Tutor

Dr. Ricard Torres Castillo
Departament of Chemical Engineering

Grau en
Enginyeria
Química

Treball Final de Grau

Introduction of simulation in the "Experimentation in Chemical Engineering I" subject.

Dolores Lipso

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"Once a new technology rolls over you, if you are not part of the steamroller, you are part of the road".

Stewart Brand

CONTENTS

SUMMARY

This project consists of elaborating a detailed, easy-to-follow, verified, versatile script for the ANSYS® *Fluid Flow (Fluent)*, dedicated for the chemical engineering students enrolled on the *"Experimentation in Chemical Engineering I"* course, which explains how to obtain a simulation of the heat transfer in the non-steady-state in a sphere body, both in 3D and 2D. The script is based on one of the laboratory practices, "*Thermal Conductivity of Solids*". Although, this simulation can be done regardless of whether the students had done the experiment or not.

First, the methodology of the whole process is explained, so the efficiency of the script can be assessed.

Second, the verification of the ANSYS® values is detailed, comparing them to the analytically obtained ones. It is proved that the software data is trustworthy as the absolute relative error is smaller than 0,2% for the approved simulations. Also, the reasoning of some of the ANSYS® chosen parameters is specified, such as the size of the element of the mesh. In case of 3D simulation, the size of the element is equal to $2 \cdot 10^{-3}$ m, whereas in 2D simulation a smaller element size of $1 \cdot 10^{-3}$ m is assigned.

Then, the testing process of the script is described, with the implemented improvements from one session to another annotated.

Finally, the definitive version of the script is attached, explaining the creation of the simulation of the sphere (3D and 2D axisymmetric), the comparison of both simulations through the temperature contour graphs as well as the comparison of experimental results with data obtained through ANSYS®.

Keywords: ANSYS, Fluent, FEM, conduction, sphere.

RESUMEN

El siguiente proyecto consiste en la elaboración de un guion detallado, fácil de seguir, verificado por los estudiantes y versátil del software ANSYS® *Fluid Flow (Fluent)*, destinado a los alumnos de la asignatura "*Experimentación en Ingeniería Química I*", en el cual se explica cómo obtener una simulación de transmisión de calor en estado no estacionario en una esfera, tanto en 3D como en 2D. El guion se basa en una de las prácticas, "*Conductividad Térmica de los Sólidos*". Sin embargo, esta simulación puede llevarse a cabo independientemente de si los estudiantes habían hecho el experimento o no.

Primero, se presenta la explicación de la metodología del proceso, para que se pueda valorar la eficiencia del guion.

Después, está detallada la verificación de los datos obtenidos con ANSYS®, comparándolos con los valores calculados analíticamente. Está comprobado que los datos conseguidos a través del software son de confianza debido a que el error relativo absoluto no supera un 0,2 % en el caso de las simulaciones aprobadas. También, se especifica el razonamiento de selección de algunos parámetros de ANSYS®, tales como el tamaño del elemento utilizado en el mallado. En el caso de la simulación 3D, el tamaño de elemento es igual a $2 \cdot 10^{-3}$ m, mientras que el mallado de la simulación en 2D tiene un tamaño de elemento menor, de $1 \cdot 10^{-3}$ m.

A continuación, se describe el proceso del testeo del guion, con las mejoras implementadas anotadas entre sesiones.

Finalmente, se encuentra la versión definitiva del guion, que consiste en la explicación de la generación de la simulación de la esfera (3D), del semicírculo (2D), la comparación de ambas simulaciones a través de los gráficos de contornos y la comparación de los valores experimentales con los datos obtenidos a través de ANSYS®.

Palabras clave: ANSYS, Fluent, FEM, conducción, esfera.

INTRODUCTION

Heat transfer is a physical phenomenon which consists in thermal energy transmission caused by temperature difference between two or more systems. Heat moves from an area of high temperature to an area with a low temperature until the thermal equilibrium is reached. It is classified into three main mechanisms: conduction, convection and radiation.

Heat transfer has a crucial role in chemical industry in heat exchangers design, evaporation and condensation units as well as in thermal insulation.

Thermal conduction is one of the mechanisms of the heat transfer that occurs due the collision of particles such as molecules, atoms and electrons in solid bodies and in hypothetical fluids at rest with a velocity vector equal to zero.

One of the important properties in conduction is a thermal conductivity, which is an ability of material to transfer or conduct heat. In other words, it is a quantity of thermal energy that flows per unit of time through a unit of area for each unit of temperature difference. The value of the thermal conductivity is an important parameter in studies of heat transfer in solids, in calculating the thickness of thermal insulation and in choosing the most suitable material. Thermal conductivity depends on the physical state of the body and on the material, which can be:

- Isotropic: it has the same material properties in all directions. There are no preferable directions in heat conduction, thermal conductivity is the same at each point of the body.
- Anisotropic: the material properties vary within the direction. There are preferable directions in heat conduction, thermal conductivity depends on the position.

In this study it has been considered that the material is isotropic.

1.1. CASE DESCRIPTION

The heat conduction study consists of a nylon sphere with a known radius (r_o = 0,065 m) at ambient temperature (T_o), which is being submerged into a perfectly stirred bath filled with water at a constant temperature (T_e). The temperature of the water is higher than the initial temperature of the sphere. The heat generation is null and the solid-liquid heat transfer coefficient, *h*, is considered infinite.

1.2. ANALYTICAL RESOLUTION

The main expression of the microscopic energy balance[1] in heat transfer is:

$$\rho c_v \frac{\partial T}{\partial t} = -\rho c_v \vec{v}.\nabla T - \vec{\nabla}.\vec{q} - T\left(\frac{\partial p}{dT}\right)_\rho \left(\vec{\nabla}.\vec{v}\right) - \left(\vec{\tau}:\vec{\nabla}.\vec{v}\right) + g_e \tag{1}$$

As the object of the study is a solid body and the main heat transfer mechanism is conduction without heat generation, the generation and the velocity terms can be neglected, which transforms the equation 1 into the following expression:

$$\rho c_v \frac{\partial T}{\partial t} = -\vec{\nabla}.\vec{q} \tag{2}$$

In order to introduce the thermal conductivity term, k (W/(m·K)), into the energy balance equation, the law of heat conduction, also known as Fourier's law, should be introduced:

$$\vec{q} = -k.\nabla T \tag{3}$$

By combining the microscopic energy balance in non-stationary state and Fourier's law, the following expression is obtained, also known as *Laplace* equation:

$$\frac{\partial T}{\partial t} = \alpha \cdot \nabla^2 T \tag{4}$$

Where α (m^2/s) is the thermal diffusivity:

$$\alpha = \frac{k}{\rho\, c_p} \tag{5}$$

For a solid body C_v and C_p are approximately equal.

The resolution of the equation 4, applying the appropriate limit conditions, provides an information about the variation of temperature with the position and time. The analytical solution for the equation 4 exists for simple geometries with the unidirectional heat conduction.

One of the geometries that presents an analytical solution is a sphere with a finite radius, which is described in the next section.

