Work with mathematical tools for prediction of fire risks

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Abstract

This work describes two major tasks. One is related to prediction of fire behavior of wall and ceiling linings in room tests by means of small scale data in which a model developed by SP was used. The model was validated against new experimental data from SwRI (South West Research Institute, Texas, USA). Another one, the most extended, was related to spontaneous ignition of biofuels. According to a survey of the risk for spontaneous ignition in various biofuel storages done in Sweden, the largest risk for spontaneous ignition would be in storages of moist bio-fuel. It has, however, been seen that wood pellet, which are a comparatively dry product, also is capable of spontaneous heat generation. Several fires have occurred in large bulk stocks of wood pellets, e.g., large quantities of pellets stored in silos have caught fire by spontaneous ignition. SP has carried out several tests, both small-scale and large-scale tests, in order to see under what conditions spontaneous ignition occurs.

Simulation of these small scale tests using a mathematical code called SMAFS (Smoke Movement And Flame Spread) allows us to see which factors are decisive for the spontaneous ignition of the wood pellets. It is more convenient to see what is favourable to a self-ignition in bio-fuels by doing numerical simulations. Then numerical results can be compared with experimental measurements.

The work presented in this Technical Note was made by Marie Guillaume as part of her undergraduate education at ENSIAME Université de Valenciennes, France. Her supervisor at SP Fire Technology was Patrick Van Hees.

Key words: Room tests, wall and ceiling linings, numerical simulation, spontaneous ignition, biofuels, CFD code

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1 Introduction

The work presented in this Technical Note was made by Marie Guillaume as part of her undergraduate education at ENSIAME Université de Valenciennes, France. Her supervisor at SP Fire Technology was Patrick Van Hees.

ConeTools
I first worked with a software called ConeTools during more than one month. This software, developed by SP, calculates the heat release rate of the SBI and Room Corner models by means of data of the Cone Calorimeter test (see Chapter 2 and reference [1] for more information). It is useful for classifying the wall and ceiling lining materials depending on their fire safety level. The purpose of this work was to do comparisons between measurement and simulation for different projects. I also tested a new version of ConeTools (ConeTools 2.4), which is more complete (see Chapter 2), and I modified it when it was necessary.

Self ignition of bio fuels
My main work was to do simulations of spontaneous ignition of bio fuels (wood pellets). Bio fuels include a large group of fuels which all originates from biological materials. In Sweden these fuels are divided in groups: wood fuels, spent liquor, straw, waste and peat.

Spontaneous ignition is a phenomenon which occurs in a material without external heat supply. Heat can be generated (through a chemical or biological process), and when it can't be dissipated into the surrounding environment, temperature rises; it eventually result in a self-ignition. The dominant source of heat is the hydrocarbon oxidation governed by the rates of diffusion and convection of air from outside, and there can also be significant influence of heat of wetting from adsorption of the inherent moisture. Various exothermic processes such as low temperature oxidation, microbial metabolism, the adsorption-desorption of water due to the difference between real and equilibrium moisture concentration in a storage and air can contribute to self-heating of materials in storage. Mainly various funguses cause microbial degradation of the fuels; microorganisms cause a temperature increase in storage piles. These funguses prefer different components of the wood, like cellulose or lignin. The main factors influencing the temperature in the stack are: moisture content, the size of the pile and density.

The self ignition of fuel storages can cause a big economic loss, and that is why it would be desirable to find out under which conditions this phenomenon can occur and how to avoid it. SP has carried out very interesting trials in order to investigate under what conditions wood pellets and other bio fuels can spontaneously ignite. SP is working in conjunction with Lund Institute of Technology and Växjö University on research into self-ignition of stocks of wood fuels, in a project financed by the Swedish Energy Agency, the Swedish Rescue Services Agency and the Swedish Fire Research Board.

I worked with a software called SMAFS (Smoke Movement And Flame Spread). It is a fully parallelized CFD code for numerical simulation of reacting flows such as building fires, spontaneous ignition in porous fuel storage (see Chapter 3).

2 Prediction of the SBI and Room Corner tests using ConeTools

2.1 Test methods

2.1.1 Cone calorimeter test

The test method describes a test specimen with an area of 100mm x 100mm, which is exposed to a constant radiant heat flux. The heat flux can be adjusted from 10 kW/m^2 to 100 kW/m^2. A spark plug positioned over the test specimen ignites any flammable gasses produced by the test specimen. A hood collects the effluents from the test. The effluents are then analyzed in the duct by a thermocouple, a pressure sensor, smoke measurement system and a sample probe (see Figure 1 and Figure 2). The mass loss is recorded during the test.

The test results are heat release rate, time to ignition, smoke production and weight loss.
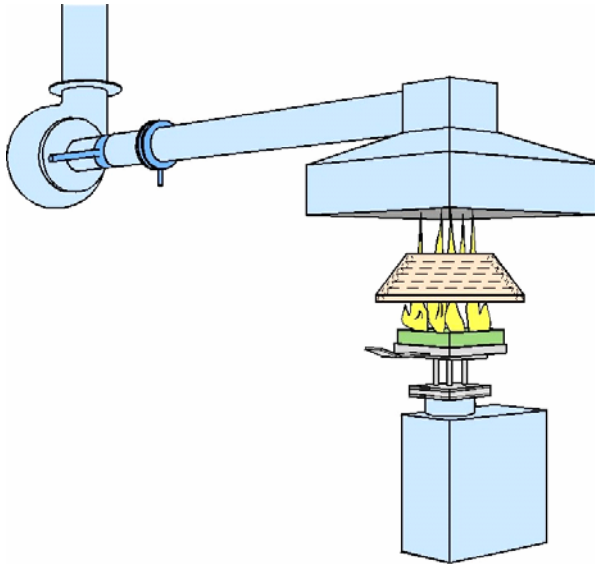
Figure 1. Cone Calorimeter test.

Figure 2. Picture of Cone Calorimeter test.

2.1.2   SBI test

The SBI (Single Burning Item) test simulates a single burning item (e.g. a waste paper basket) burning in a corner of a room and affecting a wall lining. The dimensions of the test specimen are 1.0m x 1.5m and 0.5m x 1.5m. The burner is a diffusion burner supplied with propane. It is located in the corner, and the specimen is behind it. The output of the burner is 30 kW for 21 minutes. The effluents from the fire are collected in the hood and transported through the duct, where you can find a thermocouple, a pressure sensor, a smoke measurement system and a sample probe (see Figure 3 and Figure Figure 4).

The test results are heat release rate, lateral frame spread on the large wing of the specimen, smoke production and burning droplets.
From these data, FIGRA (FIre GRowth RAte) and SMOGRA (SMoke GRowth RAte) can be calculated :

FIGRA = maximum value of 30 second averaged heat release rate / time
SMOGRA = maximum value of 60 second averaged smoke production rate / time

From this test, the major classification of building products in the European classification system can be determined. Building products are classified depending on their reaction to fire. These classes are A1, A2, B, C, D, E and F. A1 and A2 represent different degrees of limited combustibility. C to E represent products that may go to flashover in a room and at certain times, see next chapter. B means no flashover in a room corner test, and F means that no performance is determined. The tables with the classification system for wall and ceiling linings and floor coverings are given in Annex A and B. The work described here is limited to wall and ceiling linings.
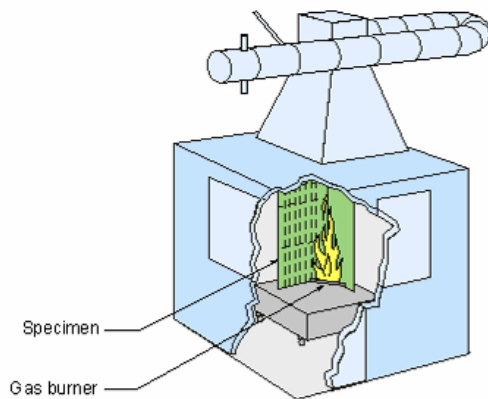
Figure 3. SBI test.Figure   **Figure 4. Picture of the SBI test.**

2.1.3   Room corner test

The dimension of the test room are 3.6m x 2.4m x 2.4m (length x width x height). The three inner walls and the ceiling are covered. The door is open, so smoke gases are vented and air is let in through it. These smoke gases are collected in a hood. The ignition source is a gas burner, and it is located in one of the corner of the room (see Figure 5 and Figure 6). Heat release rate and smoke production rate are measured continuously.
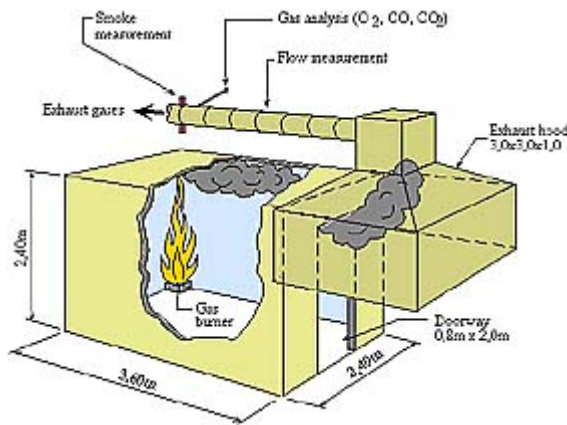
Figure 5. Room Corner test.

Figure 6. Picture of the Room Corner test.

2.2 How to use ConeTools

2.2.1 ConeTools 2.3

2.2.1.1 Principle

The software package is based on a Visual Basic program written for use under the Windows environment. It was developed in 2002. The user can simulate the results of the SBI test and the Room corner test by means of Cone Calorimeter tests: the heat release rate (HRR), the total heat rate (THR), the fire growth rate (FIGRA), and the Euroclass. First the user has to select an input file, which contains the data of the Cone Calorimeter test. Then he must choose the type of the input file (see Figure 7), or he can define his own file type.
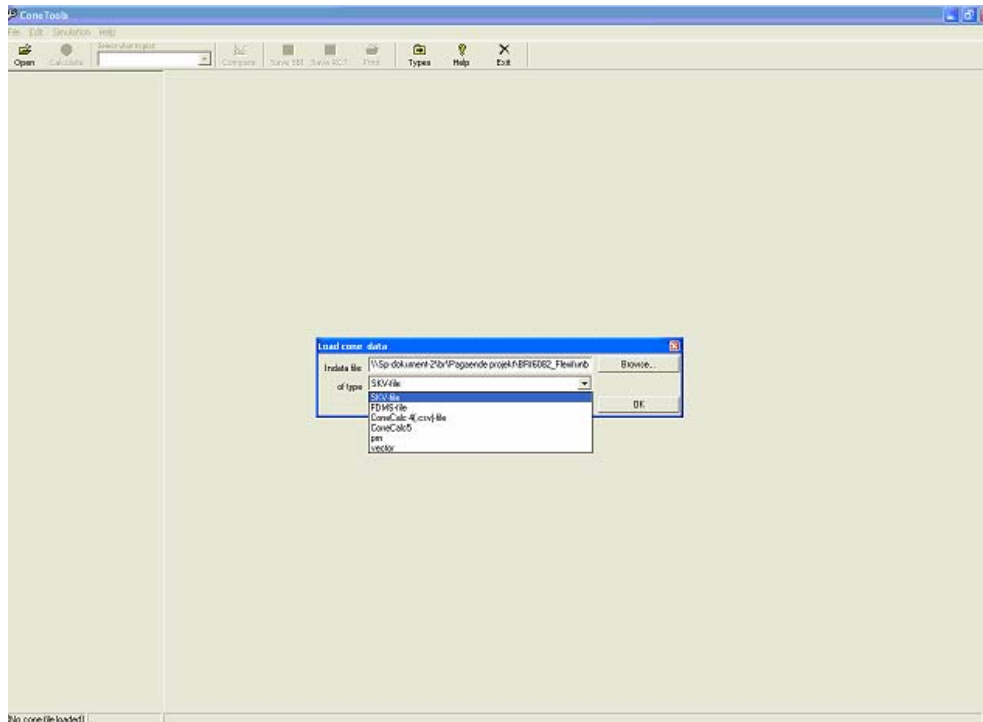
Figure 7. Open file dialog box.

From the moment a file is selected, the screen will show the HRR curve of the Cone Calorimeter test (see Figure 8).
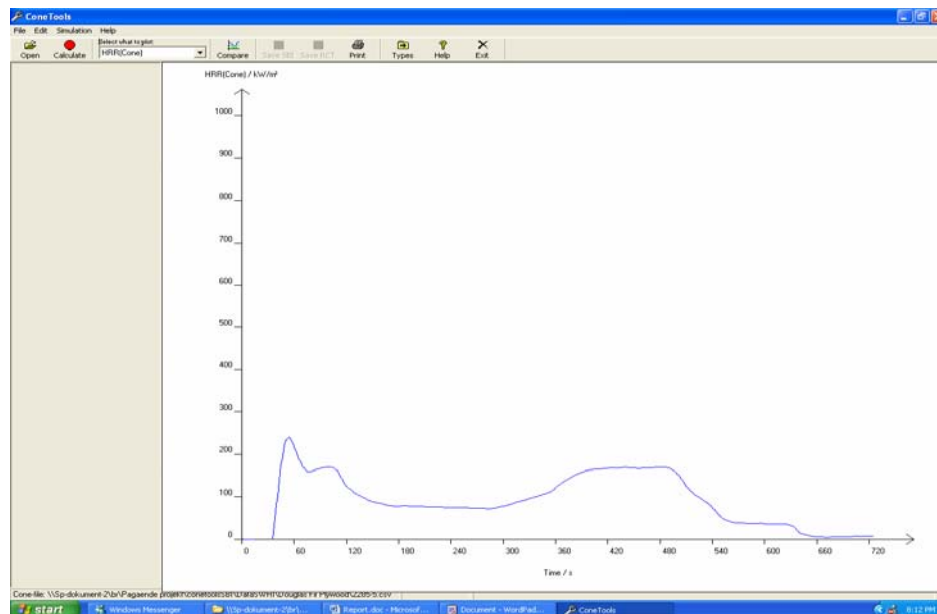
Figure 8. HRR curve of the Cone Calorimeter test.

In order to perform calculations, the user has to click on the Calculation button. Then he has to introduce the heat flux level in the Cone Calorimeter test, and a HRR threshold or a visual ignition time. Finally he can choose the simulate SBI or Room corner test results or both (see Figure 9).
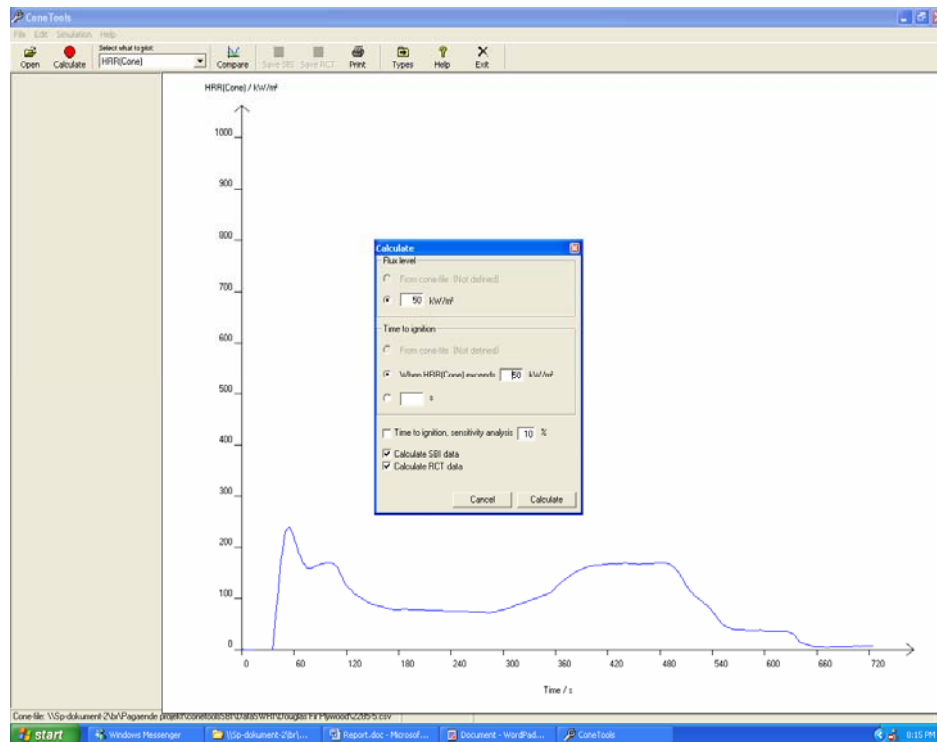
Figure 9. Calculate dialog box.

The results of the simulation and the different curves can be seen (see Figure 10).
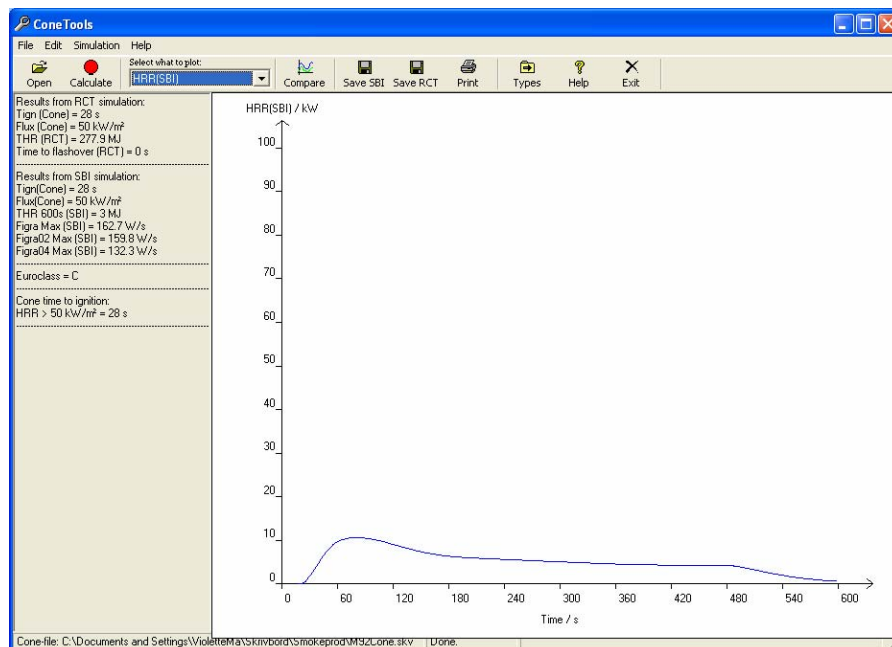
Figure 10. Results of the simulation.

With the compare button it is possible to compare two Cone Calorimeter data sets, but I never used this function.

The results from either a SBI or a RCT simulation can be saved as a vector data. The user can then print graphs and results of the simulation.

2.2.1.2   Simulations and comparisons

First I worked on the SwRI Project No.01.R9492 and No.01.11453. In January 2005 Southwest Research Institute (San Antonio, USA) initiated a research program to evaluate and improve mathematical models to predict the performance of construction products. Eight products were tested according to ISO 9705 (Room corner test), EN 13823 (Single Burning Item test) and ASTM E 1354 and ISO 5660 (Cone Calorimeter test).

The purpose of my work was to do the simulations of the SBI and Room corner tests from the Cone Calorimeter data for the eights products. Then I had to compare the results of these simulations with the tests results.

I did these calculations twice: once I took the ignition time from the Cone Calorimeter test, and once the ignition time was calculated from the HRR threshold (the user can choose it in the Calculation menu). I took the HRR threshold equal to 50 kW/m^2. I made tables in Excel who contains the FIGRA, the THR 600s, the flashover time and the Euroclass.

From these tables I did graphs, which compare the FIGRA, the THR 600s and the flashover time. Then it is easy to see the differences between the simulation and the experiment. I also wrote a little article in order to explain these curves and to analyze the results of this comparison (see Annex C, D and E). The best thing would be to obtain linear curves.

2.2.2   ConeTools 2.4

2.2.2.1   Differences with ConeTools 2.3

This new version contains a supplementary model for the heat release prediction based on the work of Anne Steen Hansen. This model is connected to a model for the smoke production. For this version the Calculate form has been modified.

The Hansen model requires, in addition of the ignition time and the heat release rate curve from the Cone Calorimeter test, the smoke production curve and the material density. This model predicts the heat release rate curve and the Euroclass inclusive the smoke class. Time to ignition here is defined as the time when the heat release rate of the Cone is more than 25 kW/m^2, and it must be include between 10 seconds and 30 seconds. These two values were chosen to give better results in the simulation according to Anne Steen Hansen.

The Smoke model was developed by the Norwegian laboratory. This model requires the smoke production rate curve. For the SBI test, it gives a range for the SMOGRA, and the smoke Euroclass (s1, s2 or s3). For the Room Corner test, it gives a range for the maximum smoke production rate, and the average smoke production rate. First the user has to select an input file, in the same way as ConeTools 2.3.

The user interface of the Calculate form has been changed (see Figure 11). New options are available. The user can choose with which model he wants to do the simulation: SP model or Hansen model (for the SBI simulation), Room Corner Test simulation, or smoke production model, but this calculation will depend on his first choice (SBI simulation or RCT simulation). For the Hansen model and the smoke production model, the user must give the density of the material.

Define your time to ignition

Define the density of material if it requires

Select smoke production

Choose the model for SBI

Start the simulation

Select RCT model
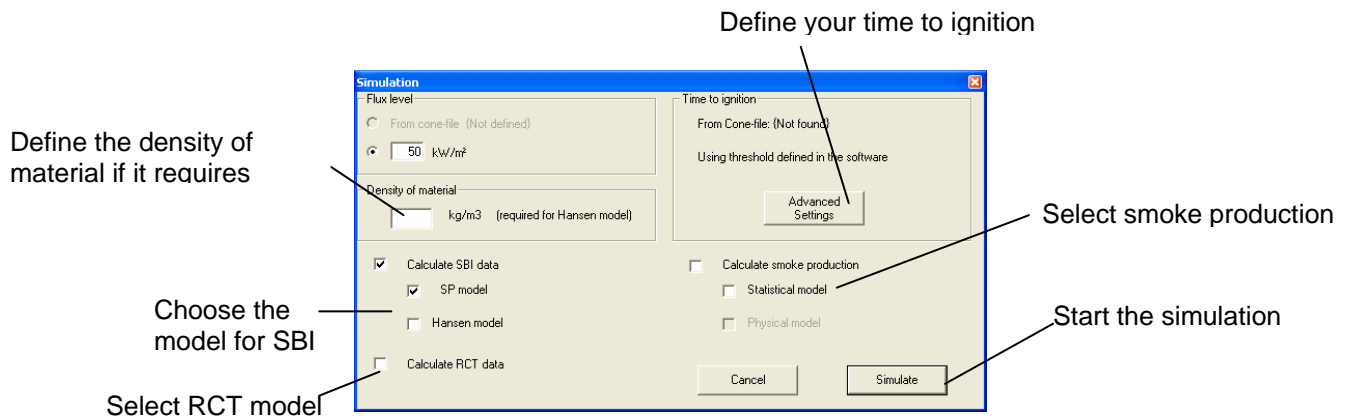
Figure 11. Interface of the Calculate form.

By clicking on "Advanced Settings", user can define different ignition time for each model (see Figure 12). For each model, it is possible to define the ignition time differently. For the three models, user can define a HRR threshold or the ignition time. For the SP model, ConeTools can recognize the ignition time in the Cone file. For the Hansen model, "by default" means that the ignition time is defined when the HRR of the Cone is higher than 25 kW/m^2. For the smoke production model, it means that the ignition time is defined when the HRR is higher than 50 kW/m^2.
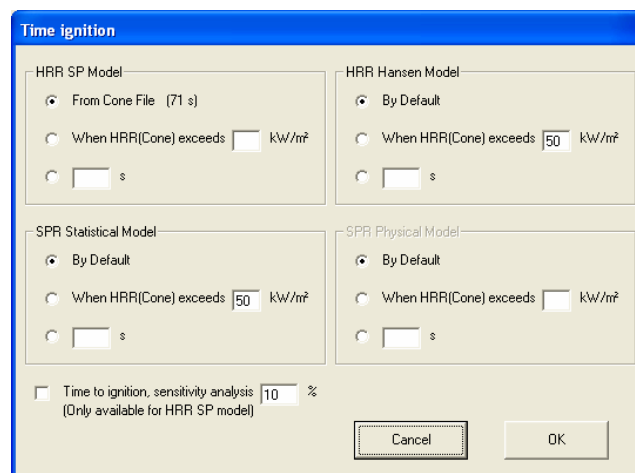
Figure 12. Interface of the ignition time.

After clicking on the "Simulate" button, results of the simulation can be seen on the screen (see Figure 13).
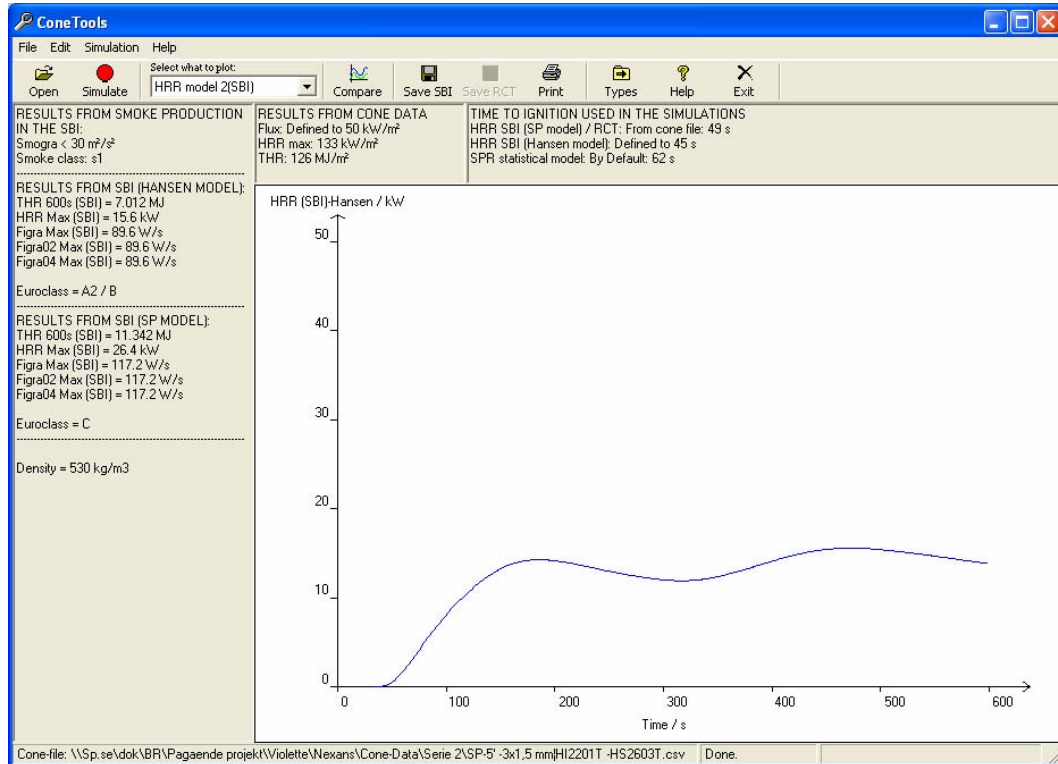
Figure 13. Interface after simulation.

But this new version was not completely finished, and it contained some errors.

2.2.2.2   Simulations, comparisons and modifications

With this new version of ConeTools, I worked on three projects. First I worked on the same project as before (SwRI Project No.01.R9492 and No.01.11453). Then I worked on two other projects, called EUREFIC project and SBI project.

With the data from the United States, I did comparisons between the results of the Hansen model and the tests results. I made tables and graphs in order to see if the Hansen model is good. But I had some problems: actually, this new version of ConeTools was not tested. I could not open certain files in ConeTools, and I didn't know why, because there was no error message. That's why I had to learn about Visual Basic, in order to find what the problem was and to correct it. For this, I used this link: http://goforit.unk.edu/vb6/default.htm.

I tried to learn the essential things, and then I looked in the code of ConeTools. I had to run ConeTools step by step, in order to find the error (see Figure 14).
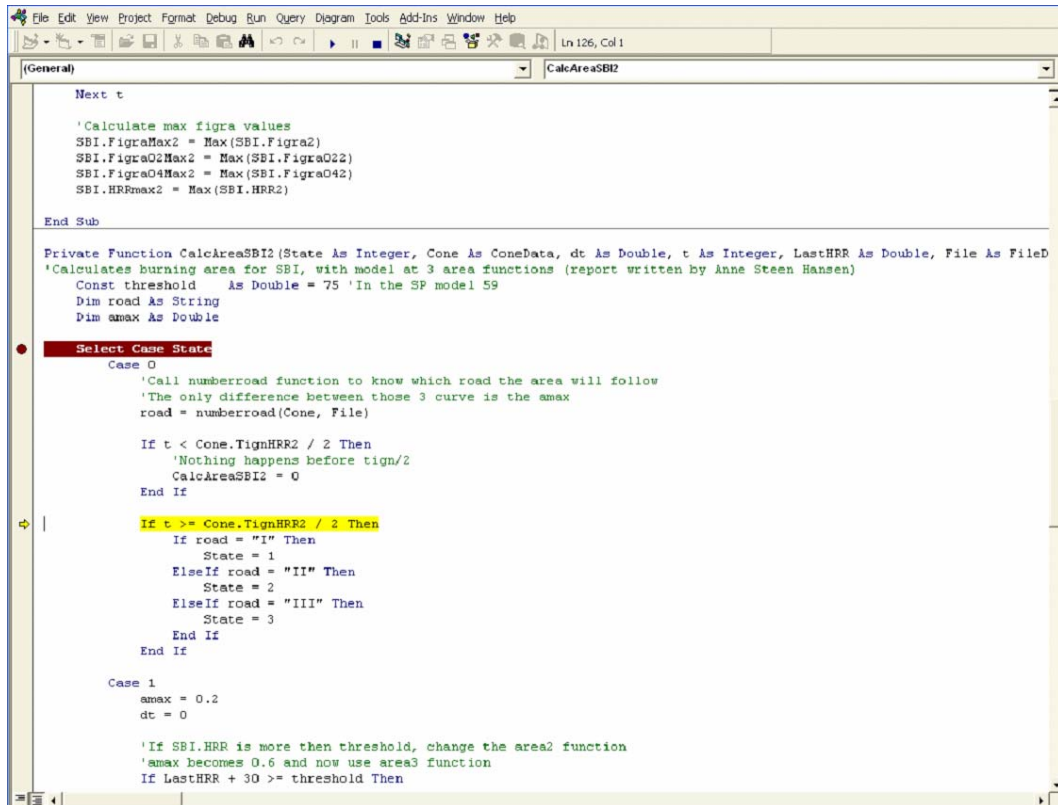
Figure 14. How to run ConeTools step by step.

