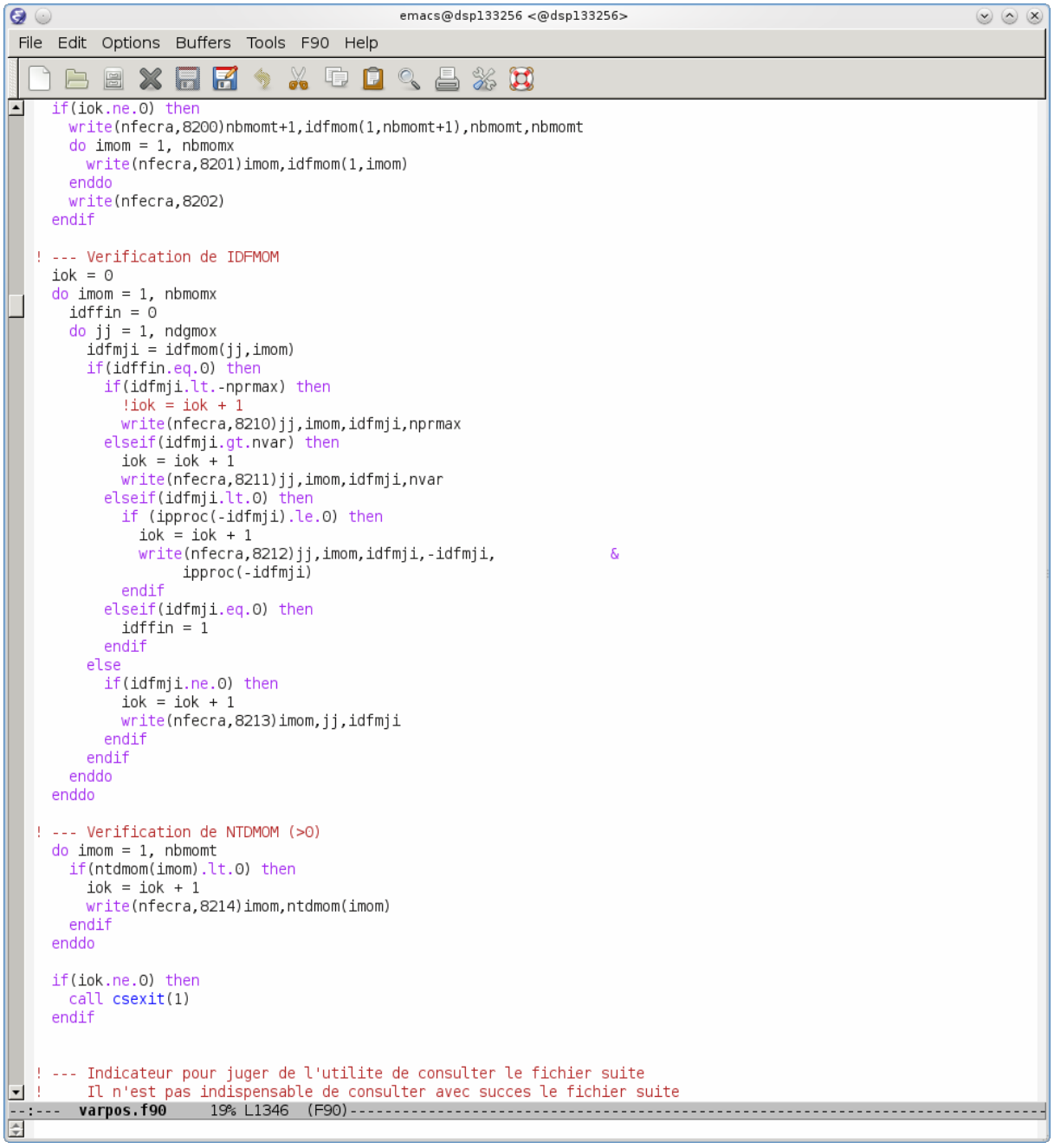

Figure 48: Edition of the subroutine *varpos* in *varpos.f90*.

8.6.2. Reuse a time-average

At the end of the calculation, the values of the time-averaged fields above the instantaneous value.