1.2.1. ANALYTICAL RESOLUTION FOR A SPHERE

There is an analytical solution for the energy balance in non-stationary state for the sphere with the finite radius r_0 at the initial temperature T_0, which is submerged in a fluid at a constant temperature T_e. The solid-liquid heat transfer coefficient, h, and the thermal conductivity, k, are assumed constant and the heat flux is radial. In this case, the resulting equation expressed in partial derivatives is:

$$\nabla^2 T = \frac{1}{r^2} \cdot \frac{\partial}{dr} \left[\frac{r^2 \cdot \partial T}{\partial r} \right]$$

(6)

In order to solve the equation 6, the following limit conditions are established:

Table 2. Limit conditions for the finite sphere.

Time	Position	Limit Condition
$t = 0$	$0 < r < r_0$	$T = T_0$
$t > 0$	$r = 0$	$\partial T/\partial r = 0$
$t > 0$	$r = r_0$	$h\,(T_e - T_w) = -k\,(\partial T/\partial r)$

Also, the analytical solution is shown through dimensionless terms for the temperature, distance and time:

$$Ys = \frac{T_e - T}{T_e - T_o}$$

(7)

$$n = \frac{r}{r_o}$$

(8)

$$F_O = \frac{\alpha \cdot t}{r_o^2}$$

(9)

Where:

Y_s – dimensionless temperature

n – dimensionless distance

Fo – dimensionless time (Fourier number)

The final expression for the analytical solution of the energy balance for the sphere with the finite radius is:

$$Ys = 4 \sum_{i=1}^{\infty} \frac{\sin(\beta_i) - \beta_i \cos(\beta_i)}{2\beta_i - \sin(2\beta_i)} \cdot \frac{\sin(\beta_i \cdot n)}{\beta_i \cdot n} \cdot \exp\left(-\beta_i^2 F_o\right) \tag{10}$$

Where β_i are the infinite solutions for:

$$1 - \frac{\beta_i}{\tan(\beta_i)} = Bi \tag{11}$$

$$0 < \beta_1 < \pi < \beta_2 < 2\pi < \beta_3 < 3\pi < \beta_4 < \cdots$$

Where:

Bi – Biot number

$$Bi = \frac{h \cdot r_o}{k} \tag{12}$$

As it was mentioned earlier in this study, the heat coefficient (*h*) is supposed to be infinite, which leads to Bi $\rightarrow \infty$.

In case the Fourier number (Fo) is higher than 0,25, all terms of the summation of the equation 8 can be neglected, except for the first one:

$$Y_s = \frac{2}{\pi \cdot n} \cdot \sin(\pi \cdot n) \cdot \exp(-\pi^2 \cdot F_o) \tag{13}$$

1.3. ANSYS® AND ITS APPLICATIONS

ANSYS® is an engineering simulation software that allows predicting how a certain body will behave and/or react in the environment that surrounds it. The program is used in different branches of science and engineering, such as thermodynamics, fluid circulation, electromagnetism, structural analysis, or heat transfer. ANSYS® simulator solves the microscopic balance equations using Finite Element Method (FEM), which consists of dividing the system of interest into a lot of small fragments.

The software has two versions: the academic one, which can be downloaded for free and allows solving problems using a maximum of 500 000 elements, and the professional one, which does not have this limitation and permits to solve much more complex simulations. The version used in this paper is an academic one as the number of elements permitted is enough to do a simulation of the case described in a section 1.1.

ANSYS® software does not stop getting better and more user-friendly. Every year several versions of the program come out. The version ANSYS® *2020 R2* was used during the elaboration of this paper, being the newest one at the outset.

2. OBJECTIVES

The main objective of this project is to explain to the students of the "*Experimentation in Chemical Engineering I*" course of the University of Barcelona, through a script, how to obtain a CFD (Computational Fluid Dynamic) simulation with ANSYS® of the temperature variation of a solid sphere submerged into the fluid. Several aims are established to achieve this objective:

- To obtain basic knowledge of ANSYS® software (in academic version).
- To generate valid simulation of the sphere body in 3D and 2D.
- To prove the accuracy of simulation data obtained with ANSYS®.
- To study the possibilities of the results representation.
- To write and test the script with the feedback of some students.
- To implement the improvements to the script and to test it again.
- To give versatility to the script, so it can be divided into smaller parts and be followed separately.

3. MATERIALS AND METHODS

3.1. WORK PROCESS APPROACH

In order to elaborate a competent script, the whole process is divided in several stages.

Initially, required knowledge of the software are obtained by reading articles[2,3], courses[4] and forums[5] related to the ANSYS®, also watching videos of the CFD simulations creation process using *Fluid Flow (Fluent)* which are related to the heat transfer and resembled the most to the case of the "*Thermal Conductivity of Solids*" laboratory practice or at least have some parts in common. In parallel, the first steps with the program are taken. Once the general knowledge of the program is gained, the script elaboration is started.

When it is proved that the created simulation gives accurate data, comparing these with the analytical ones, the results treatment is chosen and added to the script. All experimental data required for the simulation is real, obtained during the realization of the laboratory practice TCS.

Once the first version of the script is written, it is revised by a tutor in order to get first feedback, some advice and to validate its testing.

Several students who passed the "*Experimentation in Chemical Engineering I*" and "*Heat Transfer*" subjects of the Chemical Engineering Degree of the University of Barcelona are asked to follow the script and give their feedback. The testing of the script is individual in order to obtain credible data and to avoid an intersection of information among participants. Every participant has a choice to use its own data obtained during the realisation of the laboratory practice or to use the one proposed in the script in form of the examples. During each session notes are taken about the problems encountered by the student. It is decided not to implement significant changes from one session to another if possible. At the end of the session the feedback is obtained through a small questionnaire, which consists of 5 general questions, which are resumed in the following table:

Table 1. The questionnaire to the participants of the script testing.

Invested time	Are the instructions clear?	Total number of the queries	General opinion/Possible improvements	Are the results correct?

After careful examining of the questionnaires and personal observations, the improvements of the original script are made.

Once the second, better version of the script is obtained, it is tested by another group of students which meet the same criteria as the first ones. The feedback is asked to prove that the implemented changes have worked.

In the end, the questionnaires of the second group are examined and the final improvements of the second script are made if required.

The final version of the script is translated to English and presented in section 4.3.

3.2. **ANSYS® APPROACH**

A series of choices is made during the elaboration of the script, which are explained in the sections 4.1.1, 4.1.2, 4.1.3 of this paper and correspond to ANSYS'® information treatment main tools:

- Pre-processing, where the selection of the analysis system and creation of the model (geometry/sketch) takes place as well as its meshing. ANSYS® disposes of two programs to create the geometry: *DesignModeler* and *SpaceClaim*. Also, the sketch can be uploaded directly from a CAD software.

- Simulation, which is responsible for the setup of a group of parameters and conditions, such as materials and their properties, boundary conditions, etc. Once the problem is defined, the program solves a set of equations, in order to generate the simulation and obtain the results.

- Post-processing, which permits to visualize the obtained data and treat it by creating charts, contours, etc.

4. RESULTS

4.1. SCRIPT ELABORATION AND DECISION MAKING

The parameters to establish and the order to follow are taken to a large extent from a previous work of A.Monné (2019) who optimized the mesh for a cylinder.

4.1.1. PRE-PROCESSING

ANSYS® software has a variety of analytical systems which are adapted for the simulation of different natural phenomena. For this experiment *Fluid Flow (Fluent)* was chosen, as it is widely used for heat transfer simulations.