Once I found the error, I modified the code in order to fix it (in a loop, the condition was wrong, that's why I could not open some files).
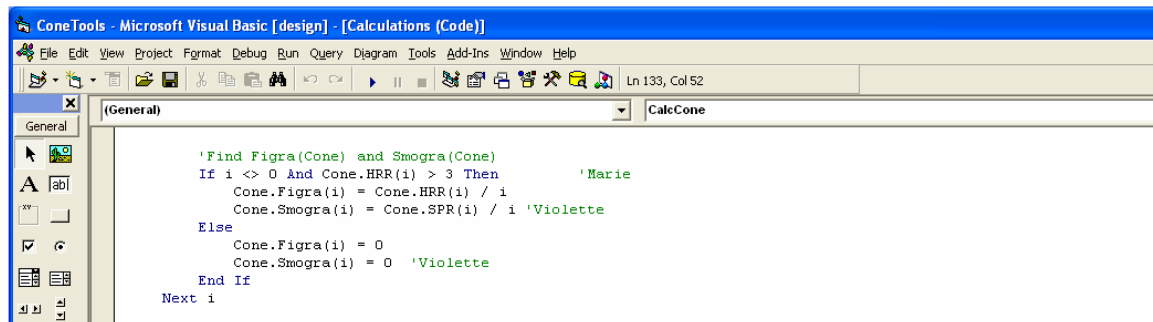
Figure 15. The loop modified.

The condition was Or, so for files who had a HRR > 3, the condition was right (see Figure 15), and the division was made for i = 0, that's why it didn't work.
I just replaced the Or by And.

I also had problems with running the Hansen model: according to Anne Steen Hansen, the ignition time must be between 10 seconds and 30 seconds. In reality, when I ran ConeTools, I could see that sometimes the ignition time was not between these two values. It was the case when the user defined the ignition time or a HRR threshold. I modified it by saying that when the ignition time was less than 10 seconds, it should be equal to 10 seconds, and when it was more than 30 seconds, it should be equal to 30 seconds (see Figure 16).

```
ElseIf frmTimeIgnition.timeHRRmodel2(1).value = True Then
    Do
        i = i + 1
        If i > UBound(Cone.HRR) Then GoTo HrrError
           Cone.TignHRR2 = i
        If Cone.HRR(i) >= Val(frmTimeIgnition.HRRlimitModel2.Text) Then Exit Do
    Loop
        If Cone.TignHRR2 < 10 Then              'Marie: for the Hansen model, the igniton time
           Cone.TignHRR2 = 10                   'should be between 10s and 30s.
        ElseIf Cone.TignHRR2 > 30 Then
           Cone.TignHRR2 = 30
        End If

ElseIf frmTimeIgnition.timeHRRmodel2(2).value = True Then
    Cone.TignHRR2 = frmTimeIgnition.timelimitModel2.Text
        If Cone.TignHRR2 < 10 Then              'Marie
           Cone.TignHRR2 = 10
        ElseIf Cone.TignHRR2 > 30 Then
           Cone.TignHRR2 = 30
        End If
End If
```

Figure 16. Modification for the ignition time in the Hansen model.

After that I could continue to do the comparisons with the data from the United Sates. I compared the test results with the Hansen model, and the SP model (it is the same model than in ConeTools 2.3) with the Hansen model. I did tables, and graphs (Annex F).
I also compared the SMOGRA and the smoke class obtained by the Hansen model with the SMOGRA and the smoke class from the experiment (Annex G).

Then I worked with data of the SBI project and the EUREFIC project, two research projects concerning the Euroclasses, see reference [2] for more information.

My task was to compare the SP model and the Hansen model, from data of the Cone Calorimeter test. I did tables and I compared the Euroclasses obtained with the two simulations with the Euroclasses obtained with the SBI test result (Annex H).

But in the data of the EUREFIC project, there was not the smoke production rate, and I needed it in order to run the Hansen model. I could calculate it, but I had to modify the code of ConeTools 2.4. Actually, the smoke production rate is the product of the mass loss rate (g/s) and the specific smoke extinction area (m2/kg), and these two data were in the files. I added a little program in the code who could calculate the smoke production rate from the mass loss rate and the specific smoke extinction area (see Figure 17).

```
'Interpolate to give Cone.HRR values with 1s timestep
For i = 0 To File.Time(UBound(File.Time))

    DoEvents

    Cone.SPR(i) = GetVal(CDbl(i), File.Time, File.SPR) 'Violette
    Cone.HRR(i) = GetVal(CDbl(i), File.Time, File.HRR)
    Cone.Time(i) = i
    Cone.MLR(i) = GetVal(CDbl(i), File.Time, File.MLR) 'Marie

    'Marie: calcul of SPR for EUREFIC project

    If Cone.SPR(i) < 0 Or Cone.MLR(i) < 0 Then
            Cone.SPR(i) = 0
    Else
            Cone.SPR(i) = (Cone.SPR(i) * Cone.MLR(i)) / 1000
    End If
```

Figure 17. Calculation of the SPR from the MLR and the SEA.

Then I could do the comparisons between the SP model and the Hansen model for the EUREFIC project, by doing tables and graphs.

The simulation of the Room Corner Test was not working. It was just an error with a name, but I should run ConeTools step by step, in order to see what was wrong. See Figure 18.
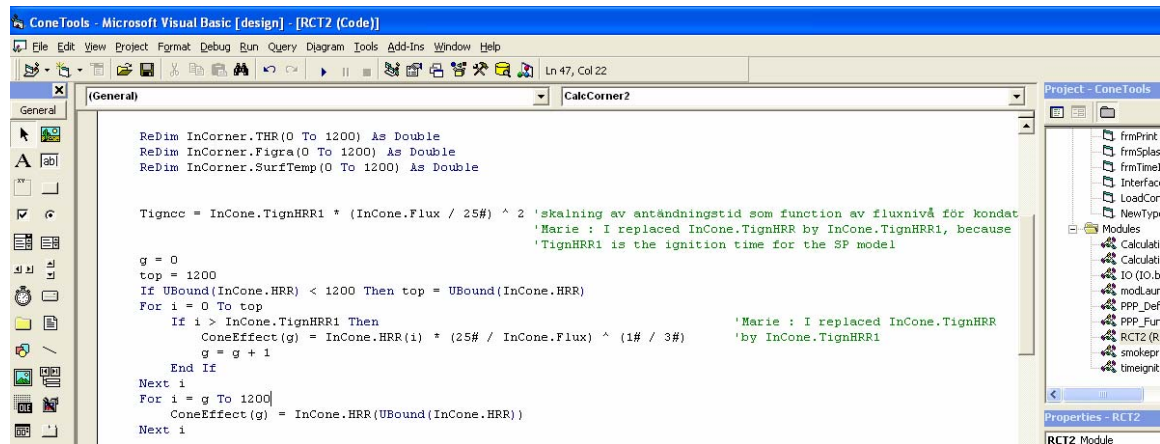
Figure 18. Solving of the problem concerning the Room Corner Test.

By definition, for the calculation of the ignition time, "by default" in the Hansen model means that the ignition time is defined when the HRR of the Cone is higher than 25 kW/m^2. But if the HRR was less than 25 kW/m^2 (it is rare but it can happen), there was no error message if "by default" was selected. It was the same thing for the smoke model if the HRR was less than 50 kW/m^2. I just added a line in the code in order to fix it (see Figure 19).
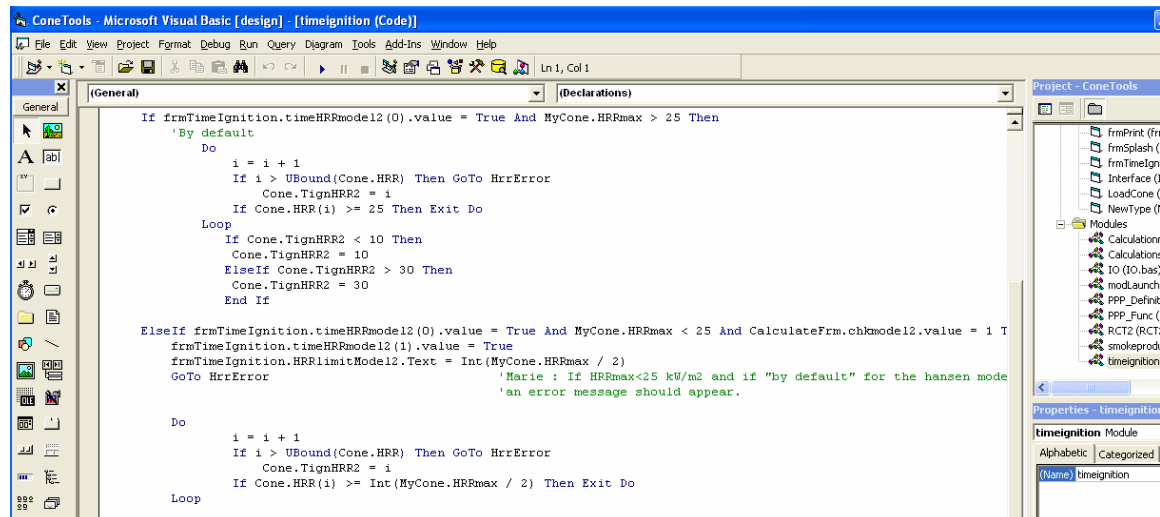
Figure 19. An error message should appears when "by default" is selected for the Hansen model.

3 Simulation of the self ignition of bio-fuels using SMAFS (Smoke Movement And Flame Spread)

After using ConeTools during approximately one month, I had to learn how to use SMAFS. This task took a while, because the manual was not detailed, and I had to understand by myself.

SMAFS is a CFD (Computational Fluid Dynamics) software package for numerical simulation of reacting flows such as building fires, spontaneous ignition in porous fuel storage and turbulent combustion in furnaces, etc. SMAFS is developed by Dr Zhenghua Yan at Lund University, Sweden. Expertise support was given by Dr Yan at some occasions during the project.

3.1 Introduction: what is CFD and how does it work?

Computational Fluid Dynamics is the analysis of systems involving fluid flow, heat transfer and associated phenomena such as chemical reactions by means of computer-based simulation (see reference [3] for details).

Some applications are:
- Aerodynamics of aircraft and vehicles
- Turbomachinery
- Chemical process engineering
- Environmental engineering (distribution of pollutants and effluents)
- Meteorology (weather prediction)
- Hydrodynamics of ships
- Etc…

CFD codes are structured around the numerical algorithms that tackle fluid flow problems. It contains three main elements: a pre-processor, a solver and a post-processor.

Pre-processing consists of the input of a flow problem to a CFD program. The user has to:
1) Define the geometry of the region of interest, called the computational domain.
2) Generate a grid.
3) Select the physical and chemical phenomena that need to be modeled.
4) Define the fluid properties.
5) Specify the boundary conditions.

Specification of the domain geometry and grid design is the most time-consuming task at the input stage.

The solver is based on numerical methods which perform the following steps:
1) Approximation of the unknown flow variables by means of simple functions.
2) Discretising the governing equations of fluid flow and heat transfer results in a system of linear algebraic equations.
3) Solution of the algebraic equations by an iterative method.

The complexity and size of the set of equations depends on the dimensionality of the problem, the number of grid nodes and the discretisation practice.

The most popular solution procedure is the TDMA solver of the algebraic equations.

The governing equations of fluid flow represent mathematical statements of the conservation laws of physics:
- o The mass of fluid is conserved.
- o The rate of change of momentum equals the sum of the forces on a fluid particle (Newton's second law).
- o The rate of change of energy is equal to the sum of the rate of heat addition and the rate of work done on a fluid particle (first law of thermodynamics).

The motion of a fluid in three dimensions is described by a system of five partial differential equations: mass conservation, x-, y-, and z-momentum equations and energy equation.

Mass conservation	Rate of increase of mass in fluid element	=	Net rate of flow of mass into fluid element	
Momentum equation	Rate of increase of momentum of fluid particle	=	Sum of forces on fluid particle	
Energy equation	Rate of increase of energy of fluid particle	=	Net rate of heat added to fluid particle	+ Net rate of work done on fluid particle

Table 1. Governing equations of the flow.

The post-processor allows the user to see the simulation results. It includes:
1) Domain geometry and grid display
2) Vector plots
3) 2D and 3D surface plots
4) Particle tracking
5) View manipulation (rotation, zoom…)
6) Animations

Once a simulation has been run, we can ask ourselves if the solution algorithm is successful. Three mathematical concepts are useful in determining the success of such algorithms:
1) Convergence. It is the property of a numerical method to produce a solution which approaches an exact solution.
2) Consistency. Consistent numerical schemes produce systems of algebraic equations which can be demonstrated to be equivalent to the original governing equations.
3) Stability. It is associated with damping of errors as the numerical method proceeds.

The solution algorithm is iterative and in a converged solution the residuals (measures of the overall conservation of the flow properties) are very small. But at the end of a simulation the user must make a judgment whether the results are "good enough".

3.2 A short presentation of the software

SMAFS has the following features:
- Parallel computing: it allows the user to use a certain number of processors to share a simulation task.
- LES and RANS: user can do simulation with LES (Large Eddy Simulations) or alternatively RANS (Reynolds Averaged Navier-Stokes).
- Cartesian and curvilinear coordinates: the user can choose between cartesian or curvilinear coordinates depending on the concerned geometry.
- Input processing: SMAFS has a powerful built-in preprocessor to process and interpret user's input.
- 3D data visualization: the postprocessor allows user to visualize the simulation results in various ways (it can plot the grid, geometry, vectors, scalar surfaces, iso-surfaces…)
- Capability of handling temporal variation of geometry.
- Variety of advanced optional models: models on turbulence, turbulent combustion, soot formation, thermal radiation, pyrolysis and flow in porous media have been incorporated.
- Dual grids system for gas and solid phases: the user can simulate both gas phase processes and solid phase processes.
- Graphical user interface (GUI): with it, the user can perform different tasks such as computations and post processing.
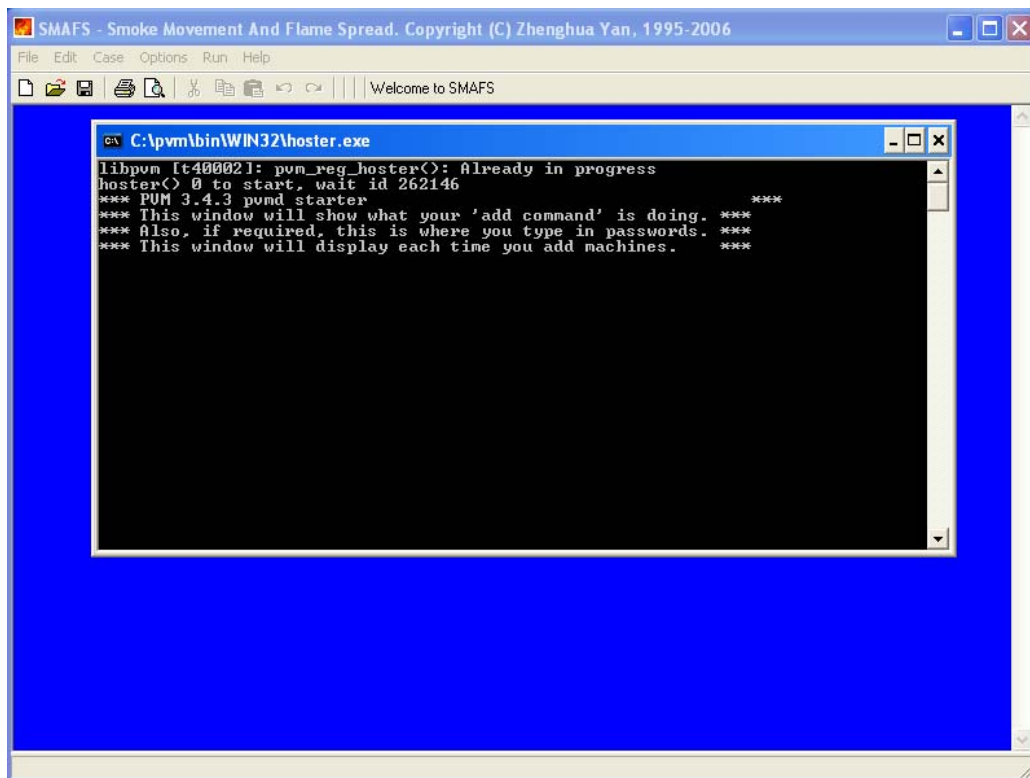
Figure 20. GUI and the communication daemon (PVM).

3.2.1 The input file

The first thing to do is to create an input file. This input file can be generated by following SMAFS instructions step by step to type in input data interactively (after starting SMAFS) or by using a text editor to modify an existing input file. The SMAFS

graphic user interface can also be used as a text editor. The user is allowed to do mistakes and errors while modifying or creating a file, but SMAFS has a self-examination function and you just have to run it in order to see if the input file will be accepted (even if the file is not terminated).

Anything starting with "!" is a comment and will be ignored by SMAFS. The input_file gives the prefix name of the input data file which will be input_file.set. SI units should be used for all inputs. See an example of an input file in Annex I and J.

As you can note, some input can be logical input. In this case, user should answer by T (True) or F (False).

An input file can have different forms, for example it depends on which mode the user wants to run the simulation: professional mode or standard mode. The professional mode allows more input and thus brings more flexibility.

3.2.2   How to run SMAFS with a Graphical User Interface (GUI)

There are two ways to run SMAFS, in command line fashion for Linux and UNIX system, and with GUI for Windows. But I used it only under Windows, that's why I will explain how to use it with GUI.

SMAFS need first to setup a communication daemon (PVM) because it is a parallel program. Every time SMAFS is started, it will check if the PVM daemon is ready (user can notice a PVM popup).

In order to run a computation, a case must be selected, and a computation can be started by clicking on "Start computation" in the "Run" menu. If the selected file is not terminated, SMAFS will invite the user to finish it. In the "Run" menu, other functions can be found, as "Interrupt computation", "Stop computation". By clicking on "Interrupt computation", a restart file will be generated before the computation is terminated: this allows you to continue the computation from the last termination point.
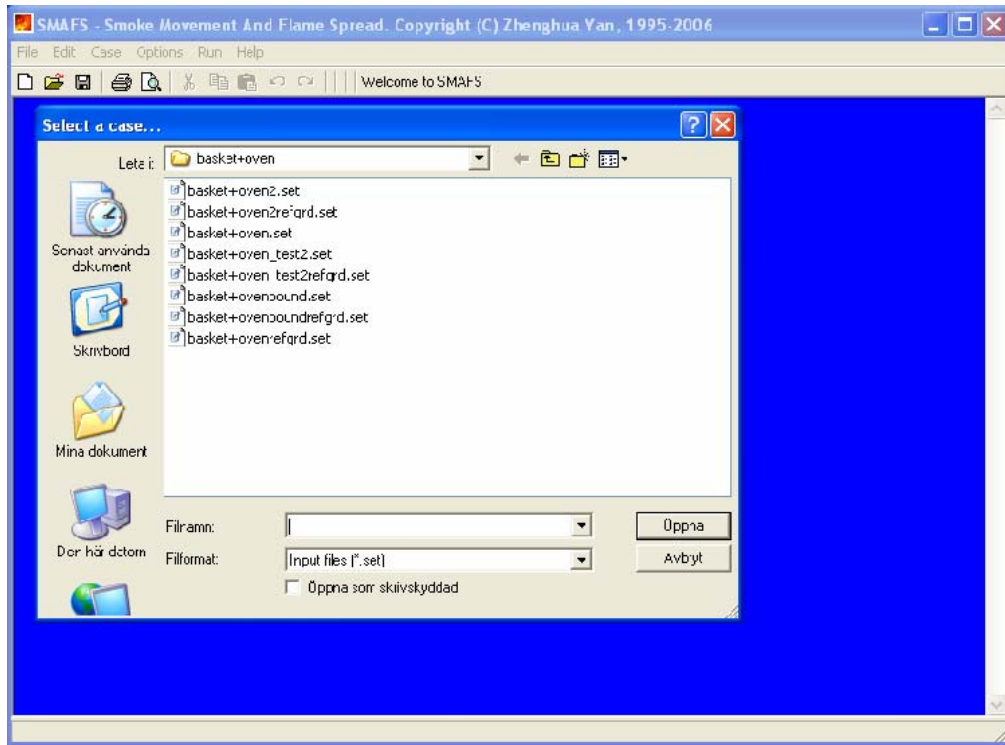
Figure 21. Open file dialog box.
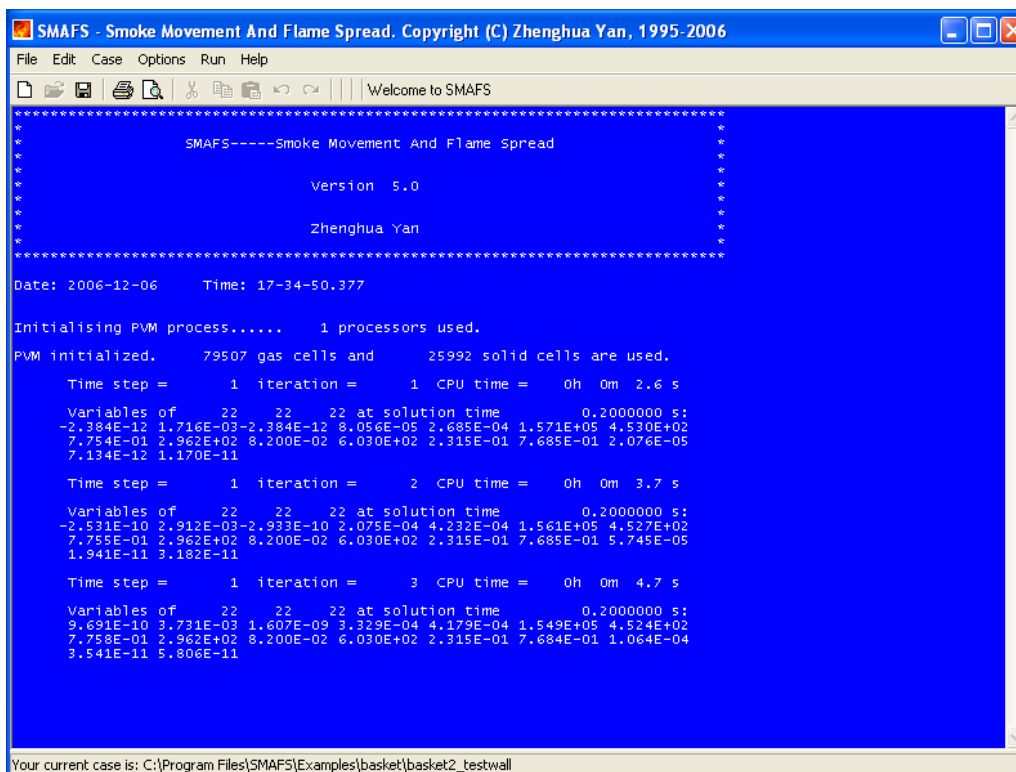
Figure 22. Interface of SMAFS when a simulation is running.

As you can see from Figure 22, a time step is composed of several iterations that the user can define. The CPU (Central Processing Unit) time is the real time, i.e. for how long the computation is running, although the solution time is the time in the simulation. The values for each variable for one specific point of the computational domain are printed

out. User can choose this monitoring point in the input file, see 4.3.1.1 (coordinate for data monitoring).

During the simulation, several files are created. If the name of your file is my_input,
- o my_input.set is the input file
- o my_input00000001, my_input00000002… are the results files for selected time steps
- o my_input.out is the running output file
- o my_inputrefgrid.set is the physical definition of the grid
- o my_inputrestart is the restart file generated when you interrupt the computation
- o my_input.res print out the residual information.

3.2.3 Post processing

In order to run the post-processing, the user has just to click on "post-processing" in the "Run" menu. Then user has to specify the first and the last time step for post-processing, and which variables he would like to study. The main menu of the post-processing is:
1. Visualization
2. Curve plot
3. Calculate flux
4. Data conversion
5. Data time averaging
6. Data spanwise averaging
7. Fieldview plot
8. Quit

Here user can choose what to do, but I essentially worked with the visualization, curve plot, and Fieldview plot. The visualization can plot the grid, geometry in different forms, vectors, scalar surfaces, iso-surfaces and iso-lines, and it can display animations. The curve plot menu can present the variables value as a function of time or as a function of space. The Fieldview plot menu allows user to export the results of the simulation into Fieldview, which is a powerful software for visualizing simulation results.
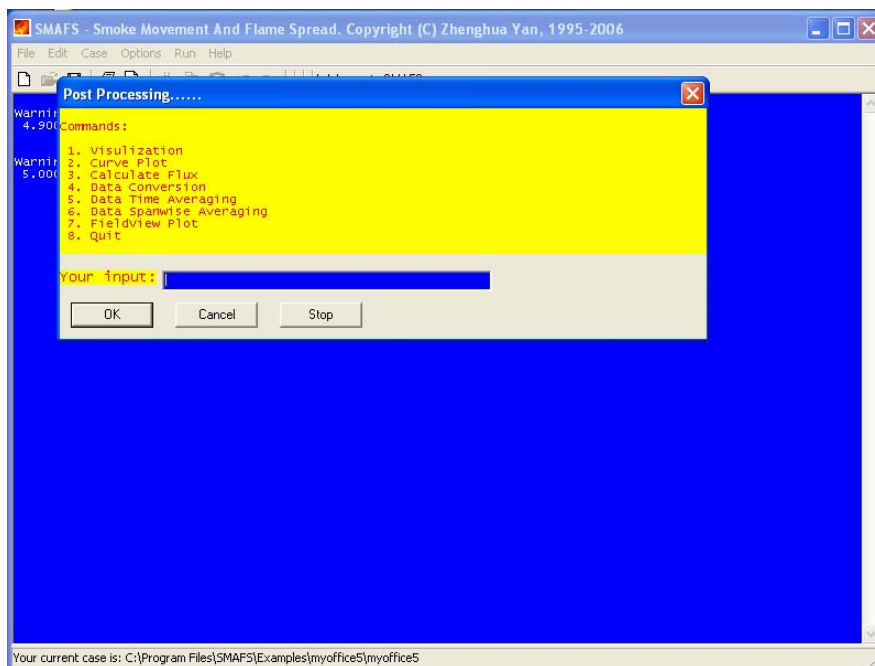
Figure 23. Post Processing.

3.3 Presentation of the simulations done with SMAFS

3.3.1 An example: my office

First I had to understand how the software works. That's why I tried to do a simple simulation, which consisted to put a propane burner in the corner of my office. The manual of SMAFS was not complete, and initially I had to understand how it works by myself.

3.3.1.1 Creation of an input file

There was an example in the manual of an input file, concerning multi-room smoke spread. I kept many values of this example in my input file. I modified the multi-room example to create the input file of my office. I tried to run the input file I created until SMAFS didn't detect any errors.

I will explain here how to do an input file through the example I made (see Annex I). I choose to run it in Standard mode, because it is sufficient for engineering computations. Less input is needed.

Physical description of the problem
The input 5 (see Annex I) concerning the porous media should be F (False), because it is a simulation of a traditional fire scenario. It should be true for example when simulating spontaneous ignition in biomass fuel storage.

A turbulence model is a computational procedure to close the system of mean flow equations (continuity, Reynolds equation, scalar transport equation) so flow problems can be calculated. There are 4 possibilities for the turbulence model. If the flow is a laminar flow (low Reynolds number), the input should be NO TURBULENCE. RANS means Reynolds Average Navier Stokes, HRN means High Reynolds Number. LES means Large Eddy Simulation, and there are two models: smagorinsky model and buoyancy modified smagorinsky model. I didn't need to know exactly what these different models were, because I was supposed to work with bio fuels, and in this case this input should be NO TURBULENCE. But for my office, I used the RANS model, as the example of the multi-room.

The next input applies only to RANS computation. It determines if a modification to the k-e models should be introduced. The k-e model focuses on the mechanisms that affect the turbulent kinetic energy.

Then I had to define the chemical species in the gas. In my office, I had air and propane (O_2, N_2, H_2O, CO_2, C_3H_8).

I had to choose between two turbulent combustion model, Flamelet model and EDC (Eddy Dissipation Concept). EDC is a popular representative method to model the mean reaction rate directly.

Then a soot model must be selected. I used the EMPIRICAL MODEL, as in the example: soot is presented in burner inflow and/or boundary inflow, or a certain amount of fuel is simply assumed to be converted to soot during combustion.

In input 11 you have to define the reaction of which the reaction rate will be explicitly computed. Only the reaction coefficients have to be specified.

In the next input, you specify if the thermal radiation has to be computed. Thermal radiation can be defined as electromagnetic waves emitted by a medium solely due to its temperature. Thermal radiation is an important heat transfer mechanism in many combustion systems.

The input 13 and 14 have to be specified only if the thermal radiation is computed. A radiation property model must be chosen. The model proposed by MODAK is simple and is used for a first rough computation (for the bio-fuels, the thermal radiation doesn't need to be computed: that's why I didn't have to know exactly the different models).

In input number 14, you specify Discrete Transfer ray's number which is defined by two integers. The Discrete Transfer method solves the radiation equation along a discrete set of directions (rays) from every element of the boundary surface.

Two pyrolysis models can be chosen: THERMAL MODEL and KINETIC MODEL. When a solid material heats up it starts to emit gases: that is the pyrolysis process. Pyrolysis usually starts at temperatures in the range from 100 to 250°C (reference [6]). The pyrolysis reaction can be described as:

Virgin material → Volatile products + Char.

Using input number 16, the user can choose a proper solver to solve the algebraic equation which results from the discretisation of a partial differential governing equation. FA is more powerful than TDMA (tri-diagonal matrix algorithm) and SIP (strongly implicit procedure), but it takes memory. Considering a system of equations that has a tri-diagonal form, the TDMA method can solve these equations by forward elimination and back-substitution.

Dimension related variables setup
The grid numbers in the three directions (if the problem is three dimensional) have to be specified. If you define n grids, it means you will have n-1 cells.

Generating grid system for computation
In Cartesian coordinates, the user has to generate the grid system along the X, Y and Z directions. This input should be defined in the following way: the start grid index should be specified, then the end grid index, the start physical location of the start grid, the start physical location of the end grid, and the cell size increment. The first grid always starts at 0. The first and the last cells are dummy cells; that is why they are so smalls. No calculations are made in these dummy cells, so they should formally be outside the computation domain. The cell increment is used in such a way that the next cell has a size increased by the increment factor relative the immediately previous neighbouring cell.
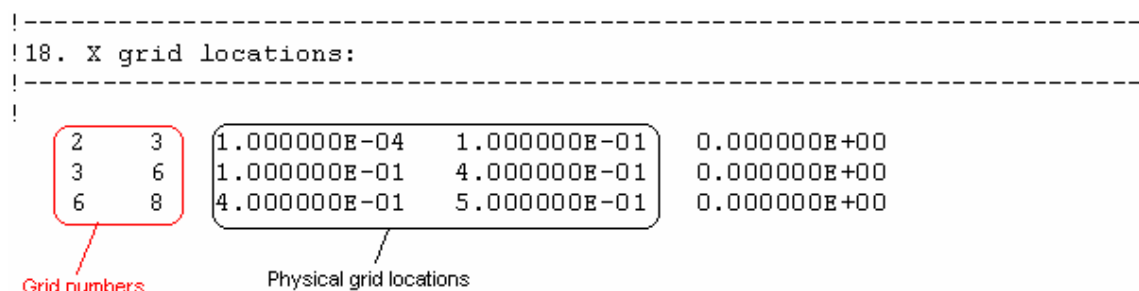
Figure 24. An example of the X grid locations.