- Edit the user-subroutine: *cs_user_extra_operation* in the file *cs_user_extra_operation.f90*
- The code to add is the following:

```
!===============================================================================
! Write the value of moments above the instantaneous values (last iterations)
!===============================================================================
if (nbmomt.gt.0 .and. ntcabs.eq.ntmabs) then
  do imom = 1, nbmomt

    ! Position in 'propce' of the array of temporal accumulation for moments,
    ! propce(iel,ipcmom)

    ipcmom = ipproc(icmome(imom))

    ! if idfmom(1,imom) > 0 : value in rtp
    !    idfmom(1,imom) < 0 : value in propce

    ! The temporal accumulation for moments must be divided by the accumulated
    ! time, which id an array of size ncel or a single real number:
    ! - array of size ncel if idtmom(imom) > 0 : propce(iel, idtcm)
    ! - or simple real     if idtmom(imom) < 0 : dtcmom(idtcm)

    if (idtmom(imom).gt.0) then
      idtcm = ipproc(icdtmo(idtmom(imom)))
      if (idfmom(1,imom).gt.0) then
        do iel = 1, ncel
          rtp(iel,idfmom(1,imom)) = &
            propce(iel, ipcmom)/max(propce(iel, idtcm), epzero)
        enddo
      elseif (idfmom(1,imom).lt.0) then
        do iel = 1, ncel
          propce(iel,ipproc(-idfmom(1,imom))) = &
            propce(iel, ipcmom)/max(propce(iel, idtcm), epzero)
        enddo
      endif

    elseif (idtmom(imom).lt.0) then
      idtcm = -idtmom(imom)
      if (idfmom(1,imom).gt.0) then
        do iel = 1, ncel
          rtp(iel,idfmom(1,imom)) = &
            propce(iel, ipcmom)/max(dtcmom(idtcm), epzero)
        enddo
      elseif (idfmom(1,imom).lt.0) then
        do iel = 1, ncel
          propce(iel,ipproc(-idfmom(1,imom))) = &
            propce(iel, ipcmom)/max(dtcmom(idtcm), epzero)
        enddo
      endif
    endif

  enddo
endif
```

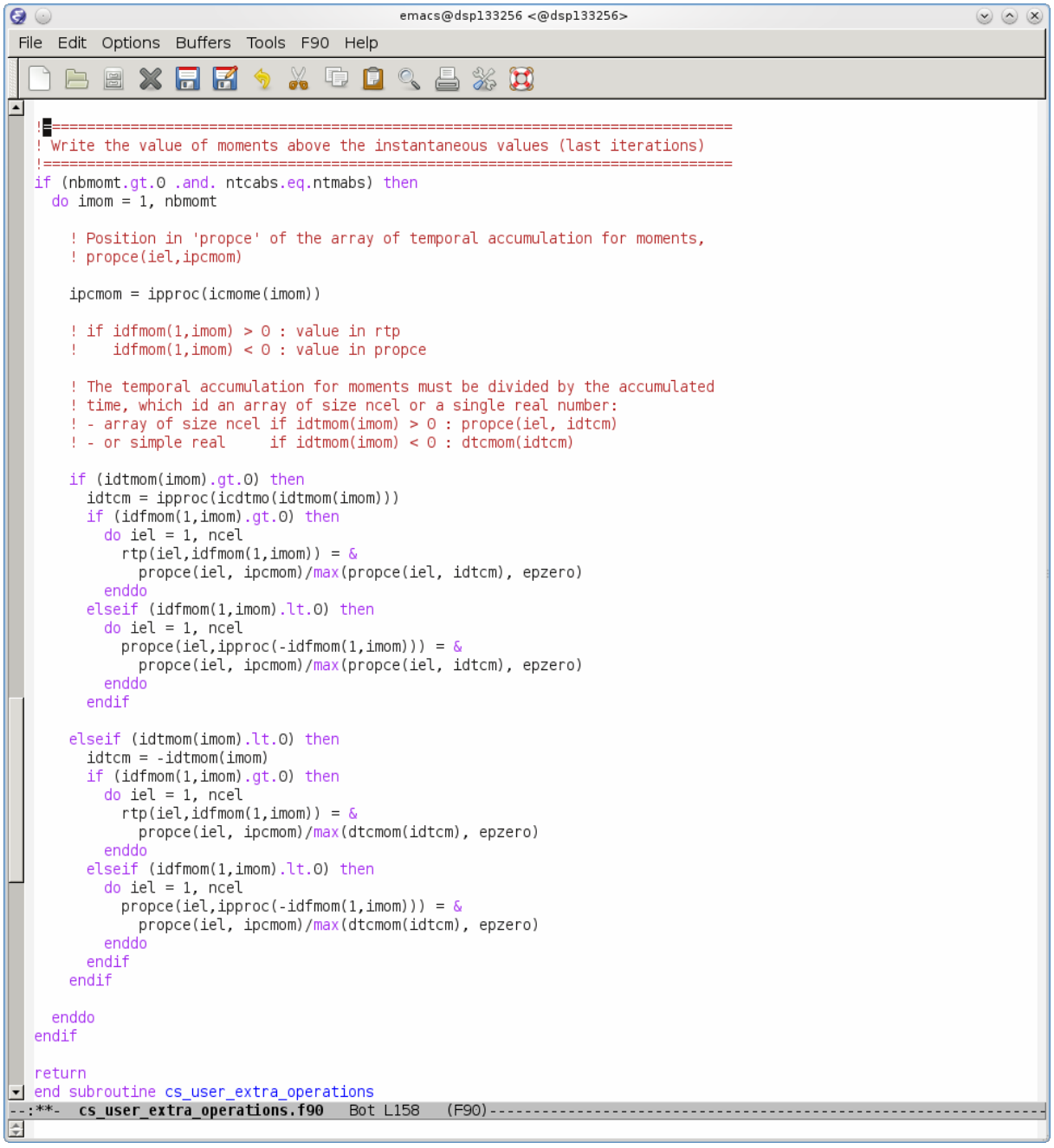

Figure 49: Edition of the subroutine *cs_user_extra_operations* in *cs_user_extra_operations.f90*.