4.1.1.1. GEOMETRY

ANSYS® offers two software to create the geometry of interest, *SpaceClaim* and *DesignModeler*. After trying both, it was decided to work with the *DesignModeler* because of its intuitive interface for someone without considerable experience in the CAD software. Also, it has a set of primitive figures that permits to obtain the sketch of a basic 3D geometry within a minute.

4.1.1.2. MESH

The mesh of the body had to meet the following criteria:

- Use the optimum number of elements, but also taking into account the time factor.
- Have more nodes on the surface of the body than in the interior.

As it was mentioned in the section 1.3, there are 500 000 elements available in the academic version. The final number of elements depends on its size, a parameter which can be defined by the user. The smaller is the size of the element, the bigger is the total number of these and the higher is the accuracy of the simulation results. The flip side is that the complexity of the mesh has a direct dependency on the time of the simulation execution.

The size of the element was chosen by recollecting the temperature data at different element sizes of the mesh and comparing them to the analytical solution. As this proof involves the results, the relevant summary table can be found in the section 4.1.3. Post-Processing.

The variation of the temperature near the surface of the sphere with time is more dynamic than inside it, which is why non-homogeneous distribution of the nodes is required. The Inflation function of the mesh program was used in order to establish more elements on the surface of the body.

4.1.2. SIMULATION

Once the mesh was created, the rest of the crucial parameters for the simulation were established in the Setup tool of ANSYS®. Detailed information about the correct setup of the simulations is described in the sections 2.3, for the 3D, and 3.3, for the 2D, of the final script, section 4.3.

4.1.2.1. MATERIALS

The properties of the nylon used during the generation of the simulations are resumed in the Table 2.

Table 2. Properties of nylon.

ρ, kg/m^3	1 165
C_p, J/(kg·K)	1 287 + 7 267·T[ºC]
k, W/(m·K)^6	0,30

ANSYS® permits to introduce the parameters of the material in form of equation if it is required. It was decided to introduce the constant value of the C_p, calculated with the equation 14, as it did not have an important impact on the results.

$$(c_p)_m = \frac{\int_{T_o}^{T} c_p \cdot dT}{\int_{T_o}^{T} dT} = 1\ 557\ J/(kg \cdot K) \tag{14}$$

The value of the $(c_p)_m$ may vary from one student to another as it depends on the experimental data.

4.1.3. POST-PROCESSING

ANSYS® results tool is used to obtain different kind of simulation data and permits its visualization.

4.1.3.1. *VALIDITY CHECK OF ANSYS® DATA, 3D SIMUALTION*

To assure that the data obtained with ANSYS® is reliable, it was decided to compare it with the analytical values, calculated with the expression 10. Table 3 summarizes some of the temperature data obtained with ANSYS®, simulation of the sphere (3D) at different element sizes and at different n values, and it also compares them with the analytical temperature values.

Table 3. ANSYS® 3D simulation and analytical temperature values comparison

			ANSYS®					
$n = r / r0$	t (min)	Analytical T (K)	$e = 1{,}852 \cdot 10^{-3}$ m 497 100 elements		$e = 2{,}000 \cdot 10^{-3}$ m 411 900 elements		$e = 1{,}123 \cdot 10^{-2}$ m 7 758 elements	
			T (K)	$|\varepsilon_r|$ %	T (K)	$|\varepsilon_r|$ %	T (K)	$|\varepsilon_r|$ %
	10	298,94	298,85	0,03	298,86	0,03	299,27	0,11
0,0	30	302,73	303,09	0,12	303,14	0,14	305,80	1,02
	60	315,32	315,02	0,09	315,03	0,09	317,33	0,64
	10	298,79	298,96	0,06	298,96	0,06	299,27	0,16
0,2	30	303,90	304,16	0,08	304,17	0,09	305,80	0,63
	60	316,31	315,98	0,10	315,99	0,10	317,33	0,32
	10	302,27	302,51	0,08	302,55	0,09	305,46	1,06
0,6	30	314,27	313,92	0,11	313,94	0,11	316,39	0,67
	60	323,05	322,78	0,08	322,79	0,08	324,05	0,31

The first column of the ANSYS® values corresponds to the element's size, which permits to use almost all elements available in the academic version. The size of the element of the right column is the one that was given by definition. The size of the element of the central column was tried as a close one to the smallest element allowed, but, at the same time, which did not reach the maximum number of elements given.

Although, in each case the absolute relative error is minor, due to the simplicity of the problem, it can be observed the direct dependency of the element size and total number of the elements on the accuracy of the obtained data. The bigger is the size of the element, the smaller is the total number of these and the higher is the absolute relative error.

It was decided to work with the central size of the element, $2 \cdot 10^{-3}$ m, as it presents high accuracy and the runtime is shorter than the execution of the simulation and posterior results treatment with the smallest possible size of the element ($1,852 \cdot 10^{-2}$ m).

Students will not be asked to do the comparison explained above and will directly use the approved value of the element size.

4.1.3.2. VALIDITY CHECK OF ANSYS® DATA, 2D SIMULATION

Any software has its own limitations and it is important to know how to make full use of the resources. The sphere is an axisymmetric body, so it can be represented in 2D as a semicircle turning around its symmetry axis. By making the simulation of the semicircle, a lot less elements are required in order to obtain reliable results and, as a consequence, it takes less time to get them. For that reason it was decided to show the generation of the simulation in 2D and to compare the results of both geometries as well as the execution times.

To prove the similarity of the results, temperatures of 3D and 2D simulations were exported, absolute relative errors were calculated at different times and radiuses and they were compared later. The comparison of some of the values is shown in the following Table 4.

Table 4. ANSYS® 3D and 2D simulations temperature values comparison.

n = r / r0	t (min)	Analytical T (K)	ANSYS® 3D $e = 2,000 \cdot 10^{-3}$ m 497 100 elements		ANSYS® 2D $e = 1,000 \cdot 10^{-3}$ m 7 417 elements	
			T (K)	$|\varepsilon_r|$ %	T (K)	$|\varepsilon_r|$ %
0,0	10	298,94	298,86	0,03	298,85	0,03
	30	302,73	303,14	0,14	303,05	0,11
	60	315,32	315,03	0,09	314,95	0,12
0,2	10	298,79	298,96	0,06	298,95	0,06
	30	303,90	304,17	0,09	304,11	0,07
	60	316,31	315,99	0,10	315,94	0,12
0,6	10	302,27	302,55	0,09	302,43	0,05
	30	314,27	313,94	0,11	313,88	0,12
	60	323,05	322,79	0,08	322,77	0,09

As 2D simulation is easier to execute, the smaller size of the element can be used. At first, the element size equal to $1 \cdot 10^{-3}$ m was chosen.

After analysing Table 4, it can be seen that the temperature values of both simulations are practically the same, meanwhile 2D simulation requires a lot less elements in order to get there. Some of the absolute relative error values are even smaller than the ones calculated for the 3D simulation. It can be concluded that the semicircle simulation data with the element size equal to $1 \cdot 10^{-3}$ m is accurate and can be used in the further studies.

Regarding time execution, it took 24 minutes to obtain simulation results in the case of the sphere and only 4 minutes in the case of the semicircle. In addition to this, it is much faster to generate graphs in order to export temperature values in the case of 2D rather than 3D.

Students will not be asked to do the same comparison explained above and will use directly the proved value of the element size.