As can be seen from Figure 24, the first cell is a dummy cell. Between 1E-04 and 0.1 meters, you can find the second cell. Between 0.1 and 0.4 meters, three cells are defined; between 0.4 and 0.5 meters, two cells are defined. Finally, eight cells and nine grids are defined, see Figure 25.
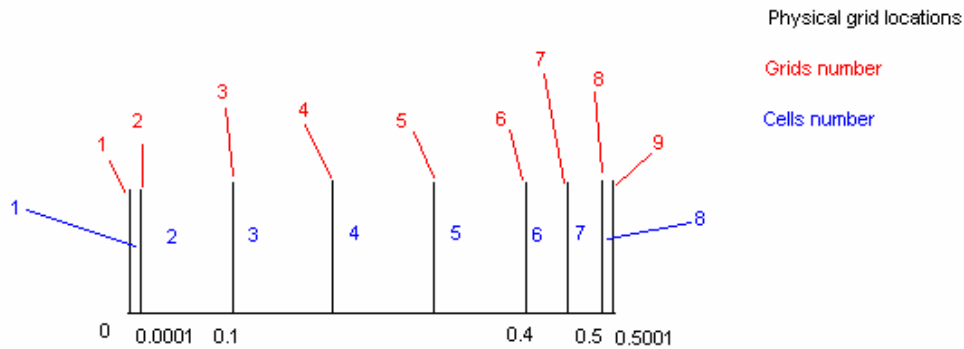
Figure 25. Visualization of the grid defined in Figure 24.

It is the same principle for the Y grid locations and Z grid locations.

Specification of blockage
In SMAFS, a blockage can be a "solid blockage" such as a solid box or a "cavity blockage" such as a void volumetric space. In this input you have to define the name of the blockage, the property (SOLID or CAVITY), the emissivity, and the coordinates of a diagonal of the blockage (a rectangular volumetric space can be created in this way). For my office, I had first to define a solid blockage, and then a cavity for the room (by making a "hole"). After that, I could specify another cavity blockage to create the door. After the blockages definition, SMAFS generates information which list all the walls created.

Specification of extra boundaries
The next input concerns the definition of the boundaries. First you have to specify the name of the boundary, then the orientation, the type, the emissivity and the coordinates of a diagonal of the boundary. The boundaries are defined in this way as planes (when using Cartesians coordinates). The computational domain must be closed by boundaries.

The boundary orientation is defined as following: if you go from neighbouring interactive gas phase to a boundary and find a decrease in the X coordinate, the orientation is WEST. Otherwise, if you find an increase in the X coordinate, the orientation is EAST. It is the same thing for SOUTH and NORTH with Y coordinates and for BOTTOM and TOP with Z coordinates.

Different types of boundaries are available:
- o   Wall: it is the default boundary condition for all fluid inactive surfaces.
- o   Symmetry: it implies zero mass flow across the interface and zero normal derivatives for all scalar variables.
- o   Extract: when the flow leaves the computational domain at a known velocity.
- o   Pressure: it allows both flow into and out of the computational domain.
- o   Inlet: when the flow comes into the computational domain at a known velocity.

- o Virtual boundary: it is just to close the computational domain and does not imply any physical implementation.
- o Entrainment: a variant of a static pressure boundary.
- o Exit: the flow is assumed to leave the computational domain.
- o CBC: convective boundary condition.
- o Non traction: not used.
- o Periodic: for different type of symmetry, for example swirling flow in a cylindrical furnace.

The boundaries are set to be subject to non-flowing ambient air condition, but user can set new values of the variables for a specific boundary.

For my office, I just defined six wall boundaries for each side of the room, and a pressure boundary at the door (the flow can go into and out of the room).
SMAFS will then automatically number the boundaries you defined and print out for reference.

Initialising the wall boundary
The wall surface is divided into many surface elements. Along the direction perpendicular to the wall surface, each wall is subdivided into a certain number of slabs, which you define here. Concerning my office, I defined six wall grids.

Then you decide for which walls you are going to assign the grid, by specifying the start wall index and the end wall index. One convenient way to cover all the walls is to set the start wall index to 1 and the end wall index to 100000000. You have to define the thickness of the cells. Since the first and the last cells are dummy cells, their thickness are zero.

For each wall, it is necessary to specify the pyrolysis temperature, the pyrolysis heat, the virgin and char densities, and the moisture content. User must first define the start wall index and the end wall index, the start slab index and the end slab index. I kept for my office the values of the example, except for the pyrolysis temperature. It is possible to change the variables values, in the same way as the extra boundary specification. For my office, the walls must be combustible walls, so I defined a lower pyrolysis temperature. If the walls are not combustibles, user has just to define a high pyrolysis temperature. To define a high pyrolysis temperature is a way to "turn off" the pyrolysis model that allows modeling of flame spread.

Then you must define the specific heat for the selected slabs in the selected walls. The specific heat is defined as: $C_p = a + bT + cT^2 + dT^3 + eT^4$. You specify in this input a, b, c, d and e. SMAFS will calculate C_p according to these coefficients. In the next input you define the thermal conductivity k in the same way as the specific heat. The thermal conductivity is expressed as: $k = a + bT + cT^2 + dT^3 + eT^4$, and user has to define the five coefficients. I took the values of C_p and k from the example.

Setting up burner parameters
You first have to define the orientation of the burner (in the same way as in the boundary definition), and two points of a diagonal of the burner. The orientation of the propane burner in my office was SOUTH (because it is on the floor), and I choose to put it in a corner of the room. It is possible to include several burners.

Then for each burner, you must define the temperature and the mass fraction of the species. I choose a temperature of 300 Kelvin and it was a propane burner, so the mass fraction of C3H8 had to be 1.

In the next input, the user has to specify a time from which the burner will have the power (in Joule) given in the same input. In this case, the power of the propane burner was 300 kJ, and it started at 0 second.

Run control parameters setting up
The user has to choose which variables he would like to save in results files, he just has to choose between T (true) or F (false).

The next input tells SMAFS for how long of physical processing time the simulation has to be performed.

Then a monitoring point must be chosen. When doing a computation, it is always useful to monitor the state change of a particular location to have some idea on how the iteration is going and how the state is developing. It is recommended to select a sensitive location where the state variation is most apparent. In this case, the monitoring point was located in the door.

In the next input, three parameters have to be specified: The first parameter determines how often the residuals will be printed out (if this parameter is n1, SMAFS will print out residual information every n1 iterations). The second parameter tells SMAFS how often the result data should be stored (if this parameter is n2, a result file will be created every n2 seconds of physical simulation time). The third parameter controls the restart file updating frequency (if this parameter is n3, SMAFS will print out update result file every n3 time step).

By setting maximum iterations for the flow computation, user can force iteration to end and go to next time step computation. But the iteration may have already converged before the tolerance has been reached. It is possible to specify a maximum of iterations for different physical simulation time periods.

In the case of my office, SMAFS will take at maximum 500 iterations when the physical simulation time is located between 0 and 30 seconds, 400 iterations between 60 and 300 seconds, 300 iterations between 300 and 500 seconds and 200 iterations between 500 seconds and the physical time specified in a previous input.

The last input concerns the variation of time step with time. It acts in the same way as the last input. In the example of my office, between 0 and 60 seconds there will be one time step each second, between 60 and 120 seconds there will be one time step each five seconds, and between 120 and 600 seconds there will be one time step each 10 seconds. The time steps should be smaller in the beginning of the simulation, as there are more physical changes during this period.

3.3.1.2   Visualization of the results : post-processing

In the visualization menu, I could see the results of the simulation.
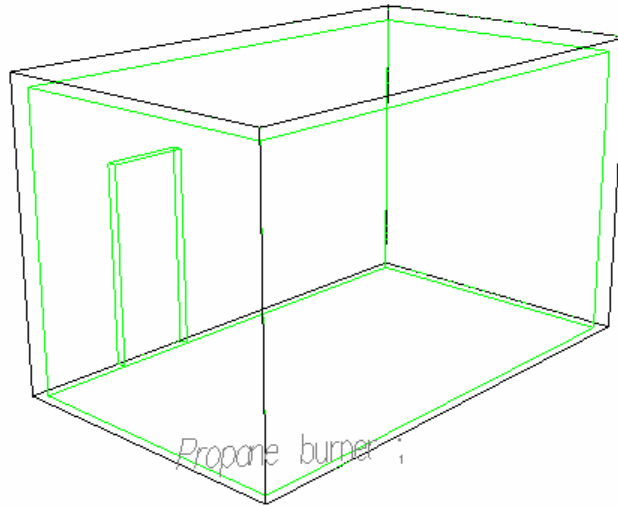
Figure 26. Configuration of my office in SMAFS visualization.
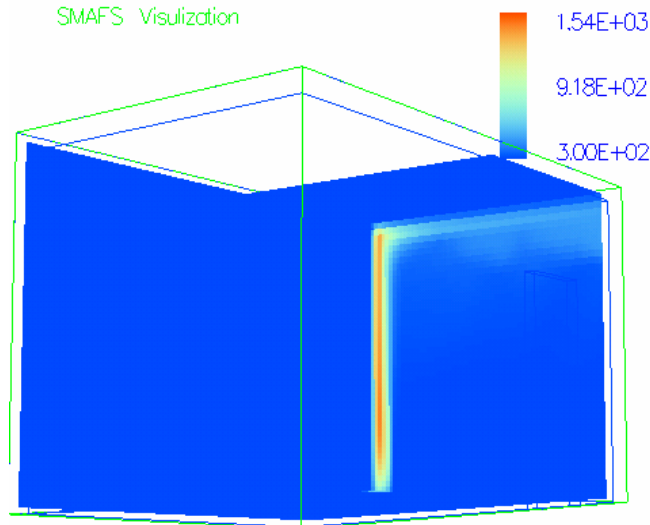
Figure 27. Visualization of the temperature in the office after 16 seconds.

I could see if the results were coherent, for example if the orientation of the burner was right, if the burner was in the corner of the room I wanted, if the temperature was not too high…

3.3.1.3 Comments

Of course, the input file you can find in the appendix is not the only input file I created. I had to try and to see what happened with the post-processing (in the visualization). For example, I tried several grids, and I could see what the grids looked like in the visualization; I changed the burner power; I changed the variation of the time step with time, the variation of maximum iterations with time.

I kept a lot of values of the example concerning the multi-room, but sometimes I saw in the post-processing that these values were wrong for my office. I had a lot of questions; I didn't know for example how to simulate the flame spread on the walls. Actually, a meeting was planed with Dr Yan, the creator of the SMAFS software. The meeting did, however, take place later when I was working with the biofuel problem. This work took almost twenty days.

I will not explain more about this example, because I spent more time on the project concerning the bio-fuels, and it was the real purpose of my placement. The input file in Annex I is thus not completely working as it should be: the flame spread in the walls was not computed.

3.3.2 Basket heating test

Wood pellets are composed of biological material that is capable of spontaneous heat generation during certain conditions. Wood pellets are a refined wood fuels. They are produced for easier handling specifically for smaller sized plants and domestic use. A number of fires have occurred in large bulk stocks of wood pellets; large quantities of wood pellets stored in a silo caught fire by spontaneous ignition. SP has carried out several experiments, both in small scale and in large scale. The experiment I tried to simulate was a small-scale basket heating test [5].

3.3.2.1 Theoretical model and presentation of the experiment

The equipment used for this test is an oven of 0.34 m x 0.40 m x 0.40 m with re-circulating air. A stainless-steel mesh basket (0.1 m x 0.1 m x 0.1 m) filled with solid fuel (wood pellets) was suspended in the oven. In order to create conditions for spontaneous ignition in this small scale, the oven was heated up at 180°C. Five type K thermocouples were placed between the centre of the basket and a surface of the basket at one side in order to monitor the temperature evolution inside the basket. The distances between these thermocouples and the center of the basket are 0 mm (point 1), 10 mm (point 2), 20 mm (point 3), 35 mm (point 4) and about 48 mm (point 5).

Two basics factors contribute to spontaneous heating and ignition: heat generation and heat dissipation. If heat generates faster than it dissipates, temperature increases. Of the many kinds of heat-generating reactions, oxidation is the most common. When wood pellets form a huge pile, self-heating is a common problem. The larger the pile is, the easier self-heating and ignition occur; it is because heat generation is proportional to the volume of the pile.

3.3.2.2 Simulation of this test

The simulation is based on solution of a set of unsteady governing equations including the continuity equation, the momentum equation, energy conservation equations for both gas and solid phases, and mass conservation equations for different chemical species. Special for this type of simulation is that the POROUS MEDIA option is selected. This

means that the transport equations are solved for a porous media, and there is e.g. no turbulent flow in such a media. The complete computational domain contains the porous media which is surrounded by boundaries. There are thus no gas phase calculations involved in this type of simulation.

    o   *Creation of the input file*

To create an input file took a long time. The professional mode was used for this simulation. The differences compared to the standard mode are:

1) <u>Gravity vector</u>: In the professional mode, the user can define his own gravity vector. In the standard mode, the gravity vector is, by default, (0,-9.81,0).
2) <u>Physical space/computational space</u>: You can choose to define your geometry in the physical space or in the computational space. In the physical space, you define the geometry with the coordinates (in meters). In the computational space, you define the geometry with the grids. By default, in the standard mode, you define the geometry in the physical space.
3) <u>Turbulent Prandtl number</u>: In the professional mode, user can set up a Prandtl number for each variable. Usually, the Prandtl number for the air is 0.7.

$$Pr = \frac{\mu c_p}{\lambda}$$, with μ the dynamic viscosity (N.s.m^{-2}), λ the thermal conductivity (W.m^{-1}.K^{-1}), and c_p the specific heat capacity (J.kg^{-1}.K^{-1}).

4) <u>Intended domain</u>: SMAFS asks you to specify an intended domain in the professional mode. The intended domain is useful if you don't need to compute the flow everywhere. You can use it for example if you have a fire in a special place.
5) <u>Initial values of the variables</u>: In the professional mode, SMAFS asks you to set up the initial values of the variables.
6) <u>Under relaxation factors</u>: User has to specify the under relaxation factors for each variables in the professional mode. The equations are susceptible to divergence unless some under relaxation is used during the iterative process, and new improved values for each variable are obtained.
7) <u>Scheme</u>: User can choose which scheme he wants to use for the computation in the professional mode. The available schemes are: Upwind, Hybrid, PLDS (Power-law Differencing Scheme), SMART, UMIST, SUPBEE. The accuracy of SMART, UMIST and SUPBEE schemes is second-order in terms of Taylor series truncation error. They belong to the class of TVD (Total Variation Diminishing) schemes.
8) <u>Residual tolerance for flows</u>: In the professional mode, user has to set up a residual tolerance for flows. It is for the mass conservation.

A new file will be created for the porous media. If the name of your input file is my_input.set, this new file will be my_input.std. It contains the data concerning the porous media: the permeability vector (the permeability can be different along each direction), the particle size, the particle porosity, the density of a dry solid particle, the conductivity of a solid particle, the specific heat of dry solid particle, and the solid heat production rate.

User has to define the conductivity of the solid particle and the specific heat of the dry solid particle 500 times, as conductivity and specific heat can change with the temperature. The user has to set up a value for each Kelvin from 1 Kelvin to 500 Kelvin.

There are 2500 values for the solid heat production rate, one for each Kelvin from 1K to 2500K. You calculate it with the Arrhenius law:

$$k = QA*\exp(-E_A/RT)$$

with k the solid heat production rate (J/kg.s)

  Q the heat of reaction (J/kg)

  A the pre-exponential factor (s^{-1})

  E_A the activation energy (J/mol)

  R the gas constant (R = 8.31 J/mol.K)

  T the temperature (Kelvin).

First I tried to define the basket and the oven. The porous media should be only inside the basket, and I didn't know how to define the porous media only in a precise place. So I first created a file without porous media, in order to see if the environment was correct. I defined the oven, with a basket inside, a slit in one of the side of the oven, and a box on a wall, for the fan of hot air (see Figure 28).
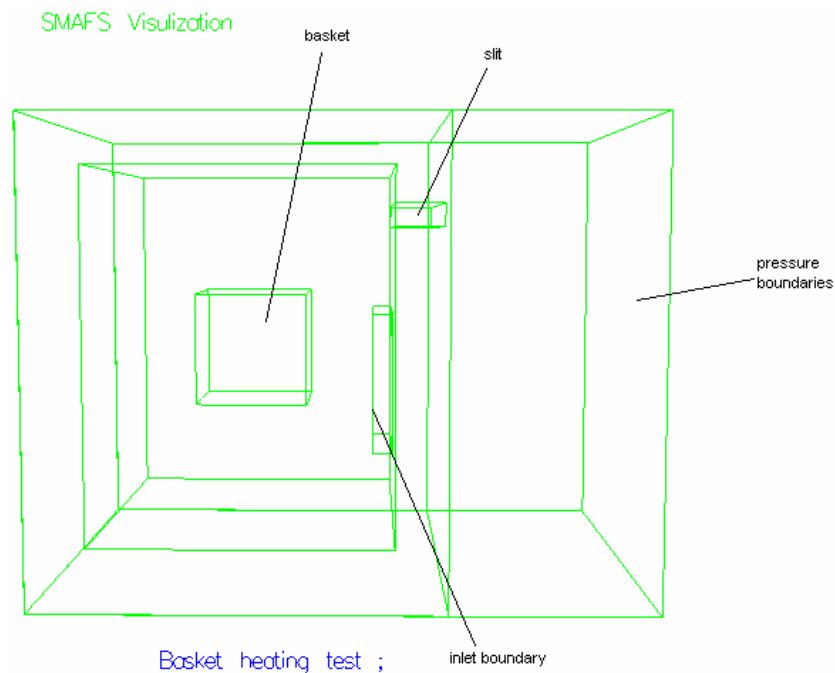
Figure 28. Visualization of the oven.

On the box, I defined an inlet boundary, with a velocity of 0.05 m/s (this velocity allows the air to be changed in the oven one time per minute). I defined five pressures boundaries placed at the side of the oven with the slit. Actually, it is better to put the pressure boundary at not exactly the same place as that of the slit. If the boundary is placed too close to solid obstacles it is possible that the flow will not have reached a fully developed state, which may lead to errors.

Furthermore, the computation domain must be closed. That's why I included the additional four pressure boundaries. The grid I defined allowed having more cells in the basket, in the slit and in front of the inlet. In these places there is more flow movement. I defined only three grids for the wall modeling (two are dummy, so there was just one real cell), as it was not really necessary to compute the heat transfer in the walls. Concerning the properties of the walls, I took the data of the mineral wool, because it was the more insulating material.

I did not run this computation until the end, I interrupted it. In fact, the solution was not convergent. The residuals were too big. When there is divergence, first you can try to change the grid, then to change the time step and finally to decrease the under relaxation factor. I changed the grid several times, because the size of the cells should not vary too much. Then I changed the time step, because it should increase more slowly.

Then I could check that all was correct in the oven in SMAFS visualization. The velocity must not be too high in the outlet for example. The temperature should be between 20°C and 180°C. The pressure should not be too high. I found some errors I could correct: the orientation of the inlet was first wrong for example.

Once everything was correct, I tried to run this simulation with the porous media. But I realized that the porous media was defined in the whole oven, because I could see that some variables (bulk density, solid temperature or solid moisture) were present in the whole geometry. It meant that the porous media was computed everywhere (see Figure 29). I realized that it was not possible to define porous media for a precise part of the geometry.
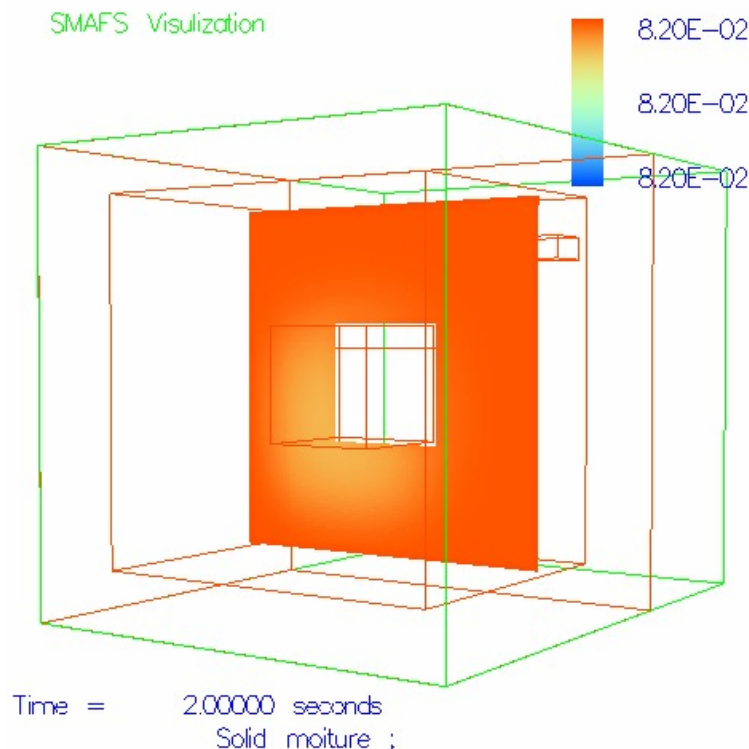
Figure 29. Distribution of the solid moisture in the oven.

That's why I had to create an input file with only a basket. I had the opportunity to speak to the creator of this software (Dr Zhenghua Yan), and I could ask him a lot of questions. He helped me in the creation of the input file that I finally used.

Background and Initial conditions

The problem was three dimensional. The porous media had to be computed. There was no turbulence, no soot, the thermal radiation didn't need to be computed and the pyrolysis model was inactive. I set up the ambient air temperature for the boundaries to 180°C (temperature of the oven). The chemical species were H_2O, O_2, N_2, CO_2 (air) and CO. The biomass fuel was at a temperature of 23°C.

The biomass fuel basket was assumed to be homogeneous and isotropic as a consequence of the definition as a porous media. The input data given for wood pellets is given in Table 1.

Table 1. Input material properties (in SI units).

Bulk permeability	6.00E-08
Bulk porosity	0.52
Compact dry density	1190
Conductivity	0.17
Specific heat	1700
QA	1.60E+09
EA	69000
Bulk density	603

Geometry

This time the geometry was easier as only the basket filled with wood pellets was included in the simulation; there was no blockage. No walls were defined.

Mesh

Twenty cells were used along each direction (twenty two with the two dummy cells). The mesh was uniform.

Boundary conditions

The conditions at the fuel basket relevant boundaries were imposed by considering the oven environment as a free space. So I set up six pressure boundaries at each side of the basket, with a temperature of 180°C. A "mini wall" which occupies one dummy cell had to be defined at one side of the basket, because the program needs to have at least one wall for the purpose of the data allocation. It didn't change anything, because there is no calculation in the dummy cell.

Numerical aspect

The simulation time was set up to 300 minutes. The time step varied from 0.5 to 2 seconds.

Comment

There was no wall modeling (no walls), and no burner. SMAFS calculates the density of the material automatically.

 o *Computation*

This simulation was very long; when the CPU time was about 56 hours, the time in the simulation was about 4800 seconds, i.e. 80 minutes. I decided to interrupt the simulation, because there was another way to simulate it which would reduce the simulation time considerably.

3.3.2.3   Comments and improvement of this simulation

It was possible to simulate only a quarter of the basket: the advantage was the simulation take in this case only a few hours. The problem is regarding geometry symmetric in both width and depth directions; because of the buoyancy, it is not symmetric in the vertical direction. But in the visualization, it was possible to see only the quarter of the basket. The differences with the previous input file were just the definition of the boundaries: I had to define two symmetric boundaries, see Figure 30. See the input file in Annex J for more details.
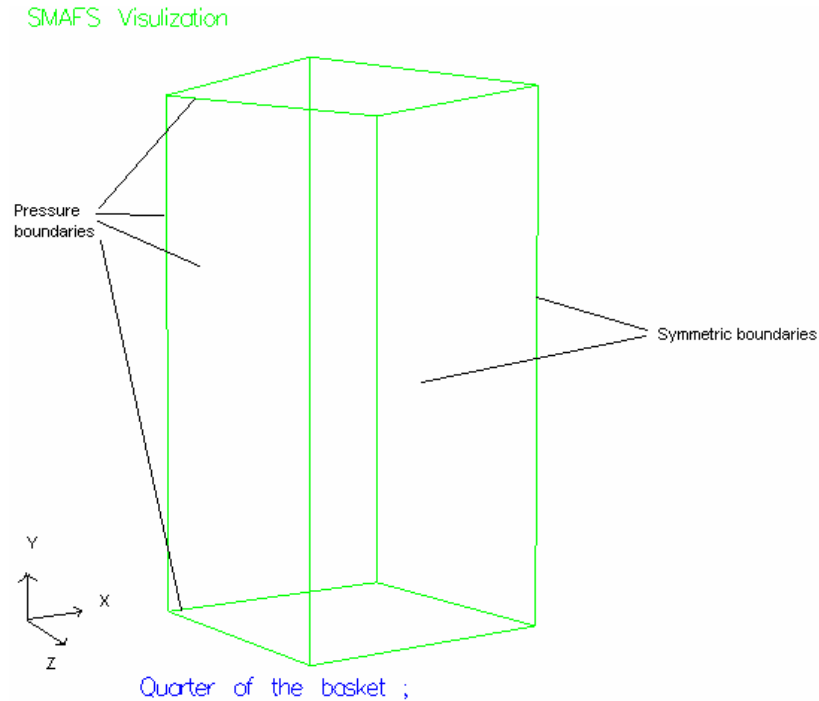
Figure 30. Visualization of the basket quarter.

In this case, the simulation took about seven hours.

I compared the results with the simulation of the entire basket, because I had to be sure that the quarter of the basket was correctly defined, and that the symmetric boundaries were at the right place. I used graphs; see Graph 1 and Graph 2.

We can see on the curves that the variation of the solid temperature with the time is the same for both simulations. It meant that the symmetric boundaries were correctly defined, and I could work with the quarter of the basket.
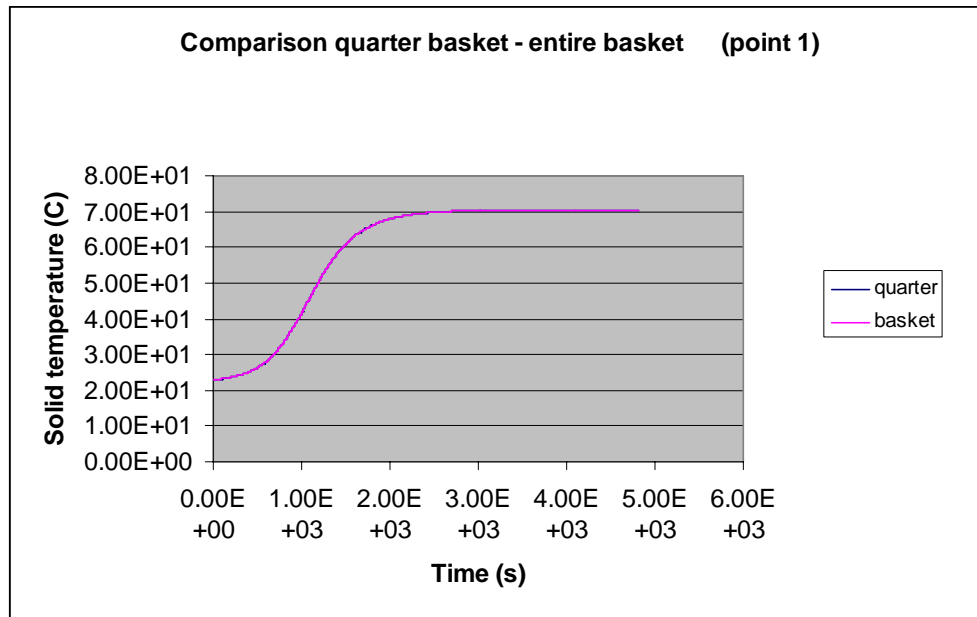
Graph 1. Comparison of the temperature between the quarter of the basket and the entire basket for the point 1 (located in the middle of the basket).
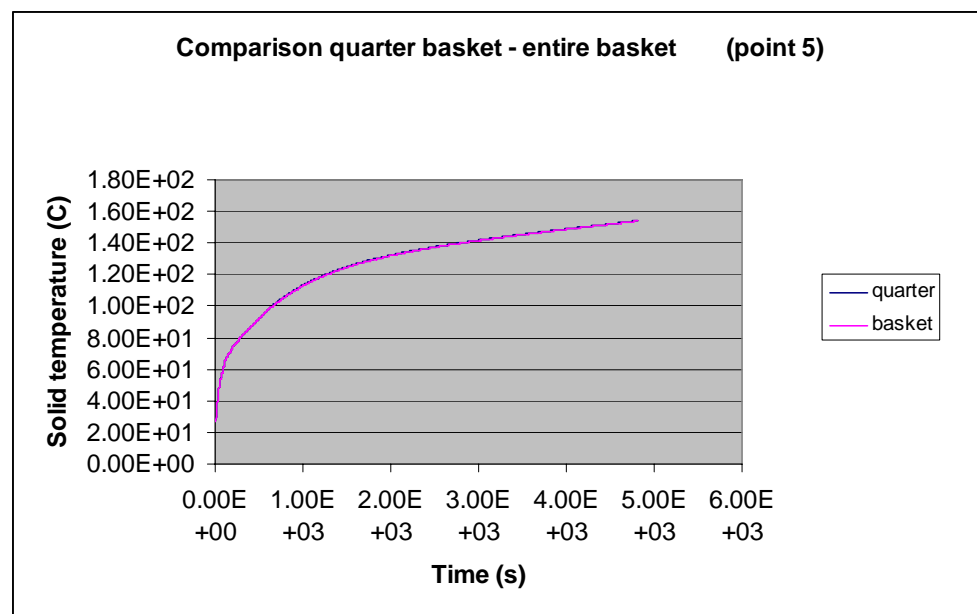
Graph 2. Comparison of the temperature between the quarter of the basket and the entire basket for the point 5 (located at the border of the basket).

3.3.2.4 Results

Basket heating test
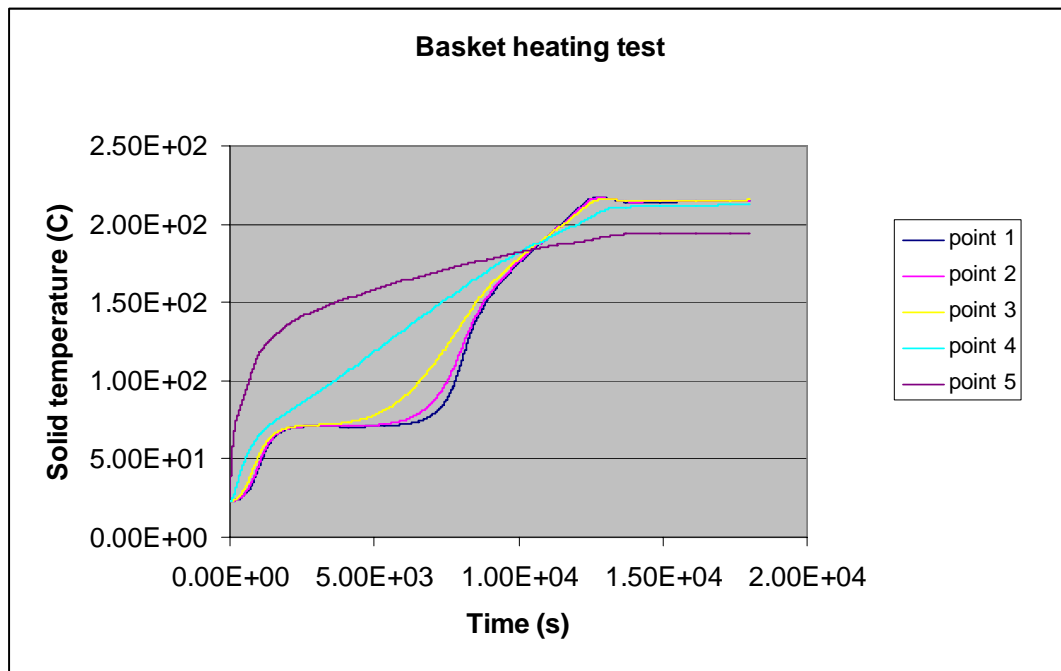
Graph 3. Plot of the solid temperature versus the time.