4.1.3.3. 3D AND 2D ANSYS® SIMUALTATIONS DATA COMPARISON

To demonstrate some of the available tools for the results representation, it was decided to explain to the students how to obtain temperature contour graphics. Students should obtain the contours at different instants of both simulations (the selected instants do not vary from 3D to 2D), compare these and conclude that 2D simulation temperature distribution is virtually the same as the one from the 3D simulation.
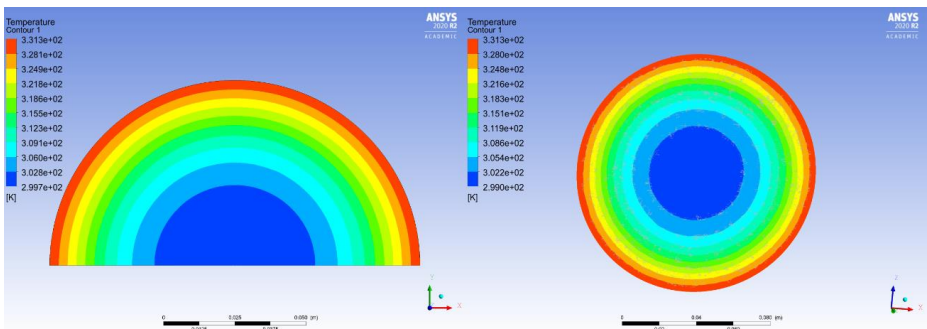
Figure 1. Temperature contour graphics at 10 minutes, a) 2D simulation; b) 3D simulation.
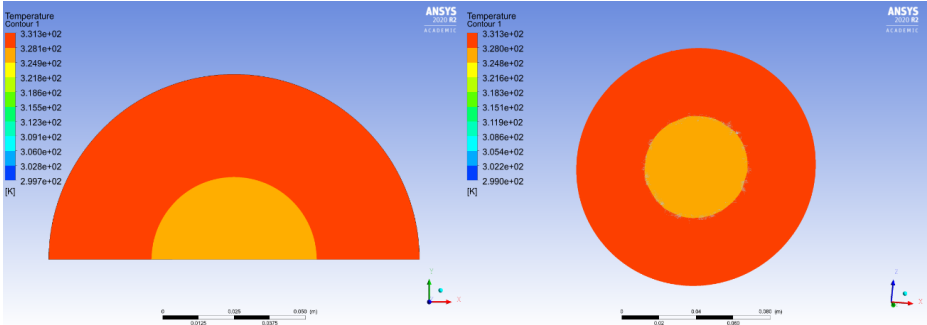
Figure 2. Temperature contour graphics at 60 minutes, a) 2D simulation; b) 3D simulation.

4.1.3.4. EXPERIMENTAL AND ANSYS® DATA COMPARISON

The main point of the original laboratory practice is to find a thermal conductivity out of experimental values of temperature. To prove the accuracy of the measured temperature, students should compare the experimental temperature with the ANSYS one. Through the point creation and chart generation student can export the temperature values and compare them to the experimental ones. This permits to observe if there is any significant deviation and what could go wrong. As an example, a comparison of the ANSYS® temperature values obtained with the 3D simulation with the size of the element equal to $2 \cdot 10^{-3}$ m and experimental values measured by a student in 2018 is shown below.
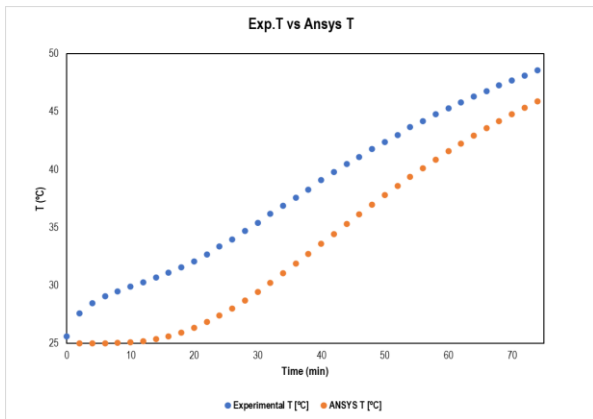
Figure 3. Plotted experimental and ANSYS® data.

It can be seen that the experimental values are above the ones obtained with the software. The initial experimental values cannot be right since, after two minutes, a significant temperature rise can be observed in the centre of the sphere. Most likely it occurred because the whole for the temperature probe was not closed properly and some water got in.

4.2. FIRST SCRIPT REVISION AND IMPROVEMENTS

The first feedback of the initial version of the script was given by the tutor who was asked to revise whether the explained steps to follow were right and accurate, as well as the clarity of these. Following his advice some changes were implemented related to the stylistics of the script and the clarity of some of the explanations.

Afterwards, it was tested by the first group, formed by 3 students. As it was mentioned in the methodology section, each session took place separately. Some changes were made after the first session:

- New image of the sphere sketch in the section 2.1. Geometry.
- In the explanation of the sketch creation, section 3.1. Geometry, the command Create was changed to Concept.
- Typos

No changes were implemented from the second session to the third one, although, some ideas of improvements were annotated based on the problems that the students had. The improvements to implement were:

- Highlight the change from steady to transient time in the General command of the Fluent program.
- Emphasize the removal of aluminium from the list of materials which is established by the definition.
- Remark the change of the analysis type from 3D to 2D at the start of the 2D simulation creation.
- Change the image of the 2D sketch to a more detailed one, which visually remarks that the drawn line to separate the circle into 2 identic parts must outstand the circumference boundary.

- Highlight the importance of the names given to the zones during the area separation process in the mesh section.

According to the questionnaires, the feedback of the first group of students was positive. Answers to some inquiry questions are summarized in the Table 5.

Table 5. Resume of the questionnaire answers of the group 1

Student	Easy to follow	Execution t (h)	Correct Results	Nº of the enquieries
1	Yes	2,25	Yes	5
2	Yes	2,50	Yes	3
3	Yes	2,25	Yes	4

The average time of the execution was about 2 hours 20 minutes and the average number of the enquiries was 4, which were the expected results for the first script testing.

In the *possible improvements* part of the questionnaire, 100% of the students suggested changing the setup and the mesh sections of the 2D simulation. Some parts of the simulation generation process are identical for the 3D and 2D cases. To avoid the repetition of the explanations, the detailed description of steps to follow was given to the 3D simulation, while in the 2D case it was asked to go back and follow the same route. Students found this way of working uncomfortable and considered it as the primary reason of the obtained errors. Also, some participants suggested the addition of more images in some sections of the script for the better understanding and process verification.

Considering personal observations and the received feedback, the changes to the original script were implemented. Apart from earlier mentioned improvements, the Setup and the Mesh sections of the 2D simulation were changed by adding more detailed explanation to both. Also, the explanation of the temperature contour diagrams comparison was modified, by making it more generic and suitable for both simulations.

The second testing of the script was carried out in order to see if the implemented changes were useful and improved the performance. Another group formed by 3 students was asked to follow the optimised script and give their feedback. Some of the inquiry answers are resumed in Table 6 below.

Table 6. Resume of the questionnaire answers of the group 2

Student	Easy to follow	Execution t (h)	Correct Results	Nº of the enquieries
1	Yes	2,00	Yes	1
2*	Yes	1,58	Yes	0
3	Yes	2,25	Yes	2

The 2nd studen had some previous knowledge of ANSYS®

Comparing these results with the previous ones, it can be seen that the implemented changes were needed and had a positive impact in the execution time, as its average decreased about 23 minutes, and the compression, as the average number of the enquiries dropped by 3.