There is a big difference in temperature between the edge point and all the other points (Graph 3). For the points 1, 2, and 3, the temperature increases and then levels off at about 71°C. With increased depth, the "level-off" period becomes longer. Then the temperature increases again, and at about 10800 seconds (180 minutes), the temperature curve crosses with each other.

When the cold pellets are placed in the oven, they are subject to external convective and radiative heating: the temperature increases. Convection is then introduced because of the buoyancy. Heat and vaporized moisture are transported to the inner parts of fuel storage trough diffusion and convection. When the water vapour meets the cold solid fuel, some water vapour condenses to release its latent heat. But when the temperature goes to a certain level, the evaporation can be fast enough to absorb the transported heat: this result in a "level-off" phenomenon. After the fuel has become dried, there is no energy sink to absorb the energy locally produced by chemical reaction, and the energy delivered by conduction and convection. The local temperature steadily increases. In the middle of the basket, the produced heat has higher resistance to be dissipated away, that is why the temperature can become higher than the temperature at outer part. When the heat cannot be sufficiently dissipated away, spontaneous ignition can occurs. When the curves cross each other, it indicates a high potential of spontaneous ignition.
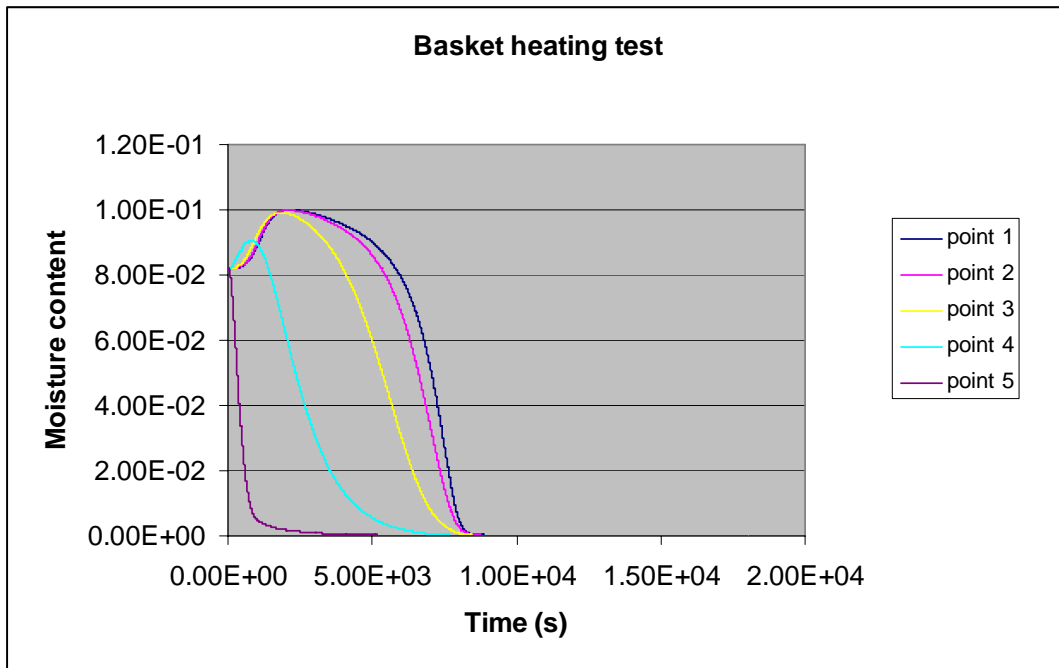
Graph 4. Plot of the moisture content versus the time.

The moisture content history shows the dying process in the fuel storage (Graph 4). When the basket is placed in the oven, the edge part dries out quickly (point 5). Because of the condensation, the moisture content of points 1, 2, 3 and 4 increases in the beginning. The condensation is due to the junction of the vaporized moisture and the cold solid fuel. Then the in-depth points start to dry slowly for a period which becomes longer with increased depth. This slow drying corresponds with the "level-off" of the temperature (Graph 3). Finally the fast drying period corresponds to the temperature's quick increase.

The results can be seen in the visualization of SMAFS, see Figure 31 and Figure 32.
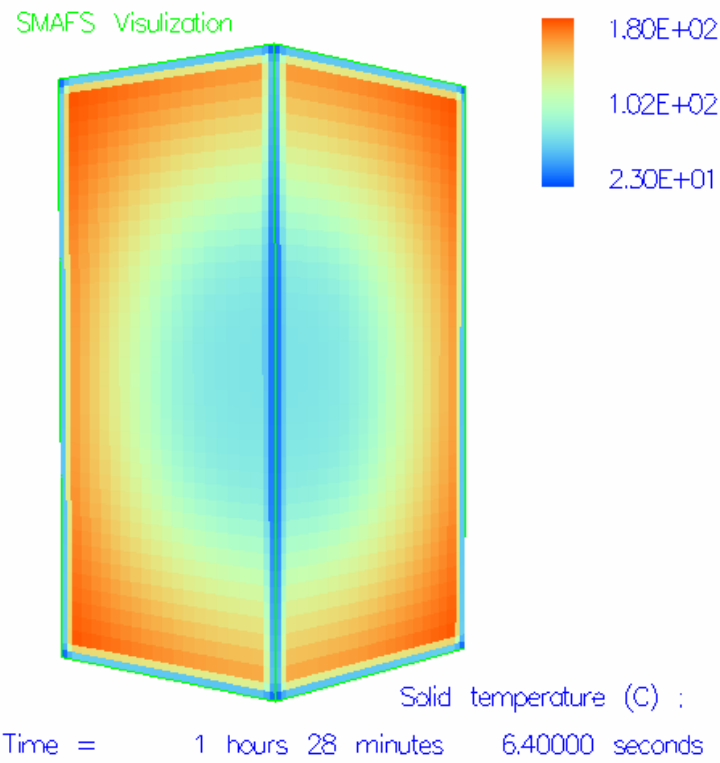
Figure 31. Visualization of the solid temperature after 5286 seconds.
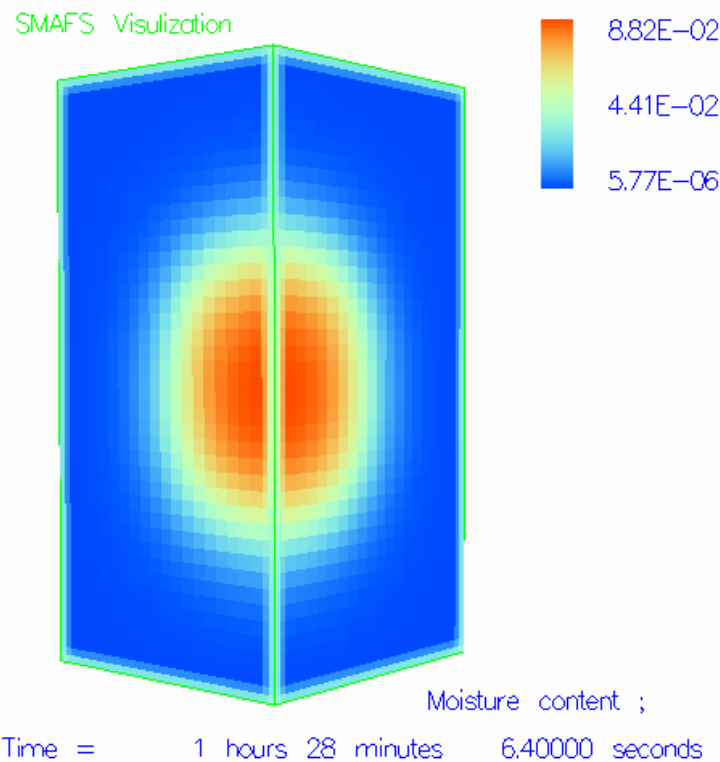
Figure 32. Visualization of the moisture content after 5286 seconds.

Then the criteria of the grid independence must be checked. The number of cells must be multiplied by two, and if the results are similar, it means that the number of cells was

enough. But if the results are really different, the number of cells should be increased, until the results are similar.

That's why I replaced the number of cells by forty along each direction for the entire basket. The simulation was longer, about 51 hours. Then I could compare the results of the two simulations.
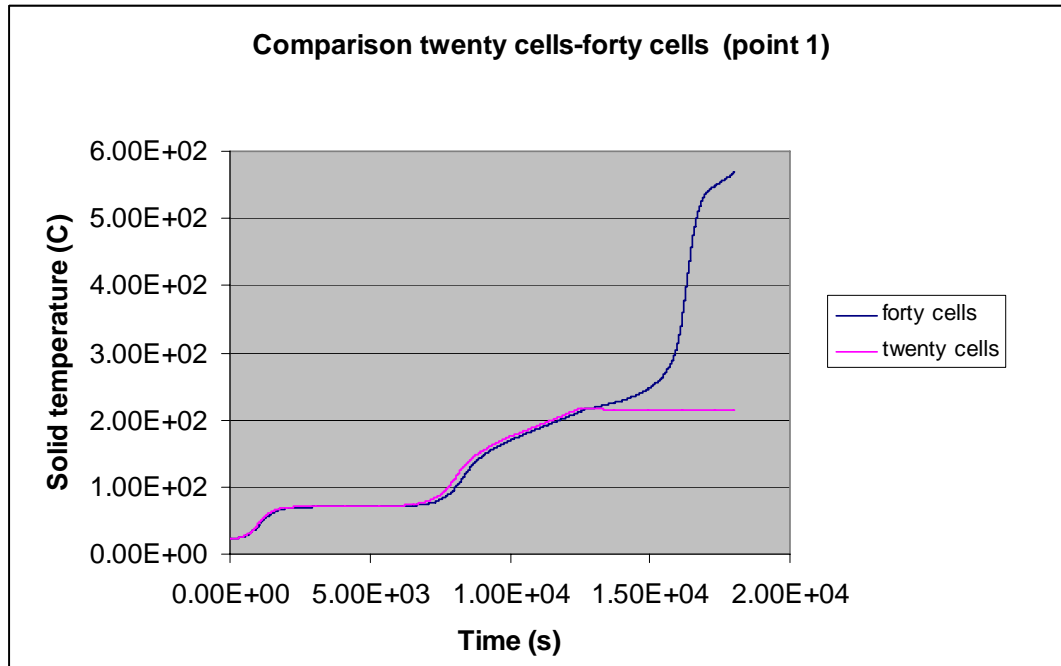
Graph 5. Comparison of the temperature between the twenty cells and the forty cells for the point 1 (located in the middle of the basket).
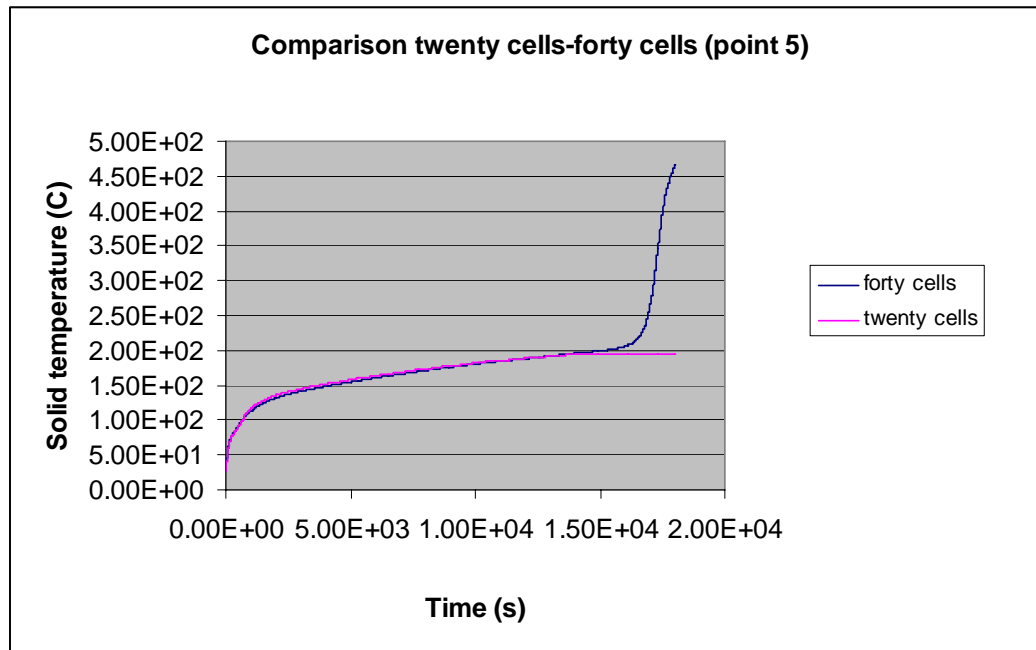
Graph 6. Comparison of the temperature between the twenty cells and the forty cells for the point 5 (located at the border of the basket).

As you can see Graph 5 andGraph 6, the temperature is similar for the two simulations until around 13000 seconds. The accuracy of the solution is governed by the number of cells in the grid: the larger the number of cells the better the solution accuracy. But it was enough to have good results until 13000 seconds, after the crossing point. In fact, the pyrolysis model was not used in this simulation, and after 13000 seconds, the temperature is higher than 200°C, so a self-ignition can occurs.

That's why I could continue to work with the first quarter I defined, with only ten cells along the X and Z directions, and twenty cells along the Y direction.

3.3.2.5   Comparison with the experiment

A comparison between the results of the simulation and the results of the experiment can be done, see Graph 7, Graph 8, Graph 9, Graph 10, and Graph 11. All the important processes are well captured by the numerical simulation (the level-off temperature, the temperature crossing time). The simulation reproduces quite well the experimental measurement.
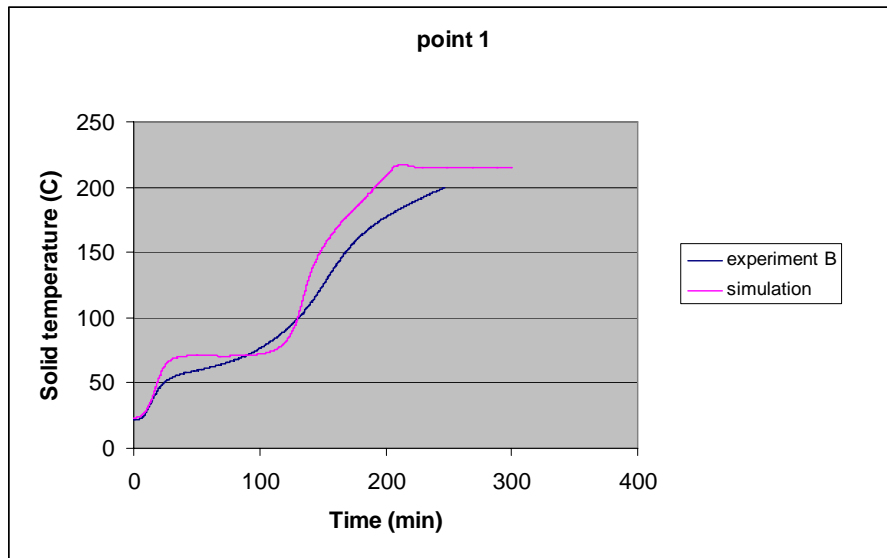
Graph 7. Comparison of the predicted and measured temperature (point 1).
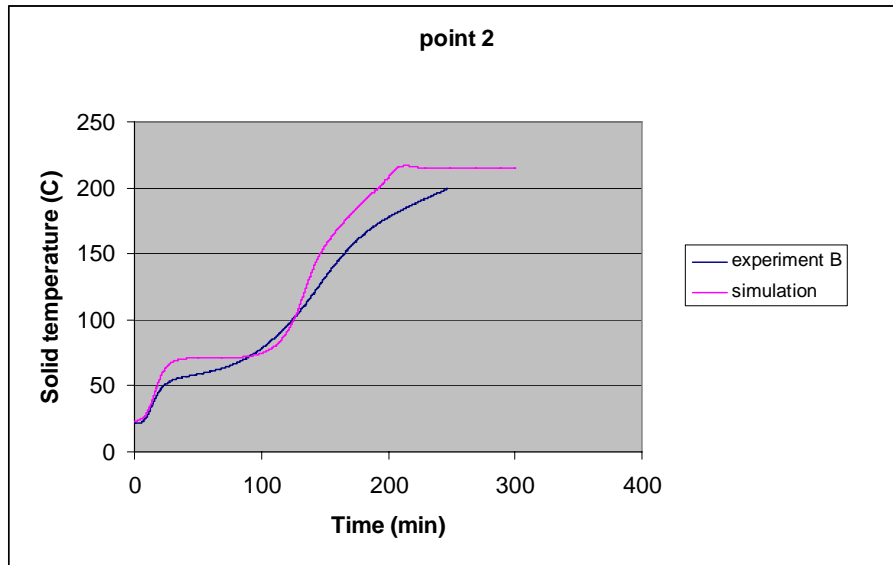
Graph 8. Comparison of the predicted and measured temperature (point 2).
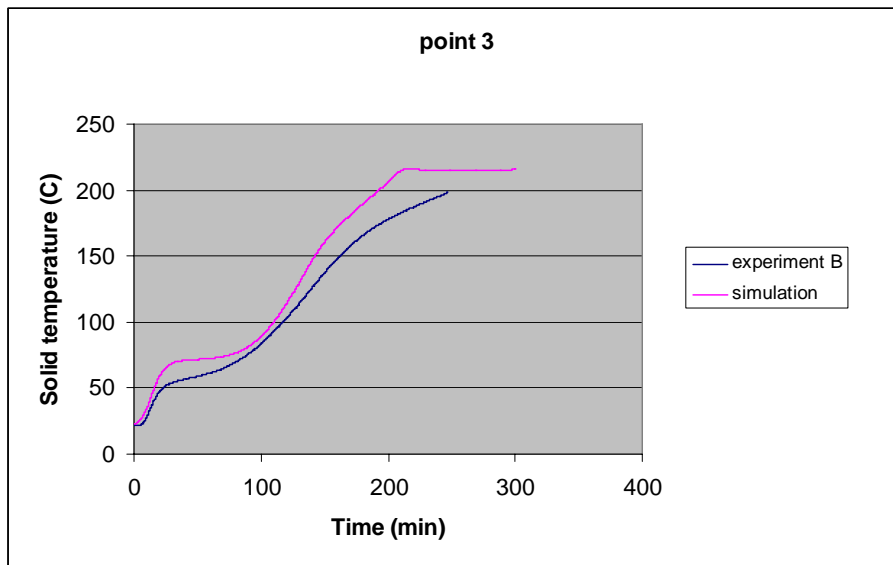
Graph 9. Comparison of the predicted and measured temperature (point 3).
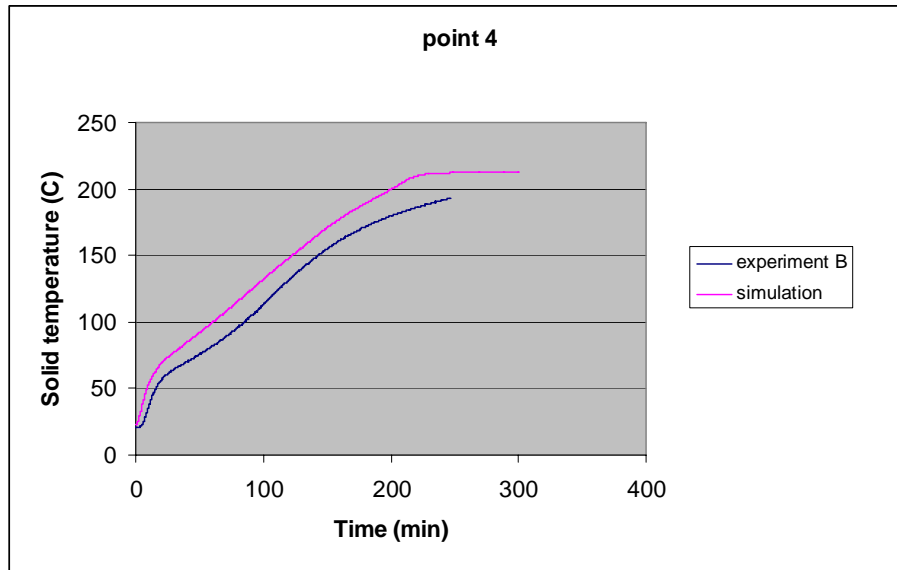
Graph 10. Comparison of the predicted and measured temperature (point 4).
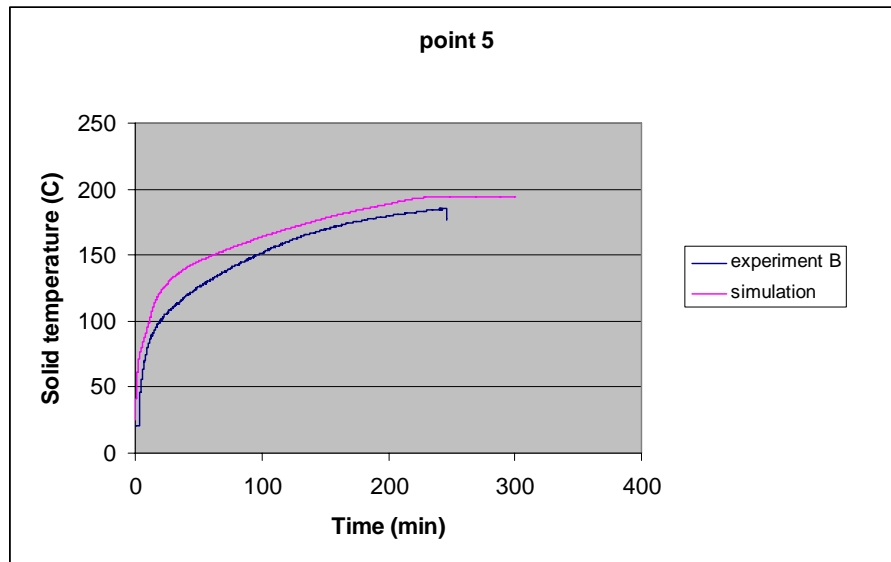
Graph 11. Comparison of the predicted and measured temperature (point 5).

3.3.2.6   Exploitation of the results

It was interesting to see the influence of some factors on the results of the simulation, for example the activation energy or QA (with Q the heat of reaction and A the pre-exponential factor of the Arrhenius law).

Influence of the factor QA
QA is difficult to calculate, that's why it is necessary to know if it changes the results, or if it is not very important. So a simulation with a QA lower of 50% (QA = 8E+08 J/kg.s) has been done (see Graph 12 and Graph 14). For the point 5, the temperature is the same. For the point 1, the temperature is the same until 8000 seconds (130 minutes), and then the temperature calculated with the lower QA is a little bit lower than the temperature calculated with QA = 16E+08 J/kg.s. But the results are similar; it means that to have a precise value for the factor QA is not so important.

Comparison of the basket heating test simulations - different QA (point 1)
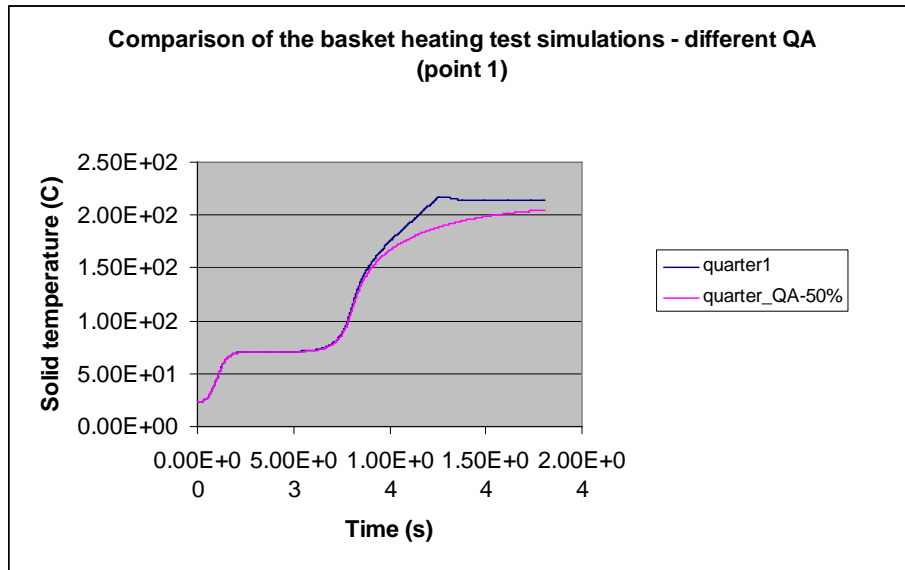
Graph 12. Comparisons of two simlations with a lower QA (point 1).

Comparison of the basket heating test simulations - different QA (point 3)
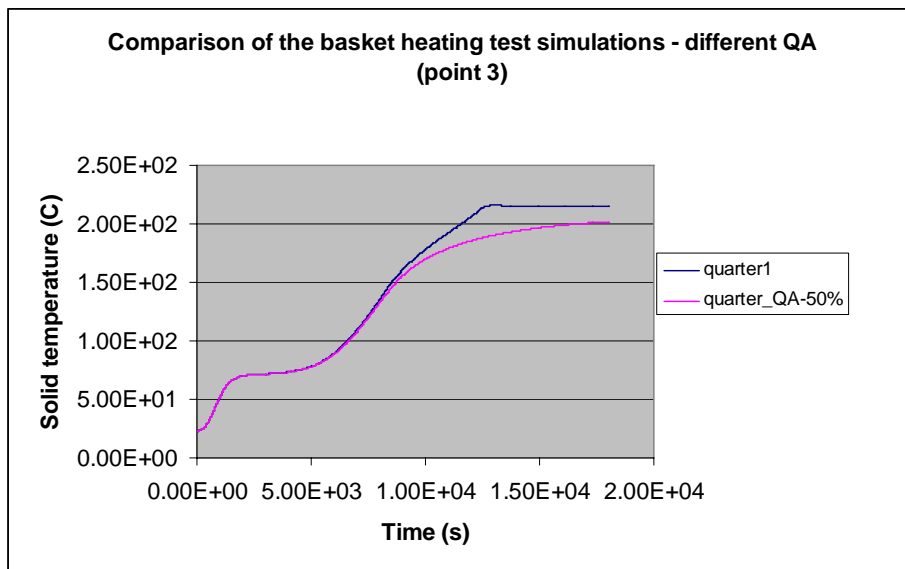
Graph 13. Comparison of two simulations with a lower QA (point 3).
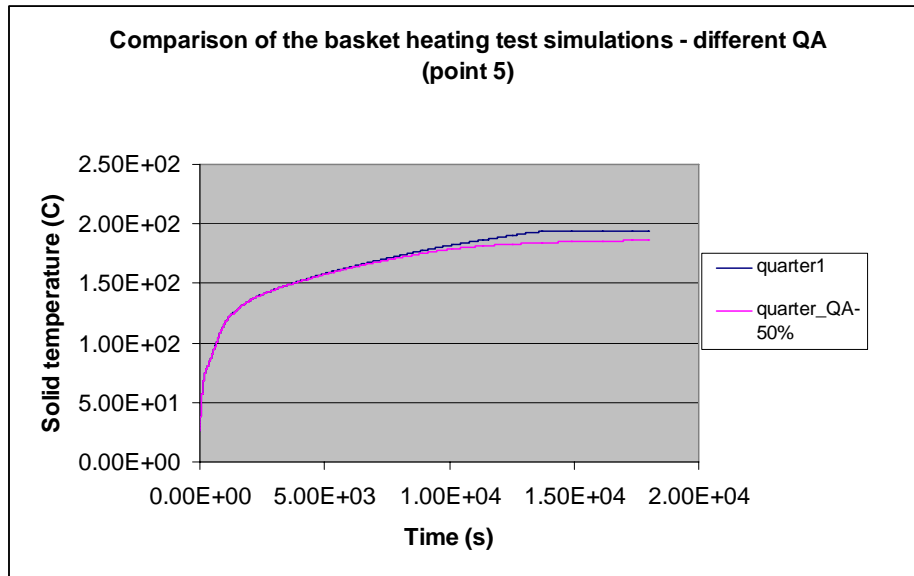
Graph 14. Comparison of two simulations with a lower QA (point 5).

We can see Graph 15, Graph 16, and Graph 17 the results of a simulation done with a QA upper of 50% (QA=24E+08 J/kg.s). We can note that after about 10000 seconds (167 minutes), the temperature for the two simulations is really different: the temperature calculated with QA=24E+08 J/kg.s is upper than the temperature calculated with QA=16E+08 J/kg.s.
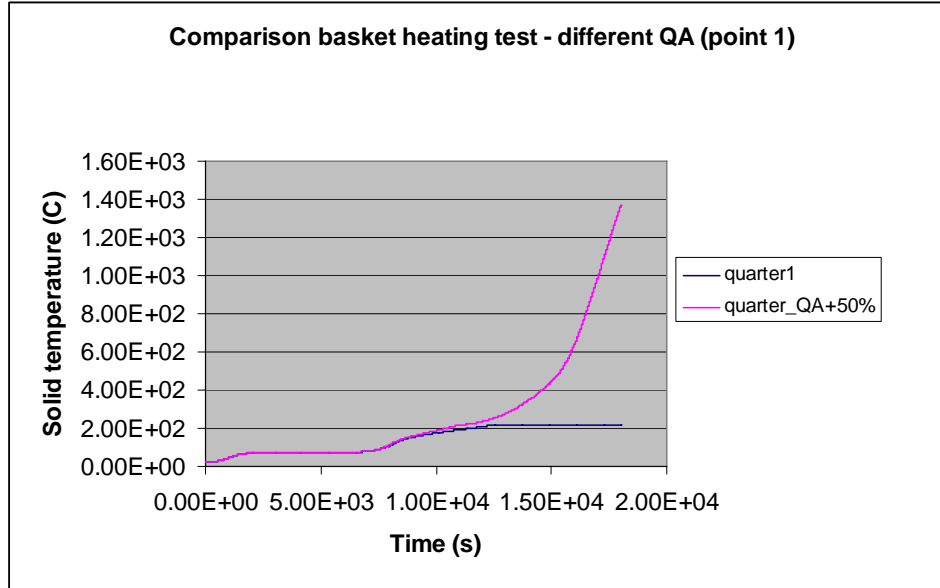
Graph 15. Comparison of two simulations with an upper QA (point 1).

Comparison basket heating test - different QA (point 3)
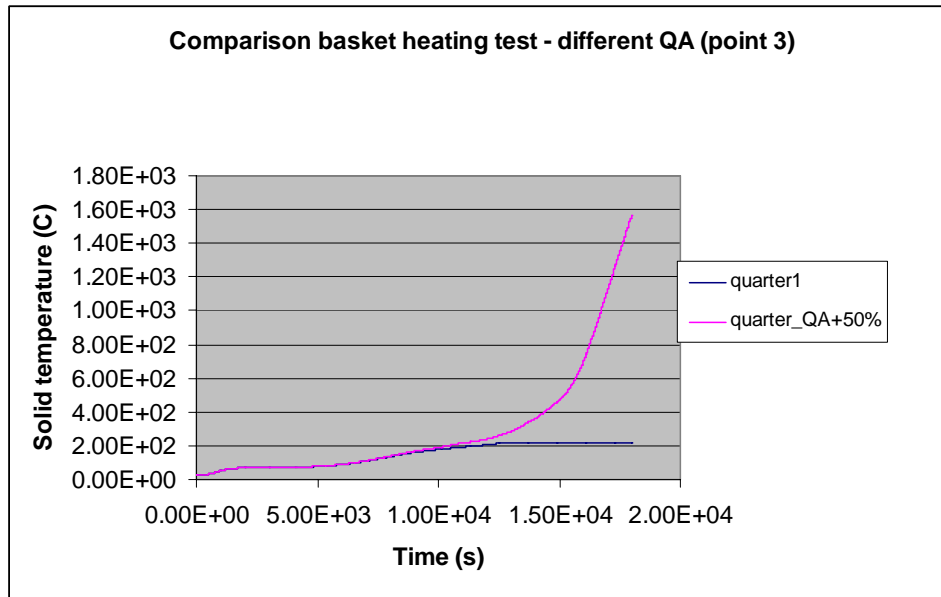
Graph 16. Comparison of two simulations with an upper QA (point 3).

Comparison basket heating test - different Q (point 5)
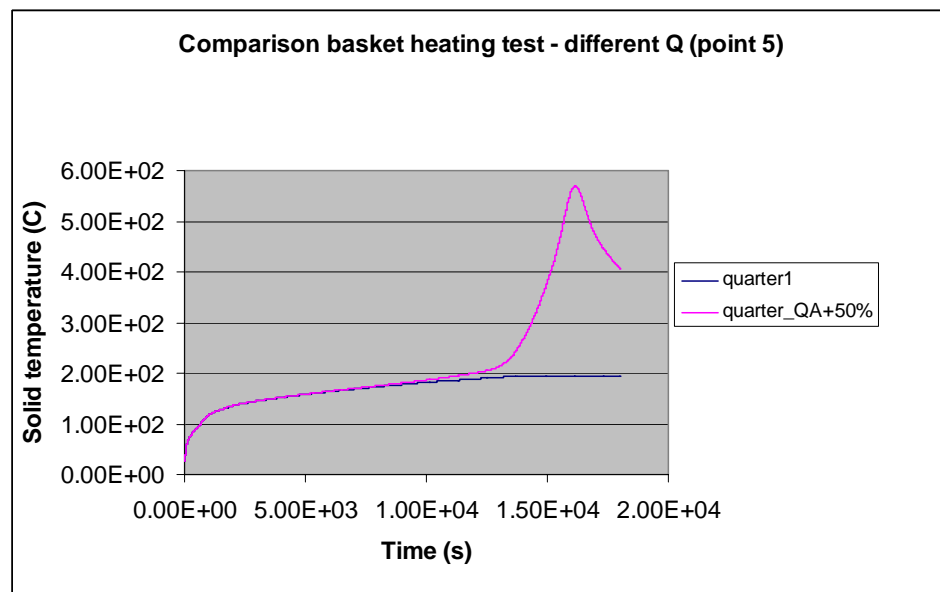
Graph 17. Comparison of two simulations with an upper QA (point 5).

It is interesting to see the influence of the factor QA on the solid heat production rate (see graphs).
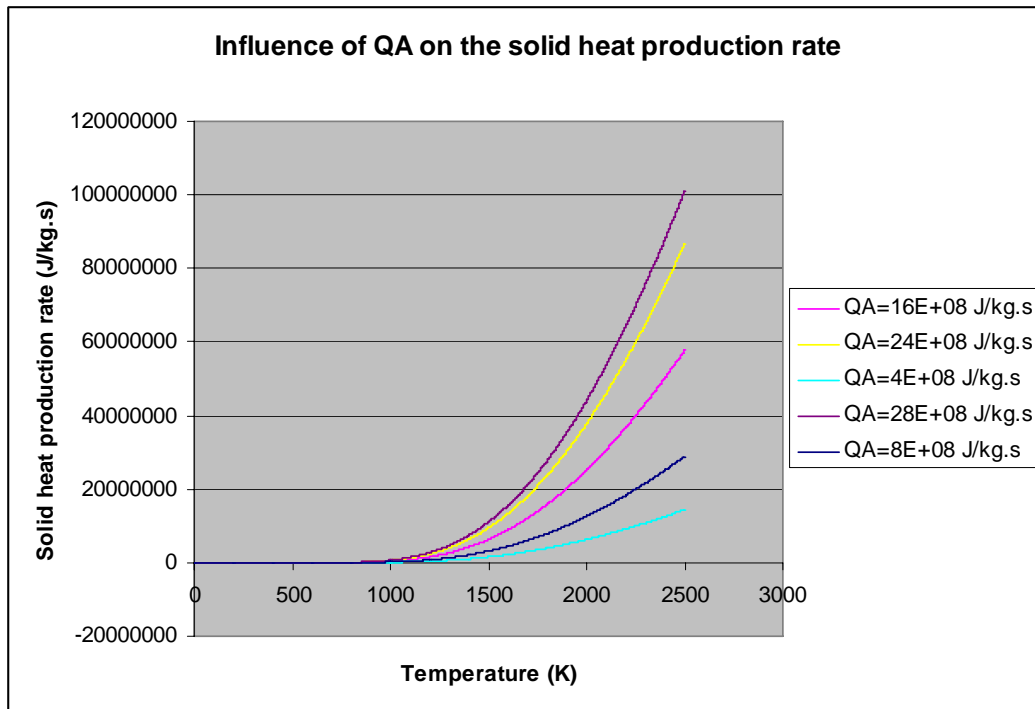
Graph 18. Influence of the QA.

The results of the simulations done with a QA lower and upper of 75% from the initial values can be seen Graph 19, Graph 20, Graph 21, Graph 22, Graph 23, andGraph 24.
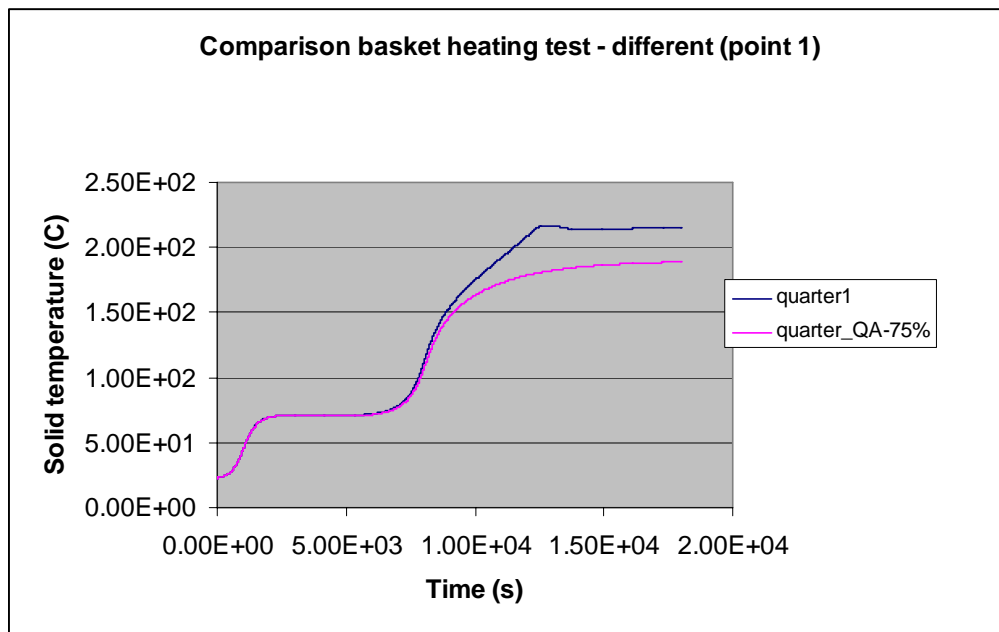
Graph 19. Comparison with a QA lower of 75% (point 1).
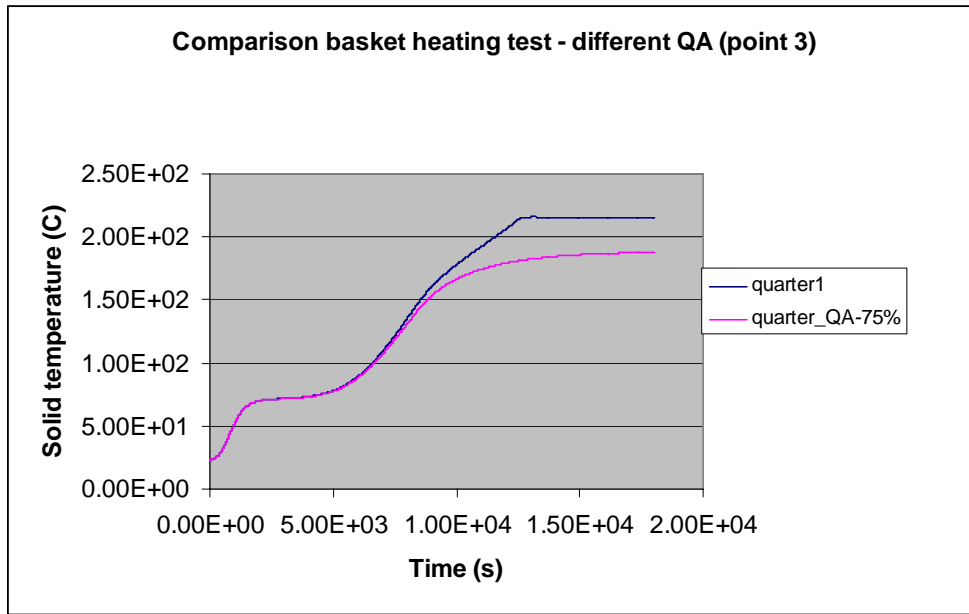
Graph 20. Comparison with a QA lower of 75% (point 3).
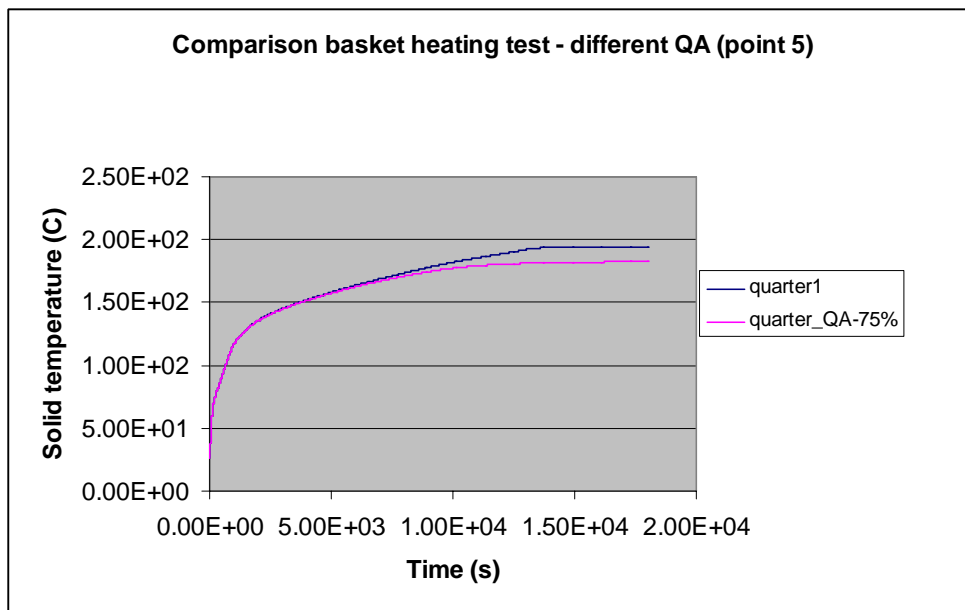
Graph 21. Comparison with a QA lower of 75% (point 5).

After 10000 seconds, the results of the simulation done with a QA upper of 75% is really different from the initial simulation.
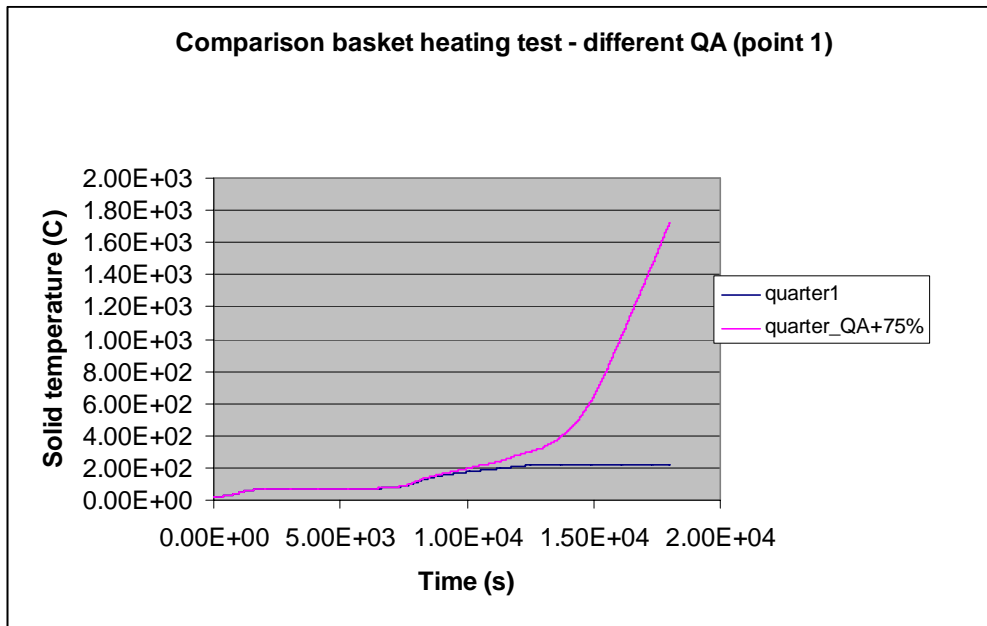
Graph 22. Comparison with a QA upper of 75% (point 1).
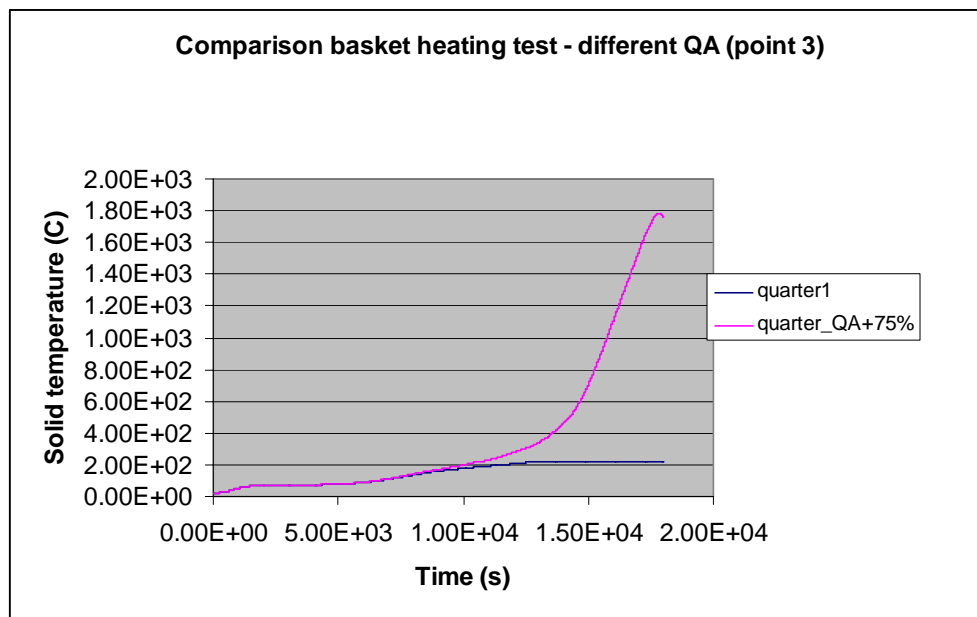
Graph 23. Comparison with a QA upper of 75% (point 3).
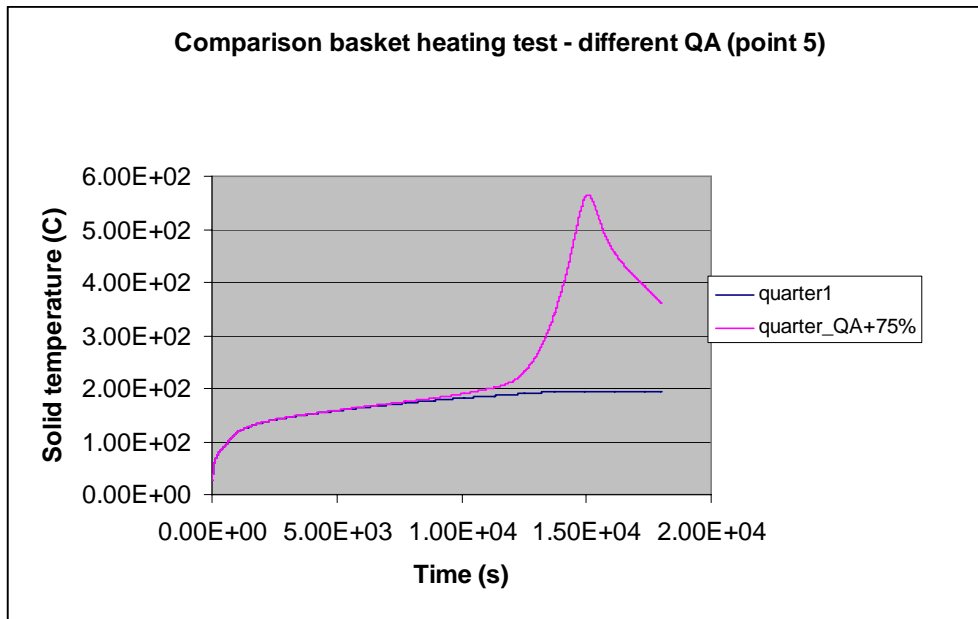
Graph 24. Comparison with a QA upper of 75% (point 5).

All these results concerning the factor QA can be summarize in the following graphs:
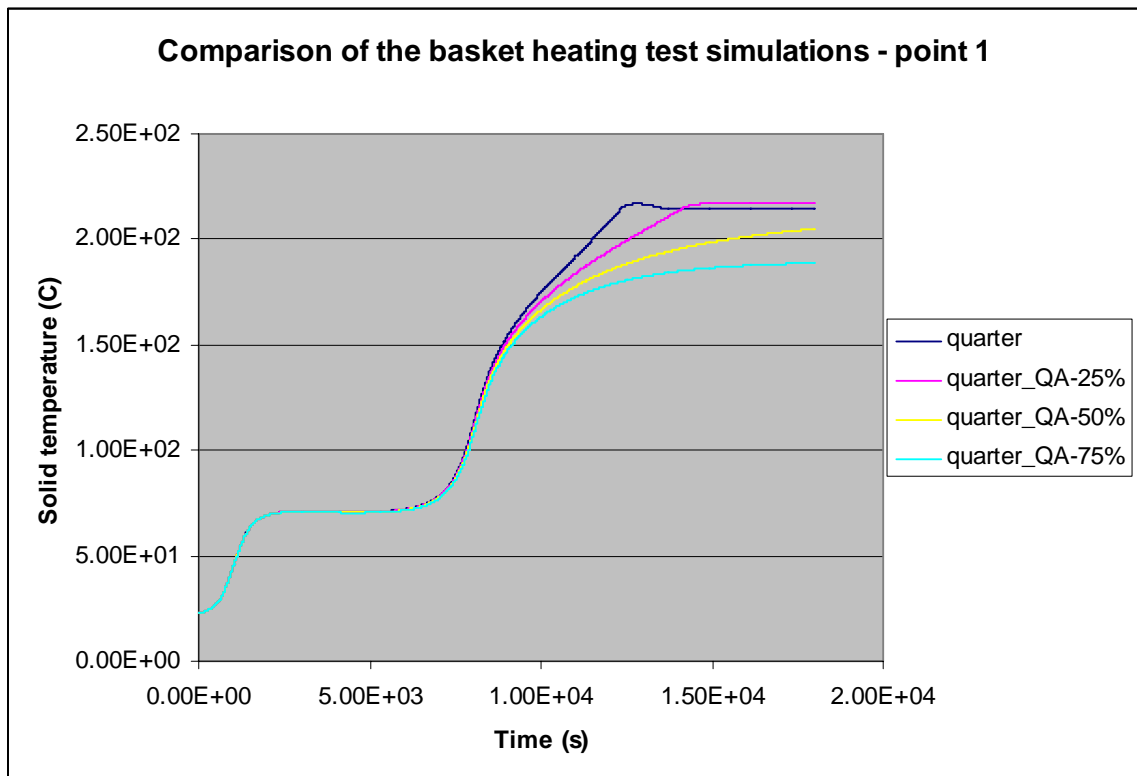
Graph 25. Plot of the simulations with different QA (point 1).

Comparison of the basket heating test simulations - point 1
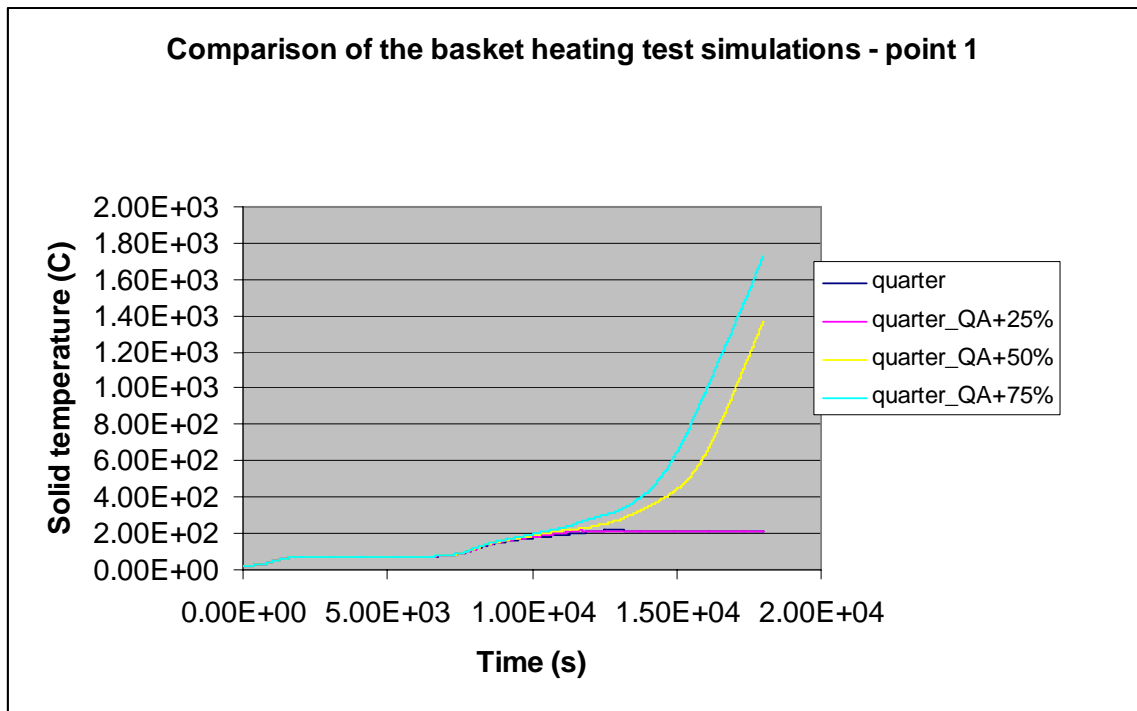
Graph 26. Plot of the simulations with different QA (point 1).

Influence of the activation energy E_a

First the simulation with an activation energy lower of 25% was made. The results are shown, Graph 27, Graph 28, and Graph 29. Before 10000 seconds, there is a big difference between the two simulations.

Comparison of the basket heating test simulations - different E (point 1)
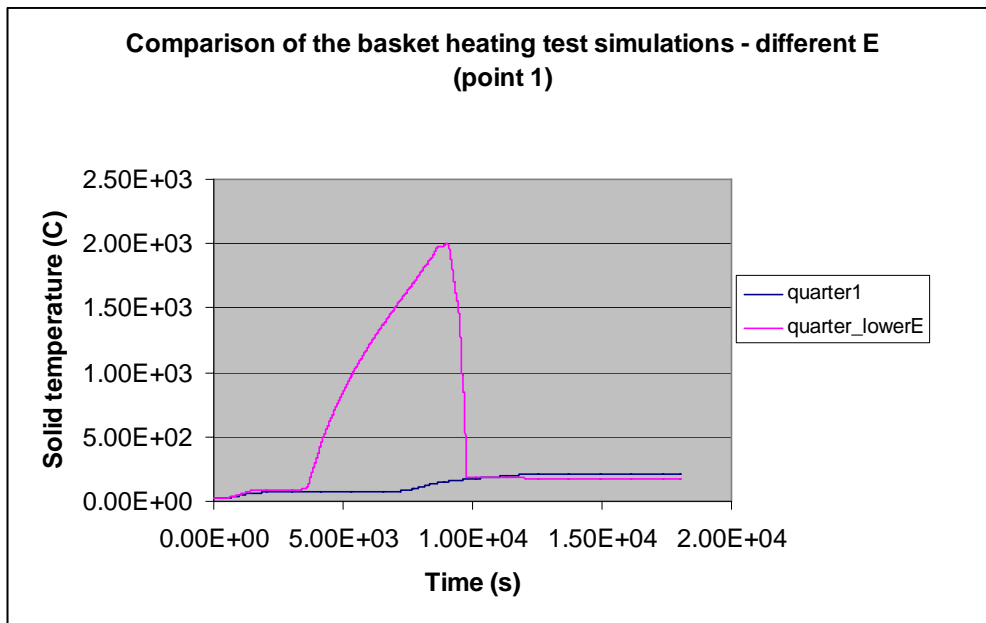
Graph 27. Comparison with a lower E (point 1).
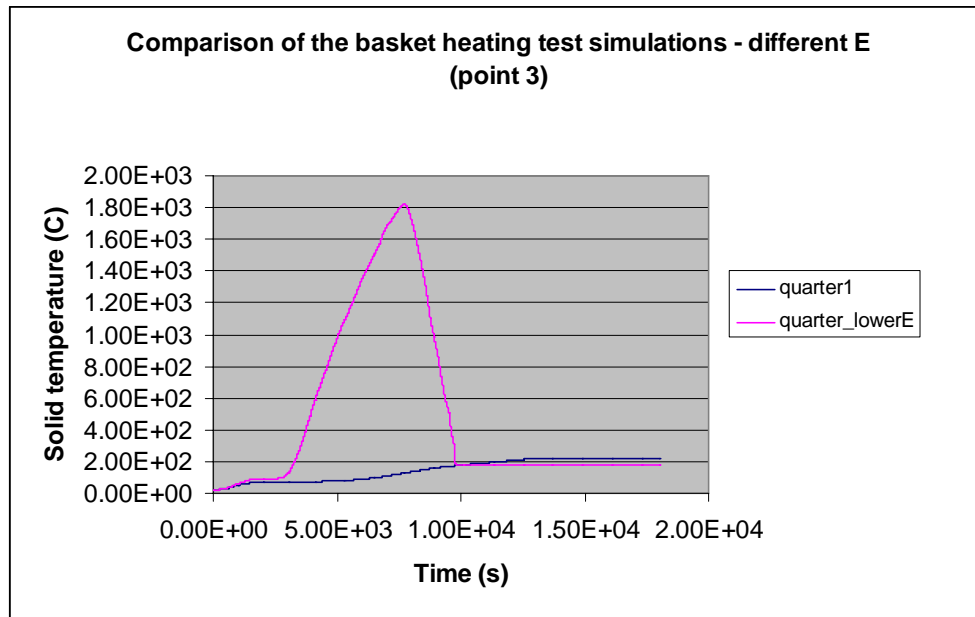
Graph 28. Comparison with a lower E (point 3).
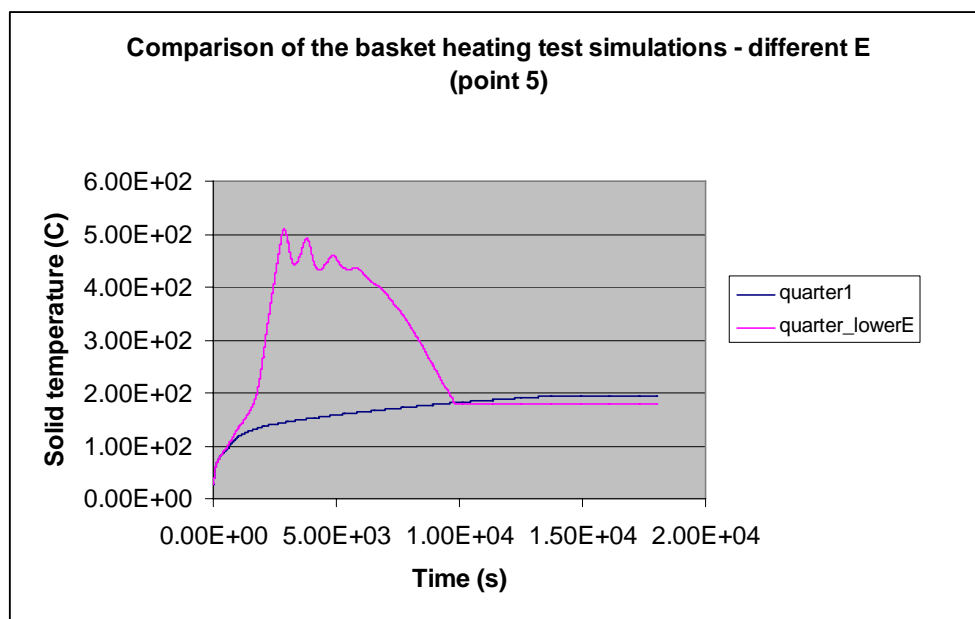
Graph 29. Comparison with a lower E (point 5).