A minor change after the second testing was implemented to the script. Even after remarking the check of the analysis type before the 2D simulation generation, one of the students did skip this step and had some problems with the execution of the simulation. As a solution, it was added a second check of this parameter, at the launch of the Fluent program.

As the final step, the final version of the script was translated to English, so in case its usage is approved by Chemical Engineering Department of UB, *"Experimentation in Chemical Engineering I"* will be the first obligatory subject to implement usage of English language in its program.

4.3. FINAL SCRIPT

This script was written as an addition to the original script of the "*Thermal Conductivity of Solids*" laboratory practice. Students can use their experimentally obtained data during the simulation generation or use those given as examples, which are real values measured by previous students. Therefore, the simulation can be done without having done the experiment beforehand.

As mentioned earlier, the script consists of 2 simulations of the sphere, the 3D and the 2D one. These simulations are independent of each other, so they can be generated separately by different students/group of students and then compared, those in charge can choose.

If the students have not carried out the experiment, for the last section of the script, *ANSYS® and experimental results comparative using 3D simulation*, the experimental data, used during the writing of this paper (attached in annex), can be provided by the person in charge of the course.

1. Introduction

1.1. Script objectives

- Run a series of simulations using data from the laboratory practice "*Determination of thermal conductivity of solids (TCS)*" in order to get familiarized with ANSYS® software.
- Compare the results obtained in the 3D simulation with those of the 2D simulation.
- Compare the experimental data with the theoretical one, gotten through ANSYS® simulation.

1.2. Work configuration and hypothesis

The following script was written using the academic version of the program, ANSYS® *Student 2020 R2*. In case there is a newer version, script validity should be checked. Through this laboratory practice (the experiment and the simulation parts), it is assumed that the involved bodies are isotropic and the solid-liquid heat transfer coefficient, *h*, is infinite.

2. Creation of the simulation in 3D

After installing ANSYS®, launch the *Workbench 2020 R2* program, which can be found in *ANSYS 2020 R2 folder*. Once opened (it may take a little while), in the **Toolbox** window choose the analytical system of interest, which in this case is *Fluid Flow (Fluent)*. Right away, in the *Project Schematic* window, the work *Module A* appears. It consists of 5 parts: geometry, mesh, setup, solutions and results. If at the beginning of the simulation the student has difficulties to locate the necessary window, screenshots of the main menus of the programs with some indications can be found in the annex of the script.

Throughout the script, system commands, buttons, options and sections are marked in **bold**, while names of work windows, tools and programs are written in *italics*.

2.1. Geometry

Once the work module has been created, right-click on the second option of the Module A: **Geometry**. Two computer-aided design software options appear: *SpaceClaim* and *DesignModeler*. Choose the *DesignModeler* option.

After the *DesignModeler* window is open (it is not immediate either), the plane of the work should be chosen. In order to do that, in the window **Tree Outline** click on the **XYPlane** option.

As a result, the coordinate system with its X-Y-Z axes appears in the Graphics window and in the **Plane** section of the window *Details View* the X-Y plane should be figured.
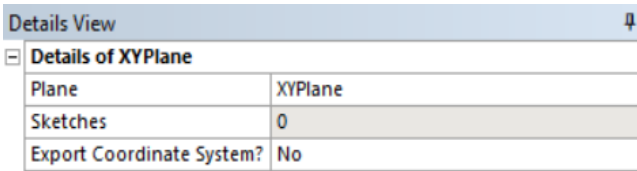

Figure 1. The "Details View" window after choosing the plane of the work.

The next step is the creation of the figure. In the top menu, click on the **Create** button. At the end of the displayed list there is a collection of basic figures, called **Primitives**, where all used figured at CTS practice can be found (sphere, parallelepiped, cylinder).
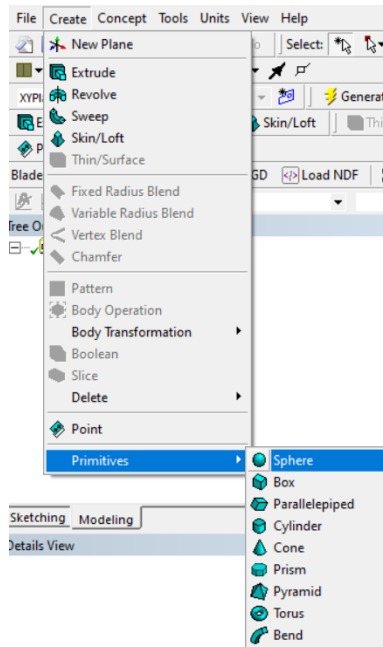
Figure 2. Basic figures collection location.

Choose the **Sphere** option. By rolling forward the mouse wheel, zoom in the figure, which, for the moment, is just a framework of the sphere (see Figure 3).
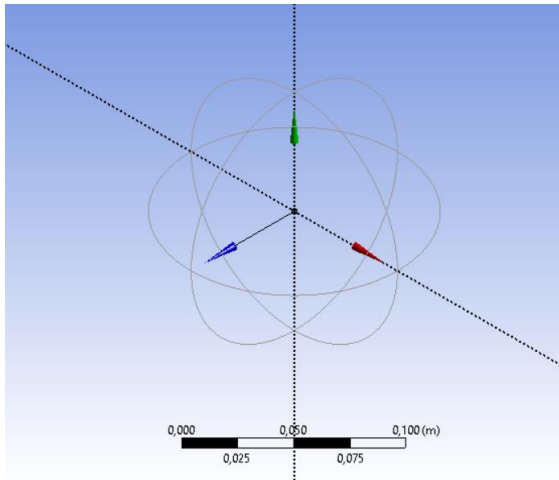
Figure 3. The framework of the future sphere before generating the figure.

In the window *Details View*, set the centre of the figure, which in this case is situated at the beginning of the coordinates, so the fields **FD3, FD4** and **FD5** should have a 0 m. In order to set the radius of the sphere, introduce it into the **FD6, Radius (>0)** field. The radius of the nylon sphere used at the practice is 0,065 m (for the decimal, the comma is used, not the period).

To generate the body, click on the button with a lightning bolt: **Generate**.
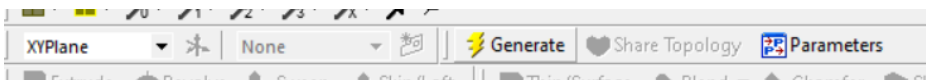
Figure 4. DesignModeler application toolbar with the Generate option.

The framework in the **Graphics** window should turn into a grey sphere.

After creating the body, close the *DesingModeler* program and return to the *Workbench*. Now, in the **Geometry** section, instead of the question mark, a green tick should appear, indicating that the body has been defined and there are no errors (see Figure 5).
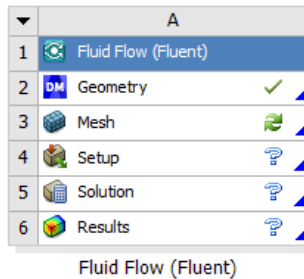
Figure 5. Module A after creating the geometry.

2.1.1. Save the project

Before proceeding with the next step, which is the meshing of the body, it is convenient to save the simulation.

In the top menu of the program *Workbench*, display the **File** option, click the **Save As** icon and choose the folder of interest. Important: once the folder for the project has been chosen, it is highly recommended not to change the location of the simulation file. This guarantees the correct execution of the simulation and avoids possible errors. Also, the project name cannot contain capital letters or symbols, such as commas, periods, accents, etc. The best option is to give it a lowercase name, for example, sphere.

2.2. Mesh

Double-click on the **Mesh** option in *Module A* to open another program (it may also take a little while) called *Meshing*, where the number of nodes and elements to be used during model resolution is determined.

Next, the basic meshing data is established: analytical model, element size, etc. In the *Outline* window, choose the **Mesh** option and in the lower work window, *Details of Mesh*, assure that the **Defaults** section has the following parameters established (see Figure 6):
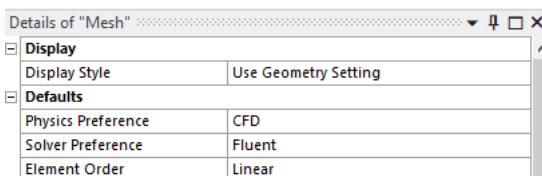
Figure 6. The parameters chosen in the Details of "Mesh" work window.

In the same window, in the **Element Size** field, write down the value of 0,002 m (again, the comma is used for the decimal).

Then, proceed to the separation of the geometry into zones[7], so the different number of nodes/elements can be used in each area. In the top bar of the window (see Figure 7) choose the **Face** command (in icon of a cube with the upper face in green) and then click on the sphere. With this step only the surface of the sphere has been selected.
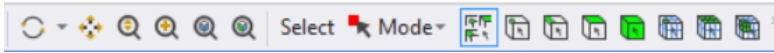

Figure 7. Part of the central work window top bar with mesh commands.

To ensure that the surface of the sphere has been chosen and not the entire body, check that the following text appears in the bottom blue bar (see Figure 8):

Figure 8. Bottom bar of the Meshing program after selecting the surface of the sphere.

Now right-click the sphere and, from the pop-up list, choose one of the last options: **Create Named Selection**. In the name field, type *surface* and click the **OK** button. The area which corresponds to the surface of the sphere has been created.

In order to select the interior volume of the figure, choose the **Body** command (green cube icon) in the top bar of the central window (see Figure 7). Now click on the sphere. Once the body is selected, right-click on it and from the pop-up list choose the command: **Create Named Selection**. To ensure that the volume of the sphere has been chosen, the following text should appear in the bottom blue bar (see Figure 9):

Figure 9. Bottom bar of the Meshing program after choosing the sphere body.

In this case, the name *volume* is given to the area.

After separating the figure into two areas, surface and interior, proceed to mesh it (fractionate the sphere into small portions). The idea is to achieve a nonhomogeneous mesh by having more nodes on the surface of the figure than in the centre. To do this, in the *Outline* window, right-click on the **Mesh** section, unfold the **Insert** option and choose the **Inflation** function.

Now, return to the top bar of the central window (see Figure 7), click on the **Body** command and then select the sphere. In the *Details of "Inflation"*, within the **Scope** section, there is a **Geometry** field marked in yellow. Click on **No selection** and then, within the same line, on **Apply**. The figure has been selected correctly if the **Geometry** field is no longer marked in yellow and it is annotated **1 Body** there. The sphere in the central window should be blue at this point.

Then, click on the **Face** command in the top bar (see Figure 7) and then select the sphere, the figure should turn green again. Go back to the *Details of "Inflation"* window and in the **Boundary field** (within **Definition** section) click on the **No selection** and then, within the same field, on **Apply**. The surface of the figure has just been selected. To prove that it has been chosen correctly, in the **Boundary** field, the following text must appear: **1 Face**. With these steps through the **Inflation** function, it has been indicated to the program that more nodes are required on the surface of the body rather inside it. Before proceeding to the next step, check that the **Inflation** function has been completely defined. If so, then the **Inflation** function (which forms a part of the Mesh section), in the *Outline* window, should have a green tick instead of the question mark.

Finally, the mesh is created by clicking on the **Generate** button in the top icon bar (see Figure 10).
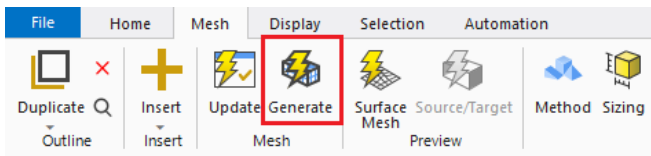

Figure 10. Generate function of the Meshing application.

The meshing process can take several minutes. Once generated, the sphere should be grey and have a net all over its surface (see Figure 11). If, in the central window, the body is still blue or green, simply click on the **Mesh** option of the *Outline* window.
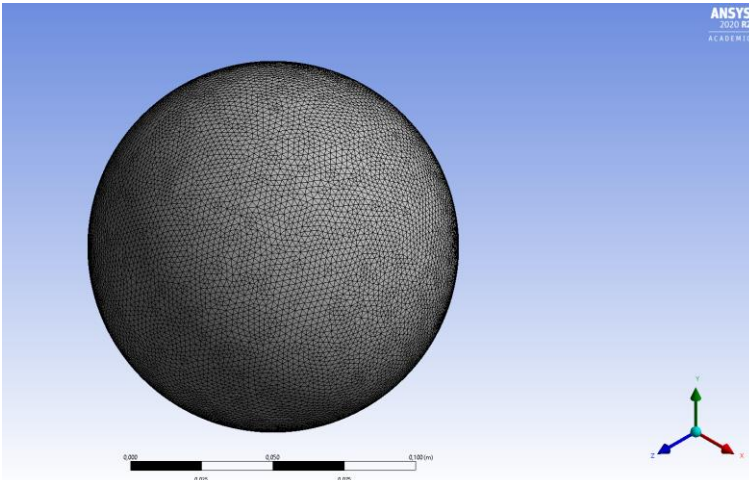
Figure 11. The surface of the sphere after mesh generation.

To see the total number of nodes and elements involved in the generated mesh, once the **Mesh** option of the *Outline* window has been selected, in the lower window, *Details of "Mesh"*, open the **Statistics** section. Considering the size of the element that had been chosen previously, the mesh should exceed 400 000 elements, which is enough to obtain reliable results.

To check that the nodes have also been generated inside the body and that they are less than on the surface, choose the **Home** option in the top bar of the program and below it, among the commands, find the **Section Plane** and click on it. Then, trace the line in the middle of the body. As now only half of the sphere remains in the central window, with the **Rotate** command (7th command of the top bar, see Figure 7), rotate the body till seeing its interior (see Figure 12).
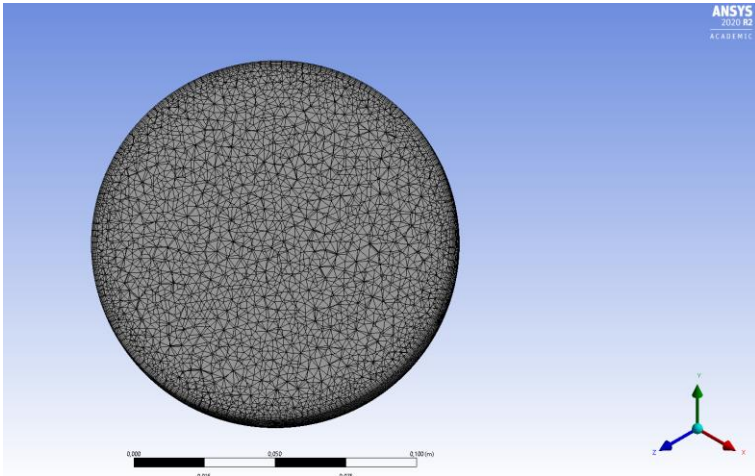
Figure 12. The meshing of the volume of the sphere.