Then a simulation with an activation energy upper of 25% was made (see Graph 308, Graph 319, and Graph 3230). The results are better that previously, they are quite similar.
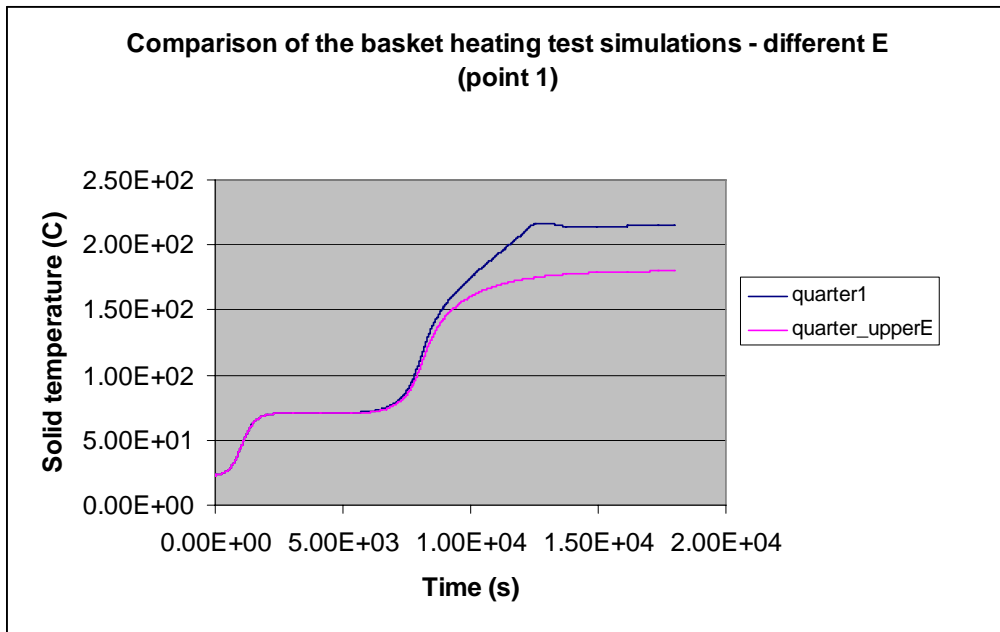
Graph 30. Comparison with an upper E (point 1).
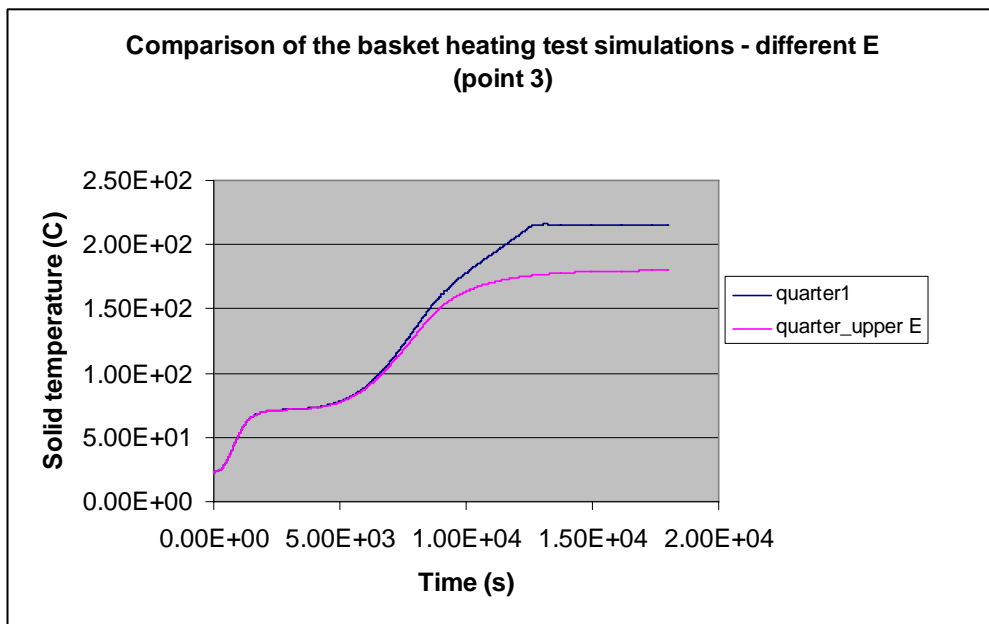
Graph 31. Comparison with an upper E (point 3).

Comparison of the basket heating test simulations - different E (point 5)
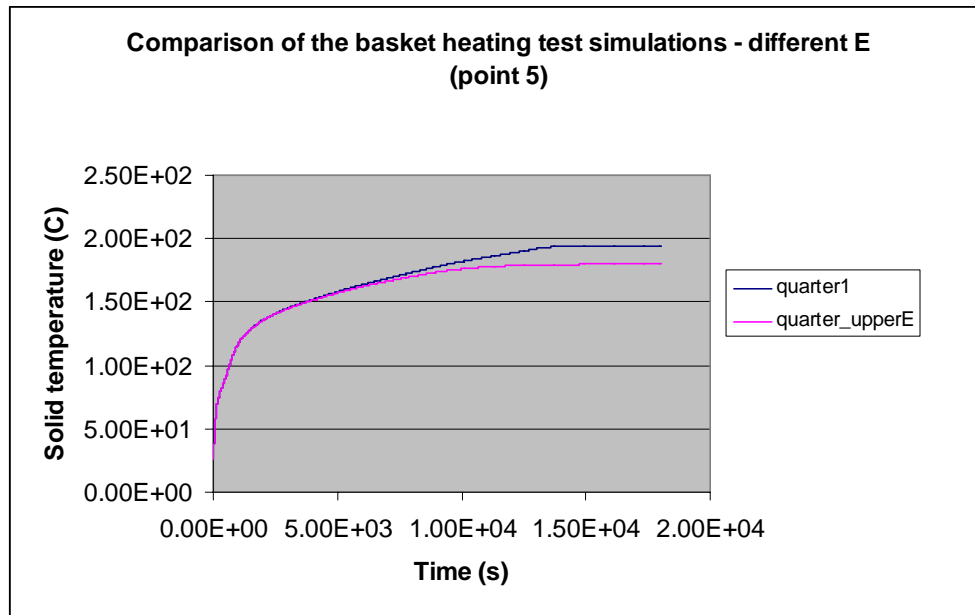
Graph 32. Comparison with an upper E (point 5).

It is possible to see the influence of the activation energy on the solid heat production rate, see graphs). The more the activation energy small is, the more the solid heat production rate changes (because of the exponential). That is why the results of the simulation made with a lower E_a are so different.

Influence of the Ea on the solid heat production rate
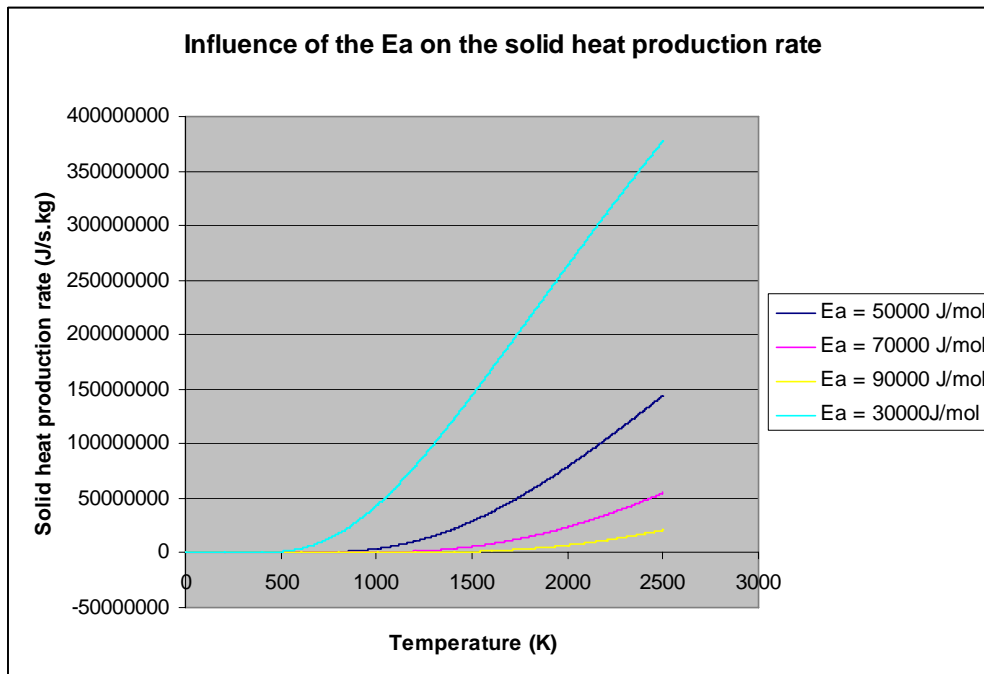
Graph 33. Influence of the activation energy.

The simulations with an activation energy lower of 50% and upper of 50% from the initial value can be done, see Graph 3432, Graph 3533, Graph 3634, Graph 3735, Graph 386, and Graph 397. We can note that the results obtained with an activation energy lower of 50% are similar of the results obtained with an activation energy lower of 25%;

and the results obtained with an activation energy upper of 50% are similar of the results obtained with an activation energy upper of 25%.
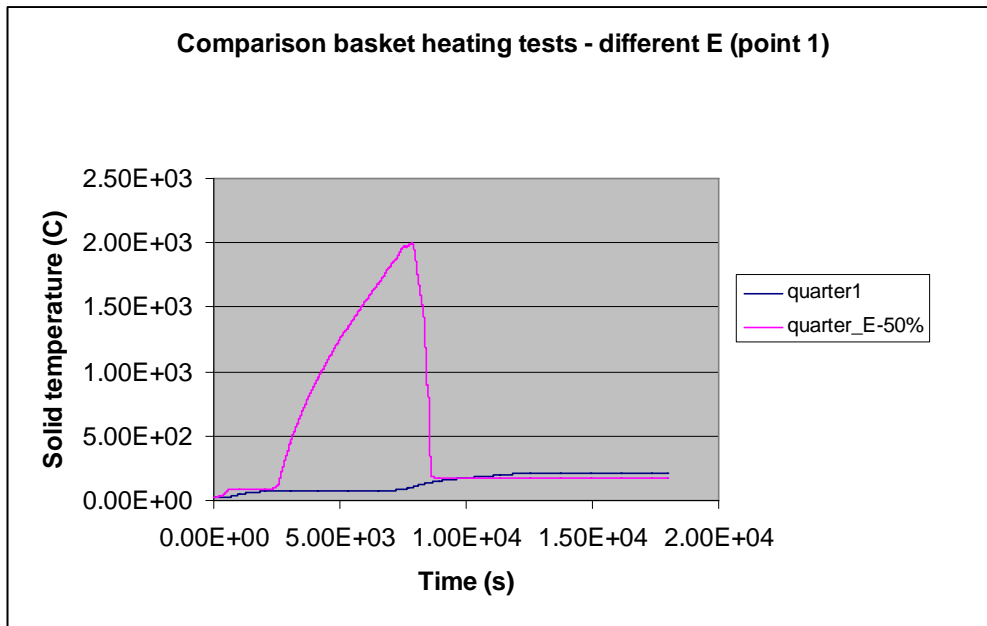
Graph 34. Comparison with an activation energy lower of 50% (point 1).
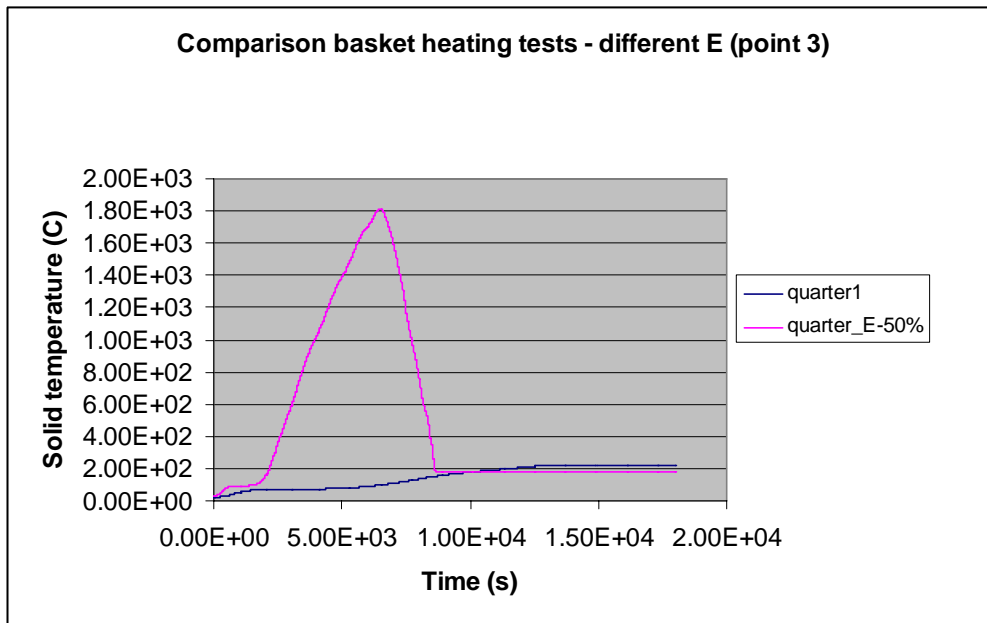
Graph 35. Comparison with an activation energy lower of 50% (point 3).
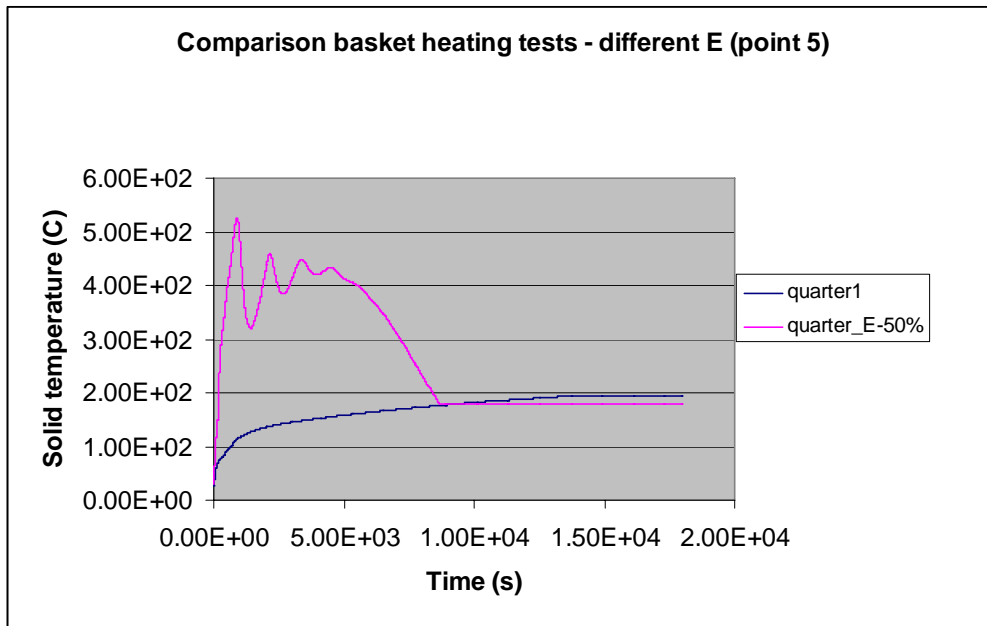
Graph 36. Comparison with an activation energy lower of 50% (point 5).
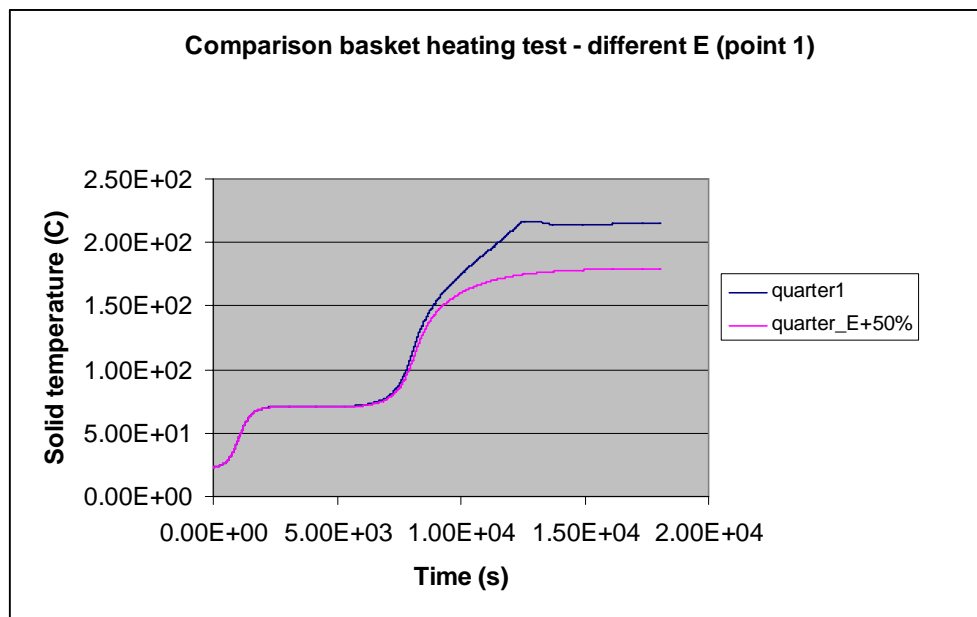
Graph 37. Comparison with an activation energy upper of 50% (point 1).
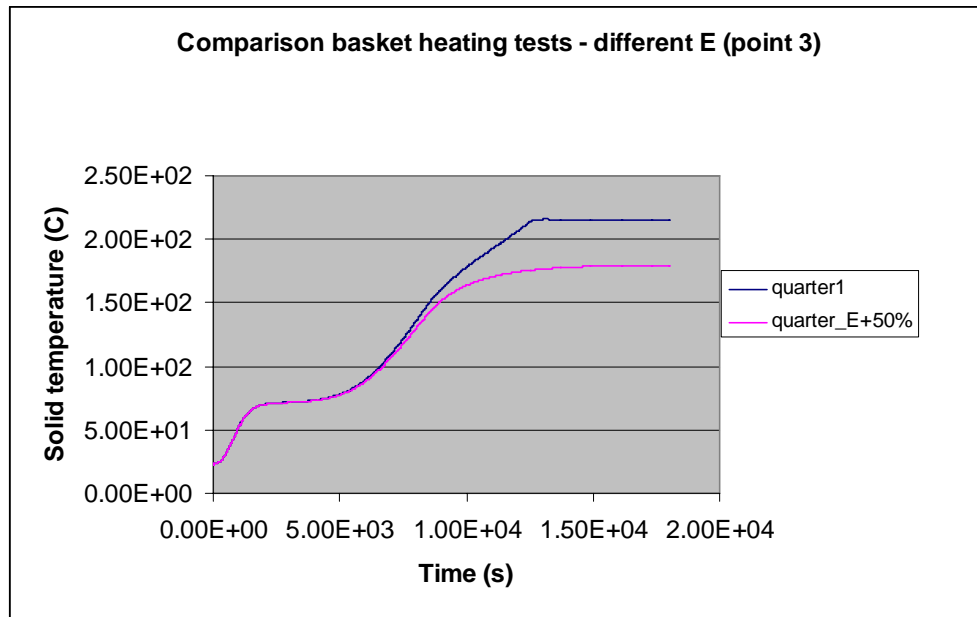
Graph 38. Comparison with an activation energy upper of 50% (point 3).
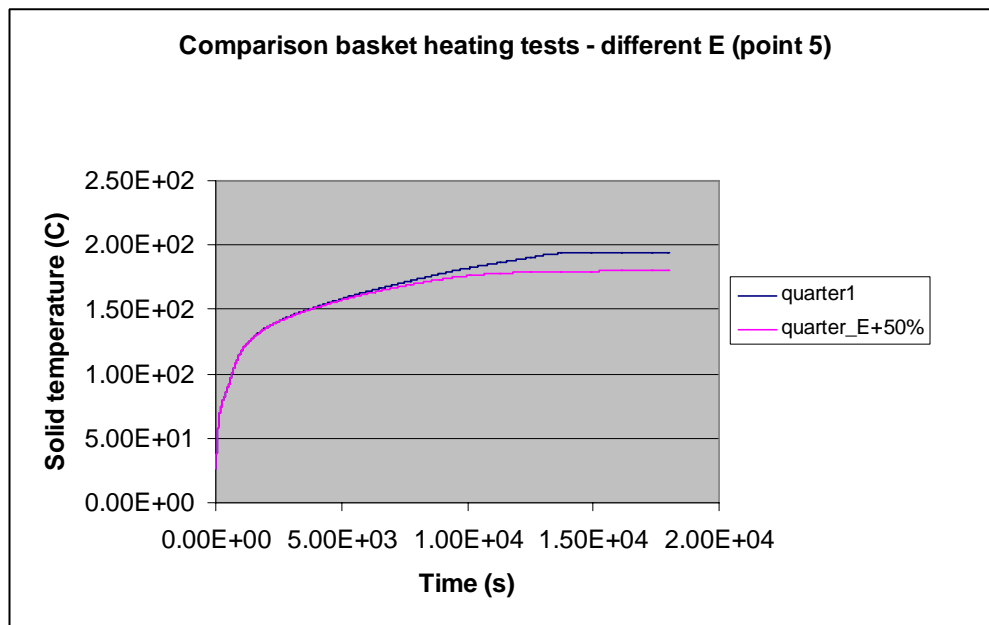
Graph 39. Comparison with an activation energy upper of 50% (point 5).

The following graphs summarize these simulations:
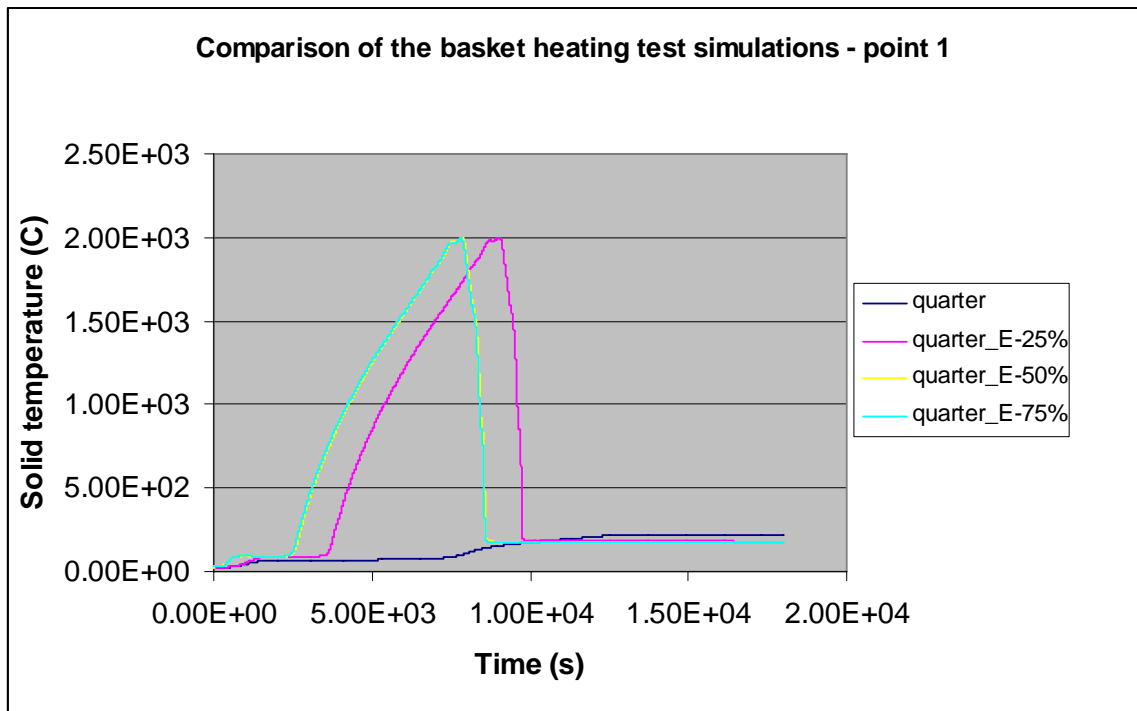
Graph 40. Plot of the simulations with different activation energy (point 1).
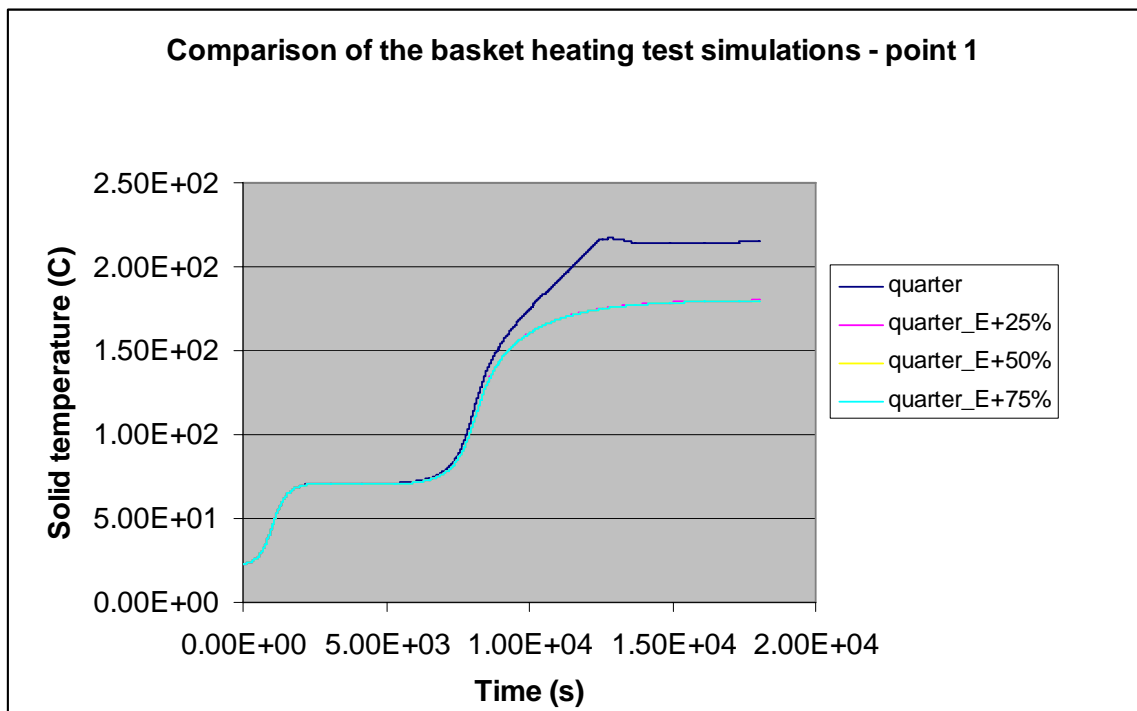
Graph 41. Plot of the simulations with different activation energy (point 1).

4   Conclusions

The new version of ConeTools, the more complete ConeTools 2.4, will be marketed as soon as possible. This new version contains:

- o   A new model for the heat release prediction (Hansen model)
- o   A model for the smoke production.

New forms are used, and it can notably recognize the ignition time in the Cone file. It is a user-friendly software program in Windows environment.

We can see the complexity of the spontaneous ignition problem, which is due to the strong coupling between flow, heat and mass transfer, water condensation/evaporation and chemical reactions. That's why it is difficult to establish a model. But the simulations done with a SMAFS seems to be a good alternative; based on numerical solution of the governing transport equations, the numerical computations were performed to simulate a small scale spontaneous ignition experiment. It has shown good results. Some factors have been modified, in order to see their influence on the results.

Following the meeting with the creator of the software, I could add some notes in the manual of SMAFS.

The next step with SMAFS will be to simulate a self ignition of bio fuels in a silo, using curvilinear coordinates.

Using ConeTools and SMAFS, I could do programming and I could learn how to use a CFD code. I think it will be useful for the following of my studies and for a job.

5   References

[1]. P. Van Hees, T. Hertzberg, A. Steen Hansen, "Development of a screening method for the SBI and Room Corner using the Cone Calorimeter", Nordtest project 1479-00, November 2002.

[2]. B. Sundström, P. Van Hees, P. Thureson, "Results and analysis from fire tests of building products in ISO 9705, the Room/Corner test", SBI Research Programme, November 1998.

[3]. H. K. Versteeg, W. Malalasekera, "An introduction to Computational Fluid Dynamics", 1995.

[4]. P. Blomqvist, B. Persson, "Spontaneous ignition of biofuels – a literature survey of theoretical and experimental methods", 2003.

[5]. Z. Yan, P. Blomqvist, U. Göransson, G. Holmstedt, L. Wadsö, P. Van Hees, "Validation of CFD model for simulation of spontaneous ignition in bio-mass fuel storage".

[6]. Z. Yan, "Numerical modeling of turbulent combustion and flame spread".

Annex A. Classes for products excluding floorings

Class	Test method(s)	Classification criteria	Additional classification
A1	EN ISO 1182 ([1]); *And*	$\Delta T \le 30°C$; *and* $\Delta m \le 50\%$; *and* $t_f = 0$ (i.e. no sustained flaming)	-
	EN ISO 1716	$PCS \le 2.0$ MJ.kg^{-1} ([1]); *and* $PCS \le 2.0$ MJ.kg^{-1} ([2]) ([2a]); *and* $PCS \le 1.4$ MJ.m^{-2} ([3]); *and* $PCS \le 2.0$ MJ.kg^{-1} ([4])	-
A2	EN ISO 1182 ([1]); *Or*	$\Delta T \le 50°C$; *and* $\Delta m \le 50\%$; *and* $t_f \le 20s$	-
	EN ISO 1716; *and*	$PCS \le 3.0$ MJ.kg^{-1} ([1]); *and* $PCS \le 4.0$ MJ.m^{-2} ([2]); *and* $PCS \le 4.0$ MJ.m^{-2} ([3]); *and* $PCS \le 3.0$ MJ.kg^{-1} ([4])	-
	EN 13823 (SBI)	FIGRA ≤ 120 W.s^{-1}; *and* LFS < edge of specimen; *and* THR$_{600s}$ ≤ 7.5 MJ	Smoke production([5]); *and* Flaming droplets/ particles ([6])
B	EN 13823 (SBI); *And*	FIGRA ≤ 120 W.s^{-1}; *and* LFS < edge of specimen; *and* THR$_{600s}$ ≤ 7.5 MJ	Smoke production([5]); *and* Flaming droplets/ particles ([6])
	EN ISO 11925-2([8]): *Exposure = 30s*	Fs ≤ 150mm within 60s	
C	EN 13823 (SBI); *And*	FIGRA ≤ 250 W.s^{-1}; *and* LFS < edge of specimen; *and* THR$_{600s}$ ≤ 15 MJ	Smoke production([5]); *and* Flaming droplets/ particles ([6])
	EN ISO 11925-2([8]): *Exposure = 30s*	Fs ≤ 150mm within 60s	
D	EN 13823 (SBI); *And*	FIGRA ≤ 750 W.s^{-1}	Smoke production([5]); *and* Flaming droplets/ particles ([6])
	EN ISO 11925-2([8]): *Exposure = 30s*	Fs ≤ 150mm within 60s	
E	EN ISO 11925-2([8]): *Exposure = 15s*	Fs ≤ 150mm within 20s	Flaming droplets/ particles ([7])
F	No performance determined		

(*) The treatment of some families of products, e.g. linear products (pipes, ducts, cables etc.), is still under review and may necessitate an amendment to this decision.

([1]) For homogeneous products and substantial components of non-homogeneous products.

([2]) For any external non-substantial component of non-homogeneous products.

([2a]) Alternatively, any external non-substantial component having a PCS ≤ 2.0 MJ.m^{-2}, provided that the product satisfies the following criteria of EN 13823(SBI) : FIGRA ≤ 20 W.s^{-1}; *and* LFS < edge of specimen; *and* THR$_{600s}$ ≤ 4.0 MJ; *and* s1; *and* d0.

([3]) For any internal non-substantial component of non-homogeneous products.

([4]) For the product as a whole.

([5]) **s1** = SMOGRA ≤ 30m^2.s^{-2} *and* TSP$_{600s}$ ≤ 50m^2 ; **s2** = SMOGRA ≤ 180m^2.s^{-2} *and* TSP$_{600s}$ ≤ 200m^2; **s3** = not s1 or s2.

([6]) **d0** = No flaming droplets/ particles in EN13823 (SBI) within 600s; **d1** = No flaming droplets/ particles persisting longer than 10s in EN13823 (SBI) within 600s; **d2** = not d0 or d1; Ignition of the paper in EN ISO 11925-2 results in a d2 classification.

([7]) Pass = no ignition of the paper (no classification); Fail = ignition of the paper (**d2** classification).

([8]) Under conditions of surface flame attack and, if appropriate to end–use application of product, edge flame attack.

Annex B. Classes of reaction to fire performance for floorings

Class	Test method(s)	Classification criteria	Additional classification
A1_{FL}	EN ISO 1182 ([1]); *And*	$\Delta T \leq 30°C$; *and* $\Delta m \leq 50\%$; *and* $t_f = 0$ (i.e. no sustained flaming)	-
	EN ISO 1716	$PCS \leq 2.0$ MJ.kg^{-1} ([1]); *and* $PCS \leq 2.0$ MJ.kg^{-1} ([2]); *and* $PCS \leq 1.4$ MJ.m^{-2} ([3]); *and* $PCS \leq 2.0$ MJ.kg^{-1} ([4])	-
A2_{FL}	EN ISO 1182 ([1]); *Or*	$\Delta T \leq 50°C$; *and* $\Delta m \leq 50\%$; *and* $t_f \leq 20s$	-
	EN ISO 1716; *and*	$PCS \leq 3.0$ MJ.kg^{-1} ([1]); *and* $PCS \leq 4.0$ MJ.m^{-2} ([2]); *and* $PCS \leq 4.0$ MJ.m^{-2} ([3]); *and* $PCS \leq 3.0$ MJ.kg^{-1} ([4])	-
	EN ISO 9239-1 ([5])	Critical flux ([6]) ≥ 8.0 kW.m^{-2}	Smoke production ([7])
B_{FL}	EN ISO 9239-1 ([5]) *and*	Critical flux ([6]) ≥ 8.0 kW.m^{-2}	Smoke production ([7])
	EN ISO 11925-2([8]): *Exposure = 15s*	$Fs \leq 150mm$ within 20s	
C_{FL}	EN ISO 9239-1 ([5]) *And*	Critical flux ([6]) ≥ 4.5 kW.m^{-2}	Smoke production ([7])
	EN ISO 11925-2([8]): *Exposure = 15s*	$Fs \leq 150mm$ within 20s	
D_{FL}	EN ISO 9239-1 ([5]) *And*	Critical flux ([6]) ≥ 3.0 kW.m^{-2}	Smoke production ([7])
	EN ISO 11925-2([8]): *Exposure = 15s*	$Fs \leq 150mm$ within 20s	
E_{FL}	EN ISO 11925-2([8]): *Exposure = 15s*	$Fs \leq 150mm$ within 20s	-
F_{FL}	No performance determined		

([1]) For homogeneous products and substantial components of non-homogeneous products.

([2]) For any external non-substantial component of non-homogeneous products.

([3]) For any internal non-substantial component of non-homogeneous products.

([4]) For the product as a whole.

([5]) Test duration = 30 minutes.

([6]) Critical flux is defined as the radiant flux at which the flame extinguishes or the radiant flux after a test period of 30 minutes, whichever is the lower (i.e. the flux corresponding with the furthest extent of spread of flame).

([7]) **s1** = Smoke $\leq 750\%$.min; **s2** = not s1.

([8]) Under conditions of surface flame attack and, if appropriate to the end–use application of the product, edge flame attack.

Annex C. Comparison of the FIGRA, the THR, the flashover time and the classes between the simulation (from the ignition time) and the experiment using ConeTools 2.3 – SwRI project

Product	FIGRA exp (W/s)	FIGRA simulation (W/s)				THR 600s exp (MJ)	THR 600s simulation (MJ)			
		run1	run 2	run 3	mean		run 1	run 2	run 3	mean
Douglas fir plywood	393	396.2	449.7	506.5	450.8	22.3	30.3	32.4	34.6	32.43333
FRT Douglas fir plywood	142	257.6	159.8	314.4	243.9333	6.5	15.3	17.6	15.6	16.16667
Glassfiber reinforced plastic	1511	936.4	720	774.7	810.3667	64.1	28.7	28.4	28.6	28.56667
Type X gypsum board	21	0	0	29.5	9.833333	0.8	0.5	0.4	0.7	0.533333
Polyisocyanurate foam	3101	3111.5	2426.3	2792.6	2776.8	5.2	8.7	11.2	9	9.633333
Vinyl wall covering	213	353.2	332.2	311.8	332.4	2.4	1	1.2	1.2	1.133333
Textile wall covering	-	402.8	469.1	486.4	452.7667	-	2.5	1.9	2.9	2.433333
Paper wall covering	-	56.7	38.9	33.9	43.16667	-	0.6	0.5	0.3	0.466667
Oriented Strand Board 1 (LP)	567	602.6	576.4	-	589.5	45.9	47.6	48.2	-	47.9
Oriented Strand Board 2 (weyerhaeuser)	458	562.2	468.9	-	515.55	36.5	42.2	41.1	-	41.65
White pine boards	455	685.3	509.2	-	597.25	25.8	28.8	28.2	-	28.5
White oak boards	286	311.6	340.6	-	326.1	22.6	24	25.9	-	24.95

Table 2. Comparison of the FIGRA and the THR.

Product	Flashover time exp (s)	Flashover time simulation (s)				Class experiment	Class simulation		
		run 1	run 2	run 3	mean		run 1	run 2	run 3
Douglas fir plywood	165	196	176	164	178.6667	D,s1,d0	D	D	D
FRT Douglas fir plywood	638	315	366	270	317	C,s1,d0	D	D	D
Glassfiber reinforced plastic	134	134	162	149	148.3333	E or F	E or worse	D	E or worse
Type X gypsum board	NF	>1200	>1200	>1200	>1200	A2,s1,d0 or B,s1,d0	A2/B	A2/B	A2/B
Polyisocyanurate foam	15	21	23	22	22	E or F	E or worse	E or worse	E or worse
Vinyl wall covering	640	668	675	687	676.6667	C,s2,d0	D	D	D
Textile wall covering	NF	119	131	129	126.3333	-	D	D	D
Paper wall covering	NF	>1200	>1200	>1200	>1200	-	A2/B	A2/B	A2/B
Oriented Strand Board 1 (LP)	-	150	158	-	154	D,s1,d0	D	D	-
Oriented Strand Board 2 (weyerhaeuser)	135	151	172	-	161.5	D,s1,d0	D	D	-
White pine boards	-	129	156	-	142.5	D,s1,d0	D	D	-
White oak boards	-	223	212	-	217.5	D,s1,d0	D	D	-

Table 3. Comparison of the flashover time and the classes.

Annex D. Plots of the FIGRA, the THR and the flashover time – SwRI Project
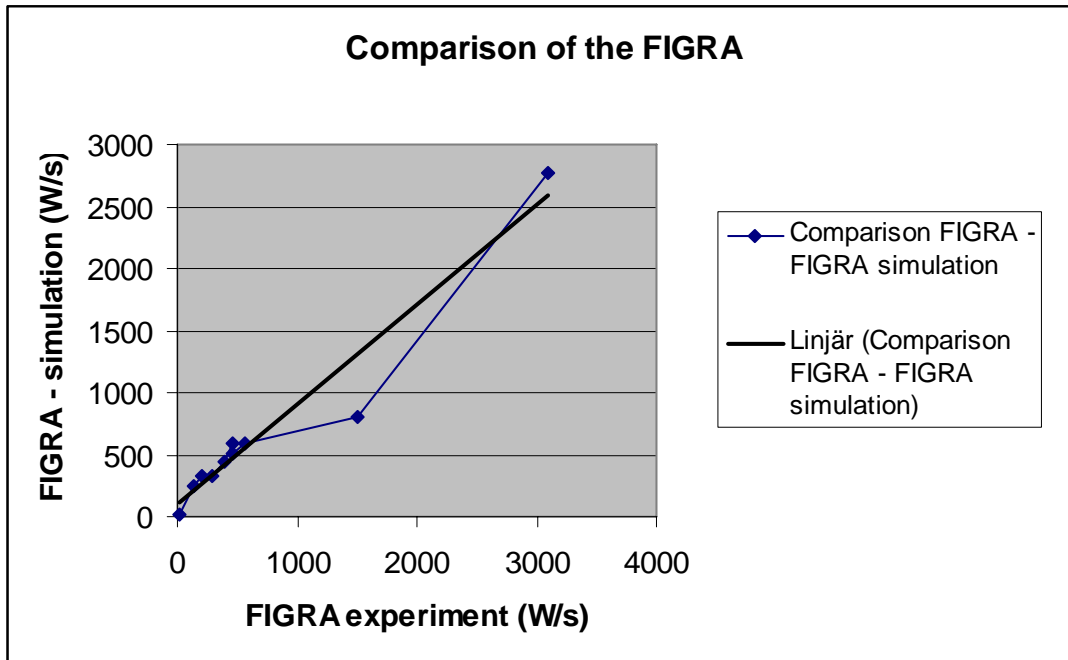
Graph 42. Comparison of the FIGRA between the experiment and the simulation.
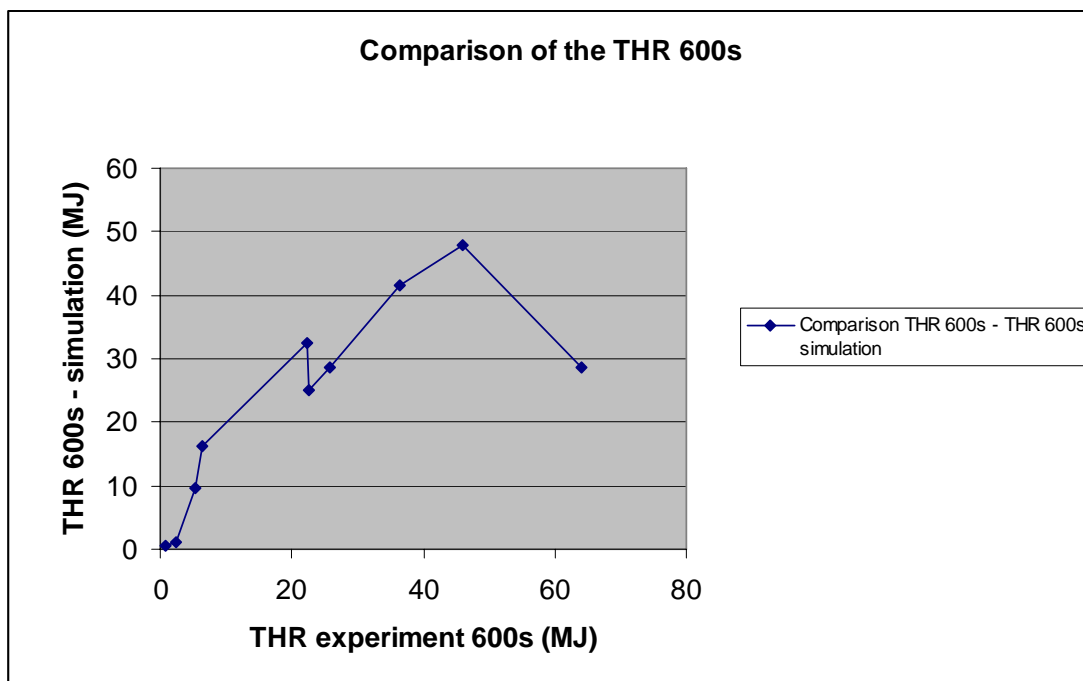
Graph 43. Comparison of the THR between the experiment and the simulation.

Comparison of the flashover times
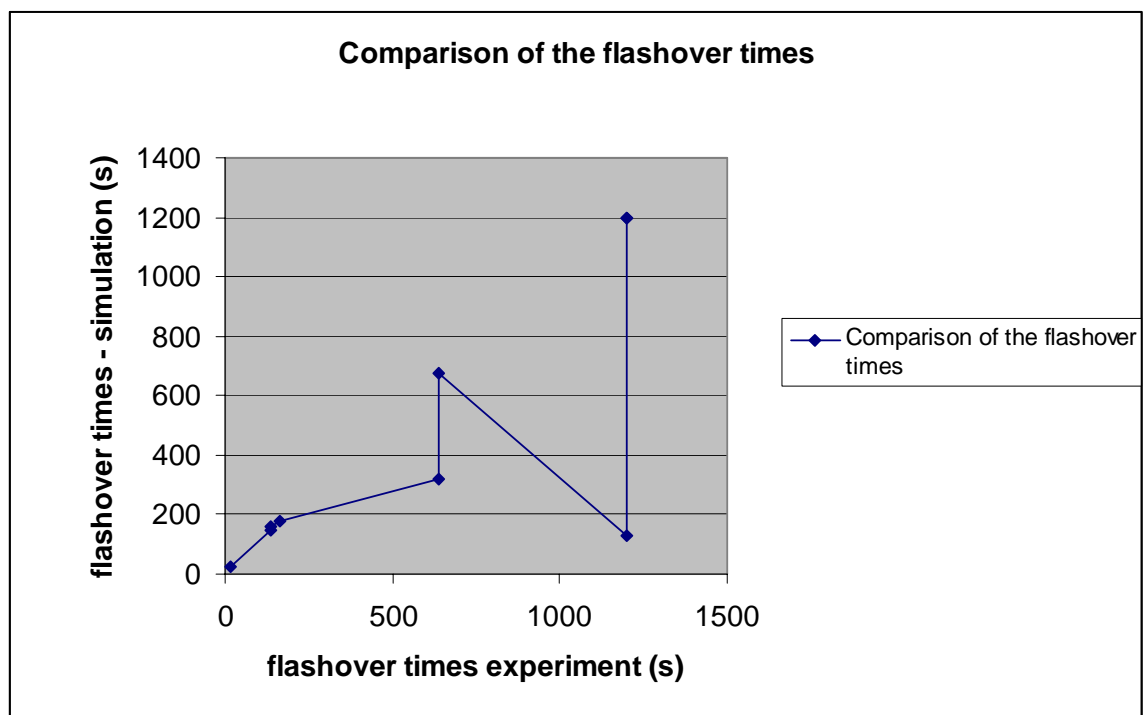
Graph 44. Comparison of the flashover times between the experiment and the simulation.

Annex E. Comparison of the FIGRA, the THR, the flashover time and the classes between the simulation (from the HRR) and the experiment using ConeTools 2.3 – SwRI project

Product	FIGRA exp (W/s)	FIGRA simulation (W/s)				THR 600s exp (MJ)	THR 600s simulation (MJ)			
		run1	run 2	run 3	mean		run 1	run 2	run 3	mean
Douglas fir plywood	393	316.5	372	424.1	370.8667	22.3	28.8	31.4	33.6	31.26667
FRT Douglas fir plywood	142	163.4	128.6	197.1	163.0333	6.5	14.2	16.7	14.9	15.26667
Glassfiber reinforced plastic	1511	823.8	644.1	678.3	715.4	64.1	28.6	28.2	28.5	28.43333
Type X gypsum board	21	0	0	23.1	7.7	0.8	0.5	0.3	0.7	0.5
Polyisocyanurate foam	3101	1292.7	820.6	987.1	1033.467	5.2	8.6	6.4	5.2	6.733333
Vinyl wall covering	213	236.7	234.2	202	224.3	2.4	0.9	1.2	1.2	1.1
Textile wall covering	-	194.9	277.5	205.7	226.0333	-	1.6	1.9	1.6	1.7
Paper wall covering	-	37.1	0	0	12.36667	-	0.6	0.4	0.3	0.433333
Oriented Strand Board 1 (LP)	567	469.4	459.6	-	464.5	45.9	44.3	45.4	-	44.85
Oriented Strand Board 2 (weyerhaeuser)	458	423.4	362.5	-	392.95	36.5	39.7	38.4	-	39.05
White pine boards	455	504	358.3	-	431.15	25.8	27.6	26.4	-	27
White oak boards	286	228.1	271.4	-	249.75	22.6	22.5	24.7	-	23.6

Table 4. Comparison of the FIGRA and the THR.

Product	Flashover time exp(s)	Flashover time simulation (s)				Class experiment	Class simulation		
		run 1	run 2	run 3	mean		run 1	run 2	run 3
Douglas fir plywood	165	230	202	187	206.3333	D,s1,d0	D	D	D
FRT Douglas fir plywood	638	443	447	418	436	C,s1,d0	C	D	C
Glassfiber reinforced plastic	134	147	176	167	163.3333	E or F	E or worse	D	D
Type X gypsum board	NF	>1200	>1200	>1200	>1200	A2,s1,d0 or B,s1,d0	A2/B	A2/B	A2/B
Polyisocyanurate foam	15	72	211	261	181.3333	E or F	E or worse	E or worse	E or worse
Vinyl wall covering	640	>1200	>1200	>1200	>1200	C,s2,d0	C	C	C
Textile wall covering	NF	>1200	683	>1200	-	-	C	D	C
Paper wall covering	NF	>1200	>1200	>1200	>1200	-	A2/B	A2/B	A2/B
Oriented Strand Board 1 (LP)	-	181	187	-	184	D,s1,d0	D	D	-
Oriented Strand Board 2 (weyerhaeuser)	135	187	210	-	198.5	D,s1,d0	D	D	-
White pine boards	-	165	207	-	186	D,s1,d0	D	D	-
White oak boards	-	289	256	-	272.5	D,s1,d0	D	D	-

Table 5. Comparison of the flashover times and the classes.

Annex F. Analysis of the results – SwRI Project

Specimens of 12 construction products were tested according to the Steiner Tunnel, the Room Corner and the Single Burning Item tests in the Southwest Research Institute, in order to predict the performance of construction products.

These test results can be compared with simulations, which are done from data of the Cone Calorimeter test. That's how we can see if simulations are close to the reality.
The simulations are made with a software named ConeTools.
There are two manners to define ignition properties: to indicate the visual ignition time or the heat release rate threshold.

First we can do the comparison between the test results and the simulations from the ignition time.

The comparison of the fire growth rating (FIGRA), the total heat release over the first 10 minutes of the test (THR $_{600s}$), the flashover time and the Euroclass is presented in table 1.
The FIGRA and the THR $_{600s}$ of the textile wall covering and the paper wall covering are missing, because the SBI tests were in progress.

We can see that the simulation is quite good concerning the class: the classes are the same as the tests results except for the FRT Douglas fir plywood, the vinyl wall covering and for the glassfiber reinforced plastic (only for the run 2).

The simulation is quite good concerning the FIGRA, we can see it on the diagram 1. The worst value is the FIGRA of the glassfiber reinforced plastic.

One of the THR $_{600s}$ values is bad, and it concerns the glassfiber reinforced plastic too (diagram 2).

We can't compare the flashover times of the tests results and the flashover times of the simulations for the white pine boards and the white oak boards, because the values of the tests results are only for the walls.

There is essentially one wrong value concerning the flashover times: it is the value of the textile wall covering. According to the RCT test, there is no flashover. But when we look at the simulations, we can see that there is a flashover at each run.

We can say, with the diagram 3, that the value concerning the FRT Douglas fir plywood is not very good.

Then we can do the comparison between the test results and the simulations from a HRR threshold, which is equal to 50 kW/m^2.
The comparison of the FIGRA, the THR $_{600s}$, the flashover time and the Euroclass is shown in table 2.

Except for the FRT Douglas fir plywood and the glassfiber reinforced plastic, the classes are the same as the test results. It is in agreement with the first simulation.

We can see on the diagram 5 the comparison of the FIGRA. Two values are worse than the others, the FIGRA of the glassfiber reinforced plastic and polyisocyanurate foam.

Concerning the THR $_{600s}$, the simulation is quite good. We can comment the THR $_{600s}$ of the glassfiber reinforced plastic, which is the worst value (diagram 6).

Three values of flashover times are worrying: the flashover times of the vinyl wall covering, the polyisocyanurate foam and the textile wall covering.

According to the RCT test, the flashover time for the polyisocyanurate foam is 15 seconds, and it is 181,3 seconds with the simulation.
Concerning the textile wall covering, the run 2 indicates there is a flashover, even though there is no flashover in reality.

But the worst value is the one of the vinyl wall covering : the simulation shows there is no flashover, contrary to the test results.

It is interesting to do a comparison between the simulation obtained with the ignition time and the simulation obtained with the HRR threshold.

The two simulations are close concerning the FIGRA and the THR $_{600s}$, but there are some differences concerning the class, especially with the vinyl wall covering. According to the first simulation, the vinyl wall covering belongs to the class D, contrary to the second simulation for which it belongs to the class C.

For the polyisocyanurate foam, the flashover time obtained with the first simulation is better than the flashover time obtained with the second simulation.

We can comment one strange thing about the textile wall covering: the first simulation shows there is a flashover. But the second simulation shows there is no flashover (run 1 and 3). In fact, it is because the input ignition time is very different for each simulation. With the first simulation, we use the ignition time of the Cone Calorimeter test (8 or 9 seconds); in the second simulation we use the HRR threshold (50 kW/m^2), and the ignition time is bigger (29, 20 and 27 seconds). We can see it on the curve which shows the HRR according to the time.

Annex G. Plots of the comparison of the FIGRA and the THR between the Hansen model and the SP model – SwRI Project
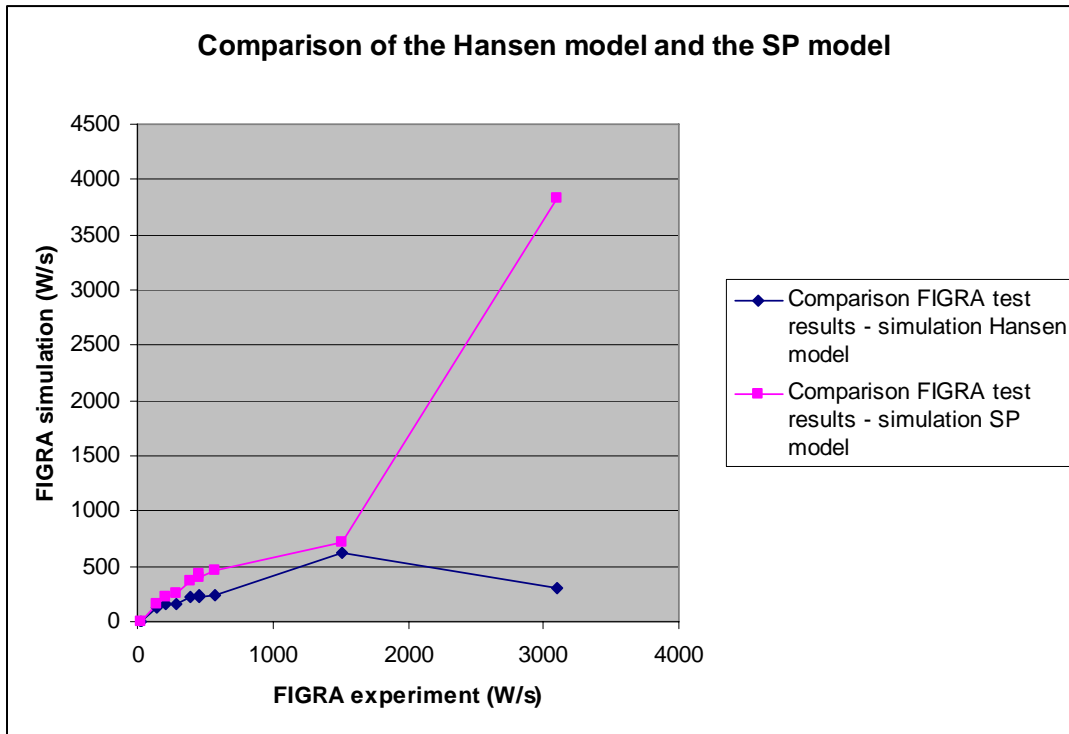
Graph 45. Comparison of the FIGRA.
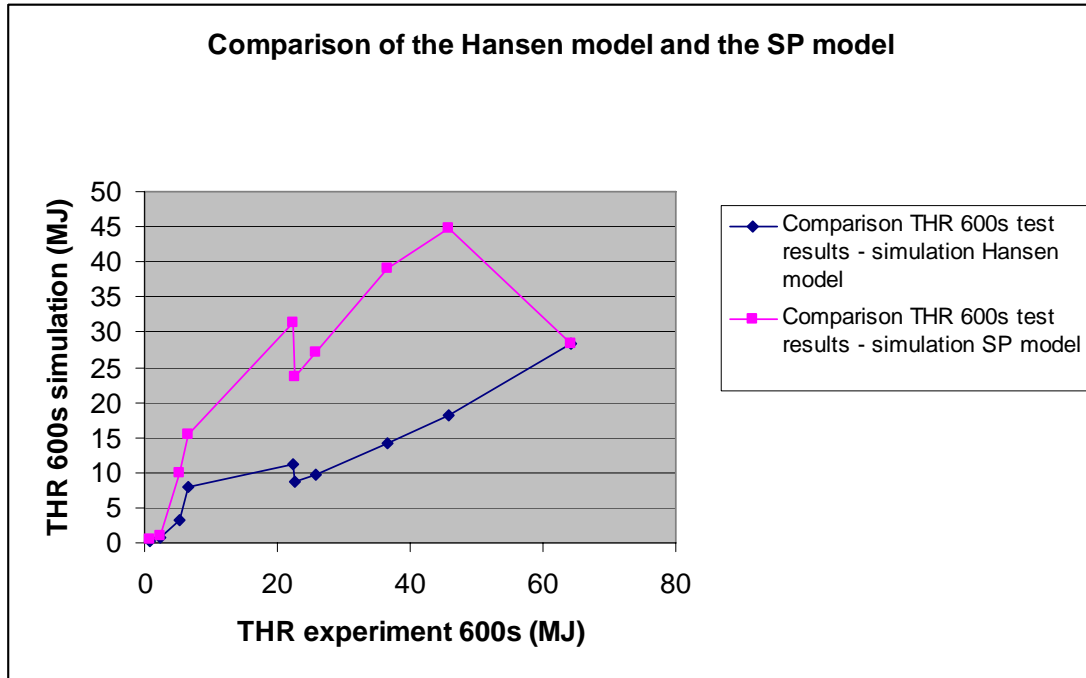
Graph 46. Comparison of the THR

Annex H. Comparison of the smoke production between the simulation and the experiment – SwRI Project

Product	SMOGRA exp(m2/s2)	SMOGRA simulation (m2/s2)		
		run 1	run 2	run 3
Douglas fir plywood	5	smogra<30	smogra<30	smogra<30
FRT Douglas fir plywood	1	smogra<30	smogra<30	30<smogra<180
Glassfiber reinforced plastic	325	30<smogra<180	30<smogra<180	30<smogra<180
Type X gypsum board	0	smogra<30	smogra<30	smogra<30
Polyisocyanurate foam	248	30<smogra<180	30<smogra<180	30<smogra<180
Vinyl wall covering	32	30<smogra<180	30<smogra<180	30<smogra<180
Textile wall covering	-	30<smogra<180	30<smogra<180	30<smogra<180
Paper wall covering	-	30<smogra<180	smogra<30	30<smogra<180
Oriented Strand Board 1 (LP)	0	smogra<30	smogra<30	-
Oriented Strand Board 2 (weyerhaeuser)	0	smogra<30	30<smogra<180	-
White pine boards	2	smogra<30	smogra<30	-
White oak boards	0	smogra<30	smogra<30	-

Table 6. Comparison of the SMOGRA.

Annex I. Comparison of the classes between the Hansen model and the SP model – SBI project

		Euroclass - Hansen model	Eurolass - SP model	Euroclass - test result
M01	C990332	A2/B	A2/B	>= B
M02	C990343	C	D	>B
M03	C990337	E or worse	E or worse	E
M04	C000501	C	D	
	C000502	C	D	E
M05	C990344	D	E or worse	D
M06	C990324	A2/B	A2/B	>=B
M07	C000401	D	D	
	C000410	D	D	
	C000414	D	D	
	C000417	D	D	>B
M08	C990333	A2/B	A2/B	>=B
M09	C990334	A2/B	C	C
M10	C990319	D	D	D
M11	C990339	A2/B	A2/B	B
M12	C000404	D	D	
	C000411	D	D	
	C000413	C	D	
	C000416	C	D	D
M13	C000418	A2/B	A2/B	
	C000503	A2/B	A2/B	>=B
M14	C990338	A2/B	A2/B	>=B
M15	C990321	A2/B	A2/B	>=B
M16	C990342	C	D	D

		Euroclass - Hansen model	Eurolass - SP model	Euroclass - test result
M19	C990347	A2/B	A2/B	
	C990348	A2/B	A2/B	>=B
M20	C990345	C	D	D
M21	C000420	A2/B	A2/B	
	C000505	A2/B	A2/B	>=B
M22	C990323	D	D	D
M23	C990325	D	D	D
M24	C990320	C	D	D
	C000403	D	D	
	C000405	D	D	
	C000412	C	D	
M25	C000415	C	D	D
M26	C990331	D	E or worse	E
	C000419	A2/B	A2/B	
M27	C000504	A2/B	A2/B	>=B
M28	C990346	A2/B	A2/B	>=B
M29	C990322	A2/B	C	C
	C000423	C	E or worse	
	C000424	C	E or worse	
	C000421	C	E or worse	
M30	C000422	C	E or worse	E

Table 7. Comparison of the classes for the SBI project.