Before closing the *Mesh* program, the created section must be deleted. In the *Section Planes* window, just below the *Outline* window, (in case the window is not open, click on the **Section Planes** tab in the lower left corner of the program), choose the previously created plane: **Section Plane1** and delete it by clicking on the red cross (**X**).
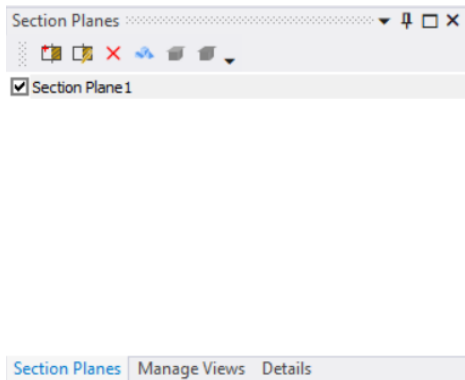

Figure 16. The Section Planes tab after creating the section.

Now close the *Mesh* program and return to the main program: *Workbench*. If a lightning bolt appears in the **Mesh** option of the *Module A*, then right-click on it and choose the **Update** command from the list. Once the mesh section has a green tick, proceed to the next step of the simulation: **Setup**.

2.3. Setup

Double-click on the **Setup** option of the *Module A* to launch the program *Fluent*. In the pop-up window, *Fluent Launcher*, in the **Options** section active the **Double Precision** option. The rest of the **Solver** options and variables are left by default. Click the **Start** button.

Once the work window of the *Fluent* is open, click the **OK** button of the pop-up *Key Behavioural Changes* window. In the bottom window **Console** appear some warnings (yellow triangle and red circle with the exclamation mark in it) related to the absence of one of the licenses, which the academic version does not have. This notification can be ignored as it does not have any influence on this simulation.

Next step consists of establishing the series of conditions for the simulation. The underlined commands in Figure 13 are the ones that are used to set up the desired simulation. The rest of the commands of the *Outline View* window are left unchanged.
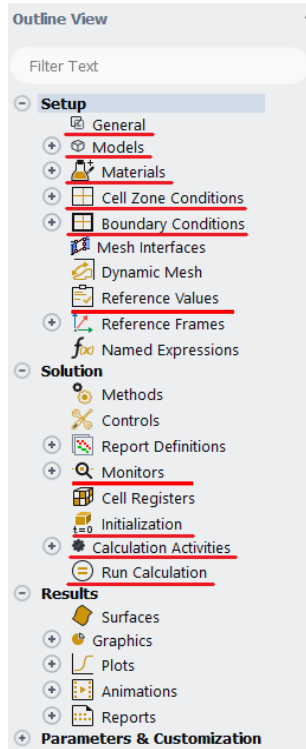
Figure 13. The Outline View window with the parameters to be defined.

Select the command **General** and in the *Task Page* window, active the non-stationary state of the system by choosing the **Transient** option in the **Time** section.
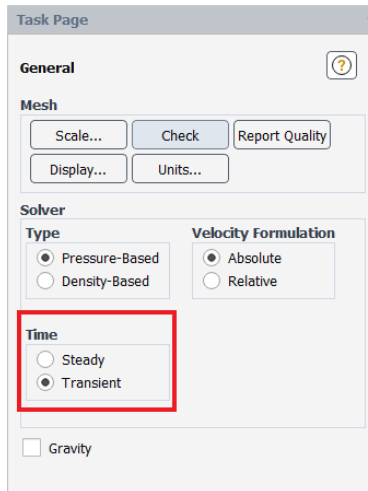

Figure 14. Configuration of the General parameters to be set.

Then, open the menu of the **Models** command of the *Outline View* window (by clicking once on the + sign or double-clicking on **Models**). Right-click on the **Energy** option and active it by choosing **On** option.

Now, display the **Materials** command menu. Two sections appear: Fluid and Solid, which by default are air and aluminium. It is not essential to change the fluid that surrounds the sphere, but it is important to establish that it is made of nylon. To do this, right-click on the **Solid** line and then click on the **New** button. In the pop-up window, *Create/Edit Materials*, enter the following data:

- Name: nylon
- Chemical Formula: c12h20n2o2
- Material Type: solid
- Density (kg/m3): constant; 1165
- Cp (Specific Heat) (j/kg-k): constant; 1557 (($c_p)_m$ of the laboratory practice)
- Thermal Conductivity (w/m-k): constant; 0.3 (mean value for practice temperature)

To save the material, click on the **Create/Generate** button and close the window. Now there are two materials in the list: aluminium and nylon. At this point, the aluminium cannot be removed because it is selected in some settings of the program. Once the boundary conditions have been established, which is the next step, it will be possible to delete the aluminium from the Materials.

Then go back to the *Outline View* window and expand the **Cell Zone Conditions** command and right-click on the **Fluid** option. In the pop-up list in the **Type** select **Solid**. In the *Solid* window, which opens immediately, before clicking the **Apply** button, confirm that in the **Material Name** field **nylon** is chosen and then close the window.

Now, open (in the same way as above) the following command: **Boundary Conditions**, display the **Wall** option and double-click on the **Surface**. In the pop-up window, *Wall*, open the **Thermal** tab and choose the **Temperature** option in the **Thermal Conditions** section, as shown in Figure 15. The temperature in the **Temperature** field corresponds to the T_e (stirred bath temperature) of the CTS practice, introduce it or use the one from Figure 15. Before closing the window, check that in the **Material Name** field the chosen material is **nylon**.
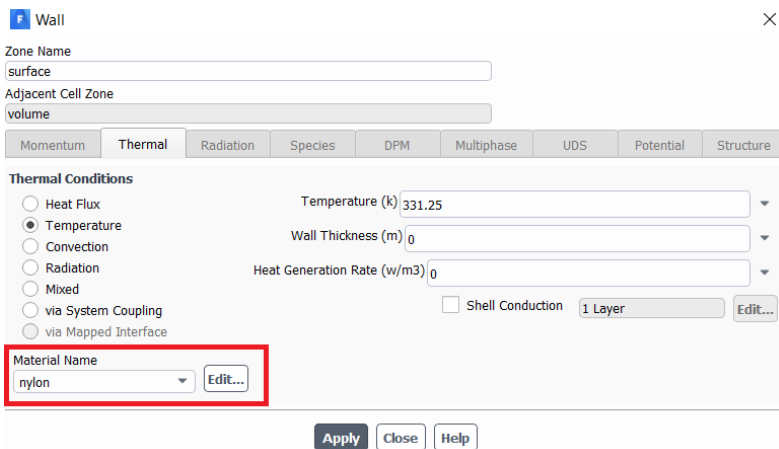

Figure 15. Configured Wall window.

To avoid possible confusions, go back to the **Materials** command and delete the aluminium from the list.

Now, open the **Reference Values** command by double clicking on it. In the *Task Page* window, display the **Compute from** option and choose the **surface** of the sphere. Repeat the

same with the last line of the menu, the **Reference Zone**, but in this case choose the **volume** of the figure. It is not necessary to change the rest of the reference values.