Annex J. Input file of the simulation of the propane burner in the office

```
!
!----------------------------------------------------------------
------
!Comments for this simulation: maximum 1500 characters.
!----------------------------------------------------------------
------
!
Example Marie : propane burner in my office.
!
!
!----------------------------------------------------------------
------
! 1. In which mode do you want to run your simulation?
!    Options: STANDARD MODE AND PROFESSIONAL MODE
!
!    You can run computation in either standard mode or
professional   mode. The
!  professional mode allows more flexible input for your
simulation.
!----------------------------------------------------------------
------
!
      STANDARD MODE
!
!----------------------------------------------------------------
------
! PHYSICAL PRESCRIPTION OF THE PROBLEM......
!----------------------------------------------------------------
------
!
!----------------------------------------------------------------
------
! 2. Cartesian coordinate? Transient? (logical input)
!----------------------------------------------------------------
------
!
  T  T
!
!----------------------------------------------------------------
------
! 3. How many dimensional?
!----------------------------------------------------------------
------
!
    3
!
!----------------------------------------------------------------
------
! 4. Ambient air temperature(K) = ?
!----------------------------------------------------------------
------
!
    3.00000E+02
!
!----------------------------------------------------------------
------
```

```
! 5. Porous media (logical input)?
!--------------------------------------------------------------
------
!
  F
!
!--------------------------------------------------------------
------
! 6. Which turbulence model?
!    Options: NO TURBULENCE  , RANS HRN K-E MODEL,
!             LES-SMAGORINSKY, LES-BUOYANCY-SMAGORINSKY
!--------------------------------------------------------------
------
!
    RANS HRN K-E MODEL
!
!--------------------------------------------------------------
------
! 7. Hybrid k-e modification? (logical)
!--------------------------------------------------------------
------
!
  F
!
!--------------------------------------------------------------
------
!8. Please specify the C H O and N atom numbers in all the
involved
!    chemical species:
!--------------------------------------------------------------
------
!
      0.000       0.000       2.000       0.000
      0.000       0.000       0.000       2.000
      0.000       2.000       1.000       0.000
      1.000       0.000       2.000       0.000
      3.000       8.000       0.000       0.000
!
!--------------------------------------------------------------
------
! 9. Which combustion model? Options: FLAMELET MODEL and EDC
!--------------------------------------------------------------
------
!
    EDC
!
!--------------------------------------------------------------
------
!10. Which soot model?
!    Options: NO SOOT            , EMPIRICAL MODEL, MOSS MODEL
!             LINDERSTEDT MODEL, MAUSS MODEL     , MAUSS LIBRARY
MODEL
!--------------------------------------------------------------
------
!
    EMPIRICAL MODEL
!
!--------------------------------------------------------------
------
!11. Please specify reaction coefficients for the following
species:
```

```
!    ( -1.0 for Fuel in each reaction. For input simplicity, soot
is
!      symbolically represented by C30.)
!----------------------------------------------------------------
------
!
!OXYG_FRACTION  NITR_FRACTION  H2O_FRACTION   CO2_FRACTION
C3H8_FRACTION
! SOOT_FRACTION
!----------------------------------------------------------------
------
!
-4.91000E+00    0.00000E+00    4.00000E+00    2.91000E+00    -
1.00000E+00
 3.00000E-03
!
!----------------------------------------------------------------
------
!12. Is thermal radiation to be computed? YES or NO
!----------------------------------------------------------------
------
!
     YES
!
!----------------------------------------------------------------
------
!13. Which radiation property model?
!    Options: MODAK, FASTNB and FASTNB APPROXIMATION.
!----------------------------------------------------------------
------
!
     MODAK
!
!----------------------------------------------------------------
------
!14. DT (Discrete Transfer) rays numbers (nth and nfi):
!----------------------------------------------------------------
------
!
   2    8
!
!----------------------------------------------------------------
------
!15. Which pyrolysis model? Options: THERMAL MODEL and KINETIC
MODEL?
!----------------------------------------------------------------
------
!
     THERMAL MODEL
!
!----------------------------------------------------------------
------
!16. Which solver?, Options: TDMA, SIP and FA
!----------------------------------------------------------------
------
!
     FA
!
!----------------------------------------------------------------
------
! DIMENSION RELATED VARIABLES SETUP......
```

```
!---------------------------------------------------------------
------
!
!---------------------------------------------------------------
------
!17. Gas grid numbers: ni=? nj=?  nk=?
!---------------------------------------------------------------
------
!
          50             30             50
!
!---------------------------------------------------------------
------
! GENERATING GRID SYSTEM FOR COMPUTATION......
!---------------------------------------------------------------
------
!
!---------------------------------------------------------------
------
!18. X grid locations:
!---------------------------------------------------------------
------
!
    2    3   1.000000E-04   1.000000E-01   0.000000E+00
    3   11   1.000000E-01   1.000000E+00   0.000000E+00
   11   41   1.000000E+00   4.000000E+00   0.000000E+00
   41   49   4.000000E+00   5.000000E+00   0.000000E+00
!
!---------------------------------------------------------------
------
!19. Y grid locations:
!---------------------------------------------------------------
------
!
    2    3   1.000000E-04   1.000000E-01   0.000000E+00
    3    9   1.000000E-01   8.000000E-01   0.000000E+00
    9   23   8.000000E-01   2.200000E+00   0.000000E+00
   23   29   2.200000E+00   3.000000E+00   0.000000E+00
!
!---------------------------------------------------------------
------
!20. Z grid locations:
!---------------------------------------------------------------
------
!
    2    3   1.000000E-04   1.000000E-01   0.000000E+00
    3   11   1.000000E-01   8.000000E-01   0.000000E+00
   11   41   8.000000E-01   2.200000E+00   0.000000E+00
   41   49   2.200000E+00   3.000000E+00   0.000000E+00
!
!---------------------------------------------------------------
------
! SPECIFICATION OF BLOCKAGE......
! In the following, blockage property is given by a key word which
can be
! SOLID or CAVITY
!---------------------------------------------------------------
------
!
!
```

```
!--------------------------------------------------------------------
------
!21.  Name, property, emissivity & phy. coords. of 2 diagonals of
blockages
!--------------------------------------------------------------------
------
!
     MAIN_FRAME                 SOLID          9.000000E-01
                   0.000000E+00   0.000000E+00   0.000000E+00
                   5.000000E+00   3.000000E+00   3.000000E+00
     ROOM                       CAVITY         9.000000E-01
                   1.000000E-01   1.000000E-04   1.000000E-01
                   4.900000E+00   2.900000E+00   2.900000E+00
     DOOR                       CAVITY         9.000000E-01
                   1.000000E+00   1.000000E-04   0.000000E+00
                   1.800000E+00   2.000000E+00   1.000000E-01
!
!--------------------------------------------------------------------
------
!    Wall     1 is identified as WEST   surface of ROOM
!--------------------------------------------------------------------
------
!
!
!--------------------------------------------------------------------
------
!    Wall     2 is identified as EAST   surface of ROOM
!--------------------------------------------------------------------
------
!
!
!--------------------------------------------------------------------
------
!    Wall     3 is identified as SOUTH  surface of ROOM
!--------------------------------------------------------------------
-----
!
!
!--------------------------------------------------------------------
------
!    Wall     4 is identified as NORTH  surface of ROOM
!--------------------------------------------------------------------
------
!
!
!--------------------------------------------------------------------
------
!    Wall     5 is identified as BOTTOM surface of ROOM
!--------------------------------------------------------------------
------
!
!
!--------------------------------------------------------------------
------
!    Wall     6 is identified as TOP    surface of ROOM
!--------------------------------------------------------------------
------
!
!
!--------------------------------------------------------------------
------
```

```
!    Wall     7 is identified as WEST   surface of DOOR
!----------------------------------------------------------------
------
!
!
!----------------------------------------------------------------
------
!    Wall     8 is identified as EAST   surface of DOOR
!----------------------------------------------------------------
------
!
!
!----------------------------------------------------------------
------
!    Wall     9 is identified as SOUTH  surface of DOOR
!----------------------------------------------------------------
------
!
!
!----------------------------------------------------------------
------
!    Wall     10 is identified as NORTH  surface of DOOR
!----------------------------------------------------------------
------
!
!
!----------------------------------------------------------------
------
! SPECIFICATION OF EXTRA BOUNDARIES......
!
!In the following, boundary orientation is given by a key word
which can be
! WEST, EAST, SOUTH, NORTH, BOTTOM or TOP
! where WEST=I-, EAST=I+, SOUTH=J-, NORTH=J+, BOTTOM=K- and TOP=K+
!
! The boundary type is given by a key word which can be :
! WALL, ENTRAINMENT    , SYMMETRY, EXTRACT    , PRESSURE,
INLET,
! EXIT, VIRTUAL_BOUNDARY, CBC     , NON_TRACTION, PERIODIC
!
!The boundary is set to be subject to non-flowing ambient air
condition.
!If this condition does not apply to your boundary,you can change
any of
! the following variables, for example, as (in SI Unit):
TEMPERATURE 300
!
! U_VELOCITY     V_VELOCITY     W_VELOCITY     PRESSURE
PRESSURE_C
!TURBULENCE_K   TURBULENCE_E   ENTHALPY       TEMPERATURE
DENSITY
!OXYG_FRACTION  NITR_FRACTION  H2O_FRACTION   CO2_FRACTION
C3H8_FRACTION
! SOOT_FRACTION
!----------------------------------------------------------------
------
!
!
!----------------------------------------------------------------
------
```

```
!22. Name, orientation, type, emissivity, coordinates of 2
diagonals of
!    boundary, and optional variable specification:
!---------------------------------------------------------------
------
!
        FLOOR                   SOUTH           WALL
        9.000000E-01   0.000000E+00   0.000000E+00   0.000000E+00
                       5.000000E+00   0.000000E+00   3.000000E+00
        DOOR                    BOTTOM          PRESSURE
        9.000000E-01   1.000000E+00   1.000000E-04   0.000000E+00
                       1.800000E+00   2.000000E+00   0.000000E+00
        EXIT_1                  WEST            WALL
        9.000000E-01   0.000000E+00   0.000000E+00   0.000000E+00
                       0.000000E+00   3.000000E+00   3.000000E+00
        EXIT_2                  EAST            WALL
        9.000000E-01   5.000000E+00   0.000000E+00   0.000000E+00
                       5.000000E+00   3.000000E+00   3.000000E+00
        EXIT_3                  TOP             WALL
        9.000000E-01   0.000000E+00   0.000000E+00   3.000000E+00
                       5.000000E+00   3.000000E+00   3.000000E+00
        EXIT_4                  BOTTOM          WALL
        9.000000E-01   0.000000E+00   0.000000E+00   0.000000E+00
                       5.000000E+00   3.000000E+00   0.000000E+00
        EXIT_5                  NORTH           WALL
        9.000000E-01   0.000000E+00   3.000000E+00   0.000000E+00
                       5.000000E+00   3.000000E+00   3.000000E+00
!
!---------------------------------------------------------------
------
!    Boundary  FLOOR                    is identified as boundary
11
!    Boundary  EXIT_1                   is identified as boundary
12
!    Boundary  EXIT_2                   is identified as boundary
13
!    Boundary  EXIT_3                   is identified as boundary
14
!    Boundary  EXIT_4                   is identified as boundary
15
!    Boundary  EXIT_5                   is identified as boundary
16
!    Boundary  DOOR                     is identified as boundary
17
!---------------------------------------------------------------
------
!
!
!---------------------------------------------------------------
------
! INITIALISING THE WALL BOUNDARY......
!---------------------------------------------------------------
------
!
!
!---------------------------------------------------------------
------
!23. Number of wall grid at the direction perpendicular to wall
surface
!---------------------------------------------------------------
------
```

```
!
           6
!
!----------------------------------------------------------------
------
!24. Wall index range & one dimensional grid thickness:
!----------------------------------------------------------------
------
!
           1      100000000
 0.00000E+00    2.00000E-03    2.00000E-03    2.00000E-03
2.00000E-03
 0.00000E+00
!
!----------------------------------------------------------------
------
!25.Wall and slab indices,pyrolysis temperature,pyrolysis
heat,virgin &
!   char densities,moisture content,and optional variable
specification:
!
! Here you can change variable values in the same way as when
specifying
! extra boundary. For combustible wall, it is important to specify
! correctly the pyrolysis gas composition so that the heat of
combustion
!    for the wall can be calculated right.
!----------------------------------------------------------------
------
!
           1      100000000              1              6
     7.730000E+02      2.636000E+03      8.000000E+02
     8.000000E+02      0.000000E+00
!
!----------------------------------------------------------------
------
!26. Wall and slab indices, five cp coefficients
!----------------------------------------------------------------
------
!
           1      100000000              1              6
   6.00000E+02    0.00000E+00    0.00000E+00    0.00000E+00
0.00000E+00
!
!----------------------------------------------------------------
------
!27. Wall and slab indices, five conductivity coefficients
!----------------------------------------------------------------
------
!
           1      100000000              1              6
   1.70000E-01    0.00000E+00    0.00000E+00    0.00000E+00
0.00000E+00
!
!----------------------------------------------------------------
------
! SETTING UP BURNER PARAMETERS......
!----------------------------------------------------------------
------
!
```

```
!------------------------------------------------------------------
------
! SPECIFICATION OF BURNER ORIENTATION AND BURNER SURFACE......
! Note: Burner orientation is given in the same way as for
boundary.
!------------------------------------------------------------------
------
!
!
!------------------------------------------------------------------
------
!28.  Orientation and physical coordinates of two diagonal points
of      burner   1
!------------------------------------------------------------------
------
!
     SOUTH                 0.000000E+00   1.000000E-04
2.700000E+00
                           3.000000E-01   1.000000E-04
3.000000E+00
!
!------------------------------------------------------------------
------
!29. Burner indices, temperature and mass fractions of following
species
!
! OXYG_FRACTION  NITR_FRACTION  H2O_FRACTION  CO2_FRACTION
C3H8_FRACTION
!   SOOT_FRACTION
!------------------------------------------------------------------
------
!
    1    1    3.00000E+02
   0.00000E+00     0.00000E+00     0.00000E+00     0.00000E+00
1.00000E+00
    0.00000E+00
!
!------------------------------------------------------------------
------
!30. Burner indices, start time and burner power
!------------------------------------------------------------------
------
!
    1    1    0.00000E+00    3.00000E+05
!
!------------------------------------------------------------------
------
! RUN CONTROL PARAMETERS SETTING UP......
!------------------------------------------------------------------
------
!
!
!------------------------------------------------------------------
------
!31. Which variables to be stored in result file? (logical)
!
! U_VELOCITY      V_VELOCITY      W_VELOCITY      PRESSURE
PRESSURE_C
! TURBULENCE_K   TURBULENCE_E   ENTHALPY        TEMPERATURE
DENSITY
```

```
!  OXYG_FRACTION  NITR_FRACTION H2O_FRACTION  CO2_FRACTION
C3H8_FRACTION
!  SOOT_FRACTION
!--------------------------------------------------------------------
------
!
   T              T              T              T              T
   T              T              F              T              F
   T              F              T              T              T
   T
!
!--------------------------------------------------------------------
------
!32. Physical time to terminate the computation:
!--------------------------------------------------------------------
------
!
    6.00000E+02
!
!--------------------------------------------------------------------
------
!33. Physical coordinate for data monitoring:
!--------------------------------------------------------------------
------
!
   1.400000E+00    1.000000E+00    0.000000E+00
!
!--------------------------------------------------------------------
------
!34. Residual print, result store & restart file update
frequencies:
!--------------------------------------------------------------------
------
!
    5     2.00000E+00      5
!
!--------------------------------------------------------------------
------
!35. Variation of maximum iterations with time:
!--------------------------------------------------------------------
------
!
    0      60     300     500
    500    400    300     200
!
!--------------------------------------------------------------------
------
!35. Variation of time step with time:
!--------------------------------------------------------------------
------
!
    0    60    120
    1    5    10
```

Annex K. Input file of the simulation of the basket heating test

```
!
!----------------------------------------------------------------
------
!Comments for this simulation: maximum 1500 characters.
!----------------------------------------------------------------
------
!
Basket heating test: 180degC, 1 dm3, 6 mm wood pellets
!
!
!----------------------------------------------------------------
------
! 1. In which mode do you want to run your simulation?
!    Options: STANDARD MODE AND PROFESSIONAL MODE
!
!    You can run computation in either standard mode or
professional mode. The
!    professional mode allows more flexible input for your
simulation.
!----------------------------------------------------------------
------
!
      PROFESSIONAL MODE
!
!----------------------------------------------------------------
------
! PHYSICAL PRESCRIPTION OF THE PROBLEM......
!----------------------------------------------------------------
------
!
!----------------------------------------------------------------
------
! 2. Cartesian coordinate? Transient? (logical input)
!----------------------------------------------------------------
------
!
  T  T
!
!----------------------------------------------------------------
------
! 3. How many dimensional?
!----------------------------------------------------------------
------
!
    3
!
!----------------------------------------------------------------
------
! 4. Gravity vector (g1, g2 and g3) = ?
```

```
!----------------------------------------------------------------
------
!
    0.00000E+00    -9.81000E+00     0.00000E+00
!
!----------------------------------------------------------------
------
! 5. Ambient air temperature(K) = ?
!----------------------------------------------------------------
------
!
    4.53150E+02
!
!----------------------------------------------------------------
------
! 6. Porous media (logical input)?
!----------------------------------------------------------------
------
!
  T
!
!----------------------------------------------------------------
------
! 7. Which turbulence model?
!    Options: NO TURBULENCE  , RANS HRN K-E MODEL,
!             LES-SMAGORINSKY, LES-BUOYANCY-SMAGORINSKY
!----------------------------------------------------------------
------
!
     NO TURBULENCE
!
!----------------------------------------------------------------
------
! 8. Please specify the C H O and N atom numbers of all the
chemical species:
!----------------------------------------------------------------
------
!
      0.000        2.000        1.000        0.000
      0.000        0.000        2.000        0.000
      0.000        0.000        0.000        2.000
      1.000        0.000        2.000        0.000
      1.000        0.000        1.000        0.000
!
!----------------------------------------------------------------
------
! 9. Which combustion model? Options: FLAMELET MODEL and EDC
!----------------------------------------------------------------
------
!
     EDC
!
!----------------------------------------------------------------
------
!10. Which soot model?
!    Options: NO SOOT            , EMPIRICAL MODEL, MOSS MODEL
!             LINDERSTEDT MODEL, MAUSS MODEL     , MAUSS LIBRARY
MODEL
!----------------------------------------------------------------
------
!
```

```
     NO SOOT
!
!----------------------------------------------------------------
------
!11. Please specify reaction coefficients for the following
species:
!    ( -1.0 for Fuel in each reaction. For input simplicity, soot
is
!      symbolically represented by C30.)
!----------------------------------------------------------------
------
!
!OXYG_FRACTION   NITR_FRACTION  H2O_FRACTION   CO2_FRACTION
CO_FRACTION
!----------------------------------------------------------------
------
!
 0.00000E+00     0.00000E+00     0.00000E+00     0.00000E+00
0.00000E+00
!
!----------------------------------------------------------------
------
!12. Is thermal radiation to be computed? YES or NO
!----------------------------------------------------------------
------
!
     NO
!
!----------------------------------------------------------------
------
!13. Which pyrolysis model? Options: THERMAL MODEL and KINETIC
MODEL?
!----------------------------------------------------------------
------
!
     THERMAL MODEL
!
!----------------------------------------------------------------
------
!14. Which solver?, Options: TDMA, SIP and FA
!----------------------------------------------------------------
------
!
     TDMA
!
!----------------------------------------------------------------
------
!16. Gas grid numbers: ni=? nj=?  nk=?
!----------------------------------------------------------------
------
!
         13            23            13
!
!----------------------------------------------------------------
------
!17. X grid locations:
!----------------------------------------------------------------
------
!
    2   12   1.000000E-04   5.010000E-02   0.000000E+00
!
```

```
!----------------------------------------------------------------
------
!18. Y grid locations:
!----------------------------------------------------------------
------
!
    2   22   1.000000E-04   1.001000E-01   0.000000E+00
!
!----------------------------------------------------------------
------
!19. Z grid locations:
!----------------------------------------------------------------
------
!
    2   12   1.000000E-04   5.010000E-02   0.000000E+00
!
!----------------------------------------------------------------
------
!20. On which space do you want to specify your geometry?
!    Options: PHYSICAL SPACE, COMPUTATIONAL SPACE
!----------------------------------------------------------------
------
!
      PHYSICAL SPACE
!
!----------------------------------------------------------------
------
! SPECIFICATION OF BLOCKAGE......
!In the following, blockage property is given by a key word which
can be
! SOLID or CAVITY
!----------------------------------------------------------------
------
!
!
!----------------------------------------------------------------
------
!21.Name, property, emissivity & coordinates of 2 diagonals of
blockages
!----------------------------------------------------------------
------
!
      BASKET                         SOLID         9.000000E-01
                0.000000E+00   0.000000E+00   0.000000E+00
                0.000000E+00   0.000000E+00   0.000000E+00
!
!----------------------------------------------------------------
------
! SPECIFICATION OF EXTRA BOUNDARIES......
!
! In the following, boundary orientation is given by a key word
which can be
! WEST, EAST, SOUTH, NORTH, BOTTOM or TOP
! where WEST=I-, EAST=I+, SOUTH=J-, NORTH=J+, BOTTOM=K- and TOP=K+
!
! The boundary type is given by a key word which can be :
! WALL,  ENTRAINMENT    ,  SYMMETRY,  EXTRACT    ,  PRESSURE,
INLET,
! EXIT,  VIRTUAL_BOUNDARY,  CBC      ,  NON_TRACTION,  PERIODIC
!
```

```
!The boundary is set to be subject to non-flowing ambient air
condition.
!If this condition does not apply to your boundary,you can change
any of
! the following variables, for example, as (in SI Unit):
TEMPERATURE 300
!
! U_VELOCITY      V_VELOCITY      W_VELOCITY      PRESSURE
PRESSURE_C
! ENTHALPY        TEMPERATURE     DENSITY         SOLID_TEMP
SOLID_MOISTURE
! BULK_DENSITY    OXYG_FRACTION   NITR_FRACTION   H2O_FRACTION
CO2_FRACTION
! CO_FRACTION
!------------------------------------------------------------------
------
!
!
!------------------------------------------------------------------
------
!22. Name, orientation, type, emissivity, coordinates of 2
diagonals of
!    boundary, and optional variable specification:
!------------------------------------------------------------------
------
!
     MINI_WALL               SOUTH           WALL
     9.000000E-01    0.000000E+00    1.000000E-04
0.000000E+00
                     1.000000E-04    1.000000E-04
1.000000E-04
     SIDE_1                  NORTH           PRESSURE
     9.000000E-01    1.000000E-04    1.001000E-01
1.000000E-04
                     5.010000E-02    1.001000E-01
5.010000E-02
     TEMPERATURE     4.531500E+02
     SIDE_2                  SOUTH           PRESSURE
     9.000000E-01    1.000000E-04    1.000000E-04
1.000000E-04
                     5.010000E-02    1.000000E-04
5.010000E-02
     TEMPERATURE     4.531500E+02
     SIDE_3                  BOTTOM          PRESSURE
     9.000000E-01    1.000000E-04    1.000000E-04
1.000000E-04
                     5.010000E-02    1.001000E-01
1.000000E-04
     TEMPERATURE     4.531500E+02
     SIDE_4                  TOP             SYMMETRY
     9.000000E-01    1.000000E-04    1.000000E-04
5.010000E-02
                     5.010000E-02    1.001000E-01
5.010000E-02
     SIDE_5                  EAST            SYMMETRY
     9.000000E-01    5.010000E-02    1.000000E-04
1.000000E-04
                     5.010000E-02    1.001000E-01
5.010000E-02
     SIDE_6                  WEST            PRESSURE
```

```
     9.000000E-01     1.000000E-04     1.000000E-04
1.000000E-04
                     1.000000E-04     1.001000E-01
5.010000E-02
     TEMPERATURE     4.531500E+02
!
!----------------------------------------------------------------
------
!    Boundary  MINI_WALL               is identified as boundary
1
!    Boundary  SIDE_1                  is identified as boundary
2
!    Boundary  SIDE_2                  is identified as boundary
3
!    Boundary  SIDE_3                  is identified as boundary
4
!    Boundary  SIDE_4                  is identified as boundary
5
!    Boundary  SIDE_5                  is identified as boundary
6
!    Boundary  SIDE_6                  is identified as boundary
7
!----------------------------------------------------------------
------
!
!
!----------------------------------------------------------------
------
!23. Turbulent Prandtl number for the following variables:
!
! U_VELOCITY      V_VELOCITY      W_VELOCITY      PRESSURE
PRESSURE_C
! ENTHALPY        TEMPERATURE     DENSITY         SOLID_TEMP
SOLID_MOISTURE
! BULK_DENSITY    OXYG_FRACTION   NITR_FRACTION   H2O_FRACTION
CO2_FRACTION
! CO_FRACTION
!----------------------------------------------------------------
------
!
  1.00000E+00     1.00000E+00     1.00000E+00     1.00000E+00
1.00000E+00
  7.00000E-01     7.00000E-01     7.00000E-01     7.00000E-01
7.00000E-01
  7.00000E-01     7.00000E-01     7.00000E-01     7.00000E-01
7.00000E-01
  7.00000E-01
!
!----------------------------------------------------------------
------
!24. Define domain for initialising the gas phase:
!----------------------------------------------------------------
------
!
!
!----------------------------------------------------------------
------
!25.Please specify phy. coords. of two diagonals of the intended
domain.
!     The coordinates of two diagnoals for the full domain are:
!                0.000000E+00   0.000000E+00   0.000000E+00
```

```
!                      5.020000E-02   1.002000E-01   5.020000E-02
!------------------------------------------------------------------
------
!
                 0.000000E+00   0.000000E+00   0.000000E+00
                 5.020000E-02   1.002000E-01   5.020000E-02
!
!------------------------------------------------------------------
------
!26. Initial values for the following involved variables:
!
! U_VELOCITY      V_VELOCITY     W_VELOCITY     PRESSURE
PRESSURE_C
! ENTHALPY        TEMPERATURE    DENSITY        SOLID_TEMP
SOLID_MOISTURE
! BULK_DENSITY    OXYG_FRACTION  NITR_FRACTION  H2O_FRACTION
CO2_FRACTION
! CO_FRACTION
!------------------------------------------------------------------
------
!
  0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
0.00000E+00
  0.00000E+00    2.96150E+02    0.00000E+00    2.96150E+02
8.20000E-02
  6.03000E+02    2.31500E-01    7.68500E-01    0.00000E+00
0.00000E+00
  0.00000E+00
!
!------------------------------------------------------------------
------
! INITIALISING THE WALL BOUNDARY......
!------------------------------------------------------------------
------
!
!
!------------------------------------------------------------------
------
!27. Number of wall grid at the direction perpendicular to wall
surface
!------------------------------------------------------------------
------
!
        3
!
!------------------------------------------------------------------
------
!28. Wall index range & one dimensional grid thickness:
!------------------------------------------------------------------
------
!
           1      100000000
   0.00000E+00    0.00000E+00    0.00000E+00
!
!------------------------------------------------------------------
------
!29.Wall and slab indices,pyrolysis temperature,pyrolysis
heat,virgin &
!  char densities,moisture content,and optional variable
specification:
!
```

```
! Here you can change variable values in the same way as when
specifying
! extra boundary. For combustible wall, it is important to specify
! correctly the pyrolysis gas composition so that the heat of
combustion
!    for the wall can be calculated right.
!-------------------------------------------------------------------
------
!
             1      100000000             1             3
       6.231500E+02     2.636000E+03     2.000000E+02
       2.000000E+02     0.000000E+00
!
!-------------------------------------------------------------------
------
!30. Wall and slab indices, five cp coefficients
!-------------------------------------------------------------------
------
!
             1      100000000             1             3
 8.40000E+02    0.00000E+00    0.00000E+00    0.00000E+00
0.00000E+00
!
!-------------------------------------------------------------------
------
!31. Wall and slab indices, five conductivity coefficients
!-------------------------------------------------------------------
------
!
             1      100000000             1             3
   4.90000E-02    0.00000E+00    0.00000E+00    0.00000E+00
0.00000E+00
!
!-------------------------------------------------------------------
------
!32. Wall and slab indices, temperature
!-------------------------------------------------------------------
------
!
           1      100000000             1             3
4.53150E+02
!
!-------------------------------------------------------------------
------
! SETTING UP BURNER PARAMETERS......
!-------------------------------------------------------------------
------
!
!
!-------------------------------------------------------------------
------
!33.  Orientation and coordinates of two diagonal points of burner
!     Note: Burner orientation is given in the same way as for
boundary.
!-------------------------------------------------------------------
------
!
      SOUTH                0.000000E+00   0.000000E+00
0.000000E+00
                           0.000000E+00   0.000000E+00
0.000000E+00
```

```
!
!----------------------------------------------------------------
------
! RUN CONTROL PARAMETERS SETTING UP......
!----------------------------------------------------------------
------
!
!----------------------------------------------------------------
------
!34. Which variables to be stored in result file? (logical)
!
! U_VELOCITY      V_VELOCITY      W_VELOCITY      PRESSURE
PRESSURE_C
! ENTHALPY        TEMPERATURE     DENSITY         SOLID_TEMP
SOLID_MOISTURE
! BULK_DENSITY    OXYG_FRACTION  NITR_FRACTION  H2O_FRACTION
CO2_FRACTION
! CO_FRACTION
!----------------------------------------------------------------
------
!
   T               T               T               T               T
   T               T               T               T               T
   T               T               T               T               T
   T
!
!----------------------------------------------------------------
------
!35. Under relax. factors for solved variables:
!
! U_VELOCITY      V_VELOCITY      W_VELOCITY      PRESSURE
PRESSURE_C
! ENTHALPY        TEMPERATURE     DENSITY         SOLID_TEMP
SOLID_MOISTURE
! BULK_DENSITY    OXYG_FRACTION  NITR_FRACTION  H2O_FRACTION
CO2_FRACTION
! CO_FRACTION
!----------------------------------------------------------------
------
!
 3.00000E-01    3.00000E-01    3.00000E-01    3.00000E-01
3.00000E-01
 3.00000E-01    3.00000E-01    3.00000E-01    3.00000E-01
1.50000E-01
 3.00000E-01    3.00000E-01    3.00000E-01    3.00000E-01
3.00000E-01
 3.00000E-01
!
!----------------------------------------------------------------
------
!36. Under relax. factors for
!    K generation, viscosity, fuel consumption rate, wall
temperature,
!    uplus and asm correction:
!----------------------------------------------------------------
------
!
 3.00000E-01    3.00000E-01    2.00000E-01    2.00000E-01
5.00000E-01
    2.00000E-01
!
```

```
!----------------------------------------------------------------
------
!37. Which difference scheme?
!    Options: Upwind, Hybrid, PLDS, SMART, UMIST, SUPBEE
!----------------------------------------------------------------
------
!
     PLDS
!
!----------------------------------------------------------------
------
!38. Physical time to terminate the computation:
!----------------------------------------------------------------
------
!
    1.80000E+04
!
!----------------------------------------------------------------
------
!39. Coordinate for data monitoring:
!----------------------------------------------------------------
------
!
   5.100000E-03   5.010000E-02   2.510000E-02
!
!----------------------------------------------------------------
------
!40. Residual print, result store & restart file update
frequencies:
!----------------------------------------------------------------
------
!
       10    5.00000E+00         10
!
!----------------------------------------------------------------
------
!41. Residual tolerance for flow:
!----------------------------------------------------------------
------
!
    5.00000E-06
!
!----------------------------------------------------------------
------
!42. Variation of maximum iterations with time:
!----------------------------------------------------------------
------
!
    0.00000E+00
    2.00000E+02
!
!----------------------------------------------------------------
------
!42. Variation of time step with time:
!----------------------------------------------------------------
------
!
    0.00000E+00    1.00000E+01    6.00000E+01    3.60000E+03
    5.00000E-01    7.00000E-01    1.00000E+00    2.00000E+00
```
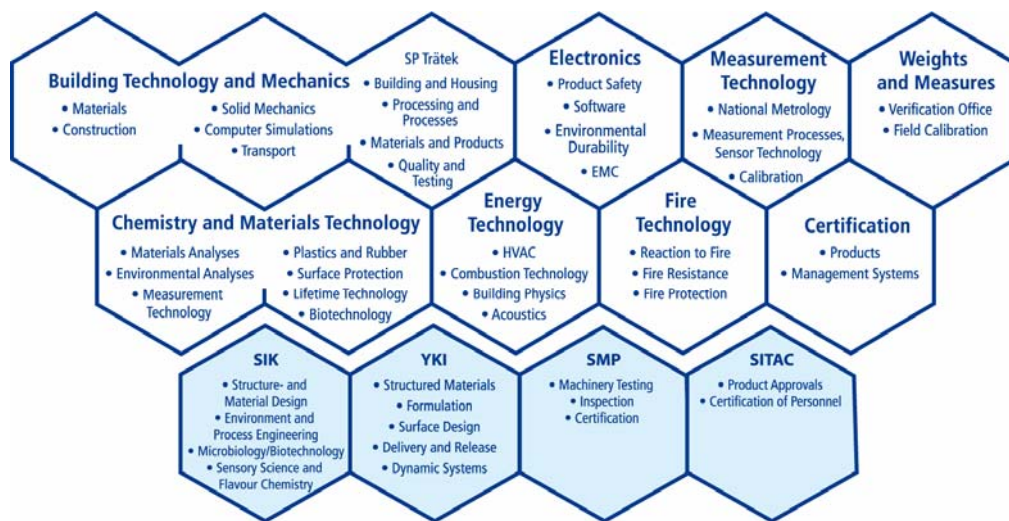
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