In the *Outline View* window, in the **Solution** section, there are many parameters that can be left at their default values. However, it should be noted that in the **Monitors** command, when displayed, the **Residuals** parameter of the **Energy** Balance is set to 10^{-6}.

Then double-click on the **Initialization** command. In the neighbouring *Task Page* window, set the following parameters:

- Initialization Method: **Standard Initialization**
- Compute from: **Surface**
- Initial Values / Temperature (k): Initial temperature value of the solid in laboratory practice, **T$_o$**. For example: 298.75 (a point is used to separate decimals).

The rest of the fields are left as they are. Click the **Initialize** button (the parameters have been saved, but the simulation has not started yet).

Then, click twice on the **Calculation Activities** command in the *Outline View* window and, in the *Task Page* window, edit the first line, **Autosave Every (Time Steps)**, by clicking on the **Edit** button. Choose the parameters shown in Figure 16:
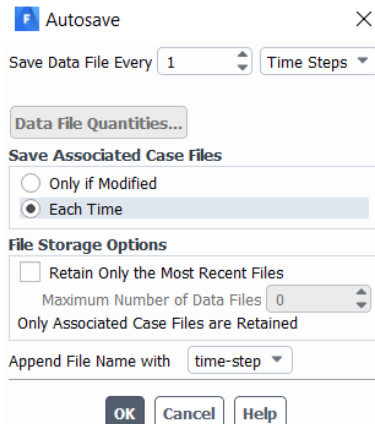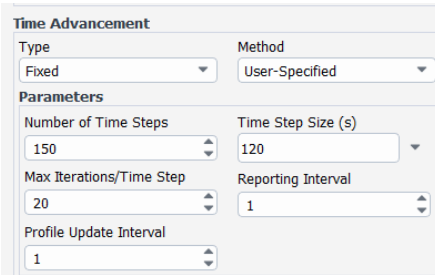

Figure 16. Calculation Activities Autosave window with set parameters.

As the last step, click on the **Run Calculation** command in the *Outline View*. In the **Task Page** window, in the **Parameters** section, enter the values shown in Figure 17.

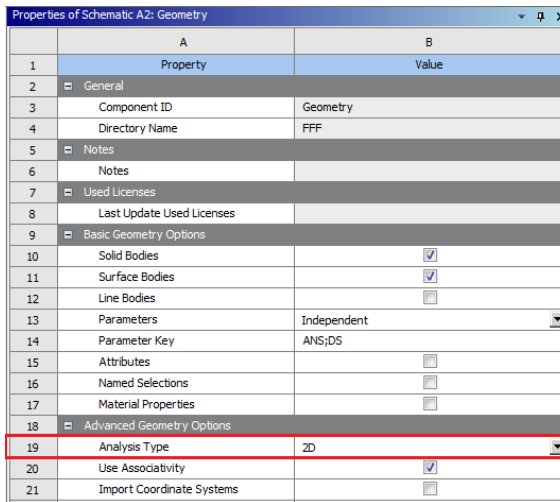Figure 17. The parameters of the Run Calculation command to be set.

Finally, the simulation can be started by clicking the **Calculate** button at the bottom of the *Task Page* window. The process can take up to 25 minutes. Once the calculation has been finished, save the project and close the *Workbench* program.

3. Creation of the simulation in 2D

A new simulation is started by re-opening the *Workbench 2020 R2* program and choosing the *Fluid Flow (Fluent)* analytical system.

3.1 Geometry[8]

Click once the left mouse button on the **Geometry** option of the *Module A*. <u>Important:</u> In the **Properties of Schematic A2: Geometry** window (see Figure 18) in the **Advanced Geometry Options** section, choose **2D** as the **Analysis Type** (line number 19).

	A	B
	Property	Value
2	General	
3	Component ID	Geometry
4	Directory Name	FFF
5	Notes	
6	Notes	
7	Used Licenses	
8	Last Update Used Licenses	
9	Basic Geometry Options	
10	Solid Bodies	☑
11	Surface Bodies	☑
12	Line Bodies	☐
13	Parameters	Independent
14	Parameter Key	ANS;DS
15	Attributes	☐
16	Named Selections	☐
17	Material Properties	☐
18	Advanced Geometry Options	
19	Analysis Type	2D
20	Use Associativity	☑
21	Import Coordinate Systems	☐

Figure 18. Properties of Schematic A2: Geometry" window after choosing 2D in the analysis type.

Right-click on the second option of the Module A: **Geometry**. Two computer-aided design software options appear: *SpaceClaim* and *DesignModeler*. Choose the *DesignModeler* option. Sphere is an axisymmetric body figure, so its 2D representation is a semicircle rotating around its axis of symmetry.

Once *DesignModeler* program has been opened, choose the working plane, **XY Plane,** in the *Tree Outline* window. To see the plane in 2D, click on the **Z** axis of the plane controller (see Figure 19).
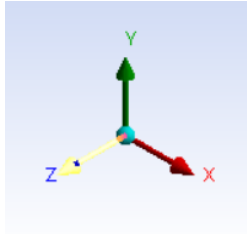
Figure 19. Plane controller.

Once there is the XY plane in the centre window, click on the **Sketching** tab in the *Tree Outline* window. To draw a semicircle quickly, follow the steps below:

- Choose **Circle** in the **Draw** menu of the *Sketching Toolboxes* window.
- In the central **Graphics** window, place the cursor in the centre of the axes and draw the circle (of any diameter).
- Select the **Dimensions** menu in the *Outline* window and click first on the surface of the drawn circle and after moving the cursor click again, this time outside the surface of the figure. The diameter of the drawn circle just has been measured.
- In the *Details View* window in the **Dimensions: 1** menu, the diameter of the circumference is set to 0.13 m in the **D** field. Zoom the sketch by scrolling forwards the mouse wheel.
- Go back to the **Draw** menu, choose the **Line** option and draw a horizontal line on the X - axis (see Figure 20). The line must extend outside the circumference. For the correct functioning of the simulation, the X - axis must be the symmetry axis.
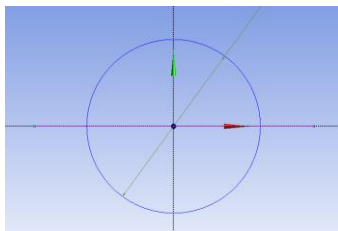

Figure 20. Circle divided into two symmetrical parts by a straight line.

- Open the **Modify** menu of the *Outline* window and use the **Trim** command to trim the circle by eliminating the part of the circle below the X - axis and the excess parts of the line (see Figure 21).
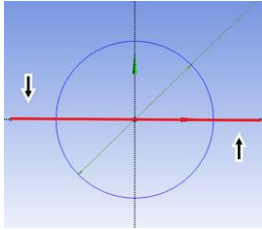
Figure 21. Resulting semicircle after using the Trim command.

- Open the **Modeling** tab of the *Outline* window and click on the **Concept** option in the top bar of the *DesignModeler* work window. In the pop-up list, choose the **Surfaces From Sketches** command.
- In the *Tree Outline* window, select the sketch by clicking on the **Sketch1** line.
- In the *Details View* window, in the **Base Objects** line, click on **Apply**.
- Click on the **Generate** button to create the figure.

Now, the *DesignModeler* program can be closed and it is proceeded to the next step, meshing.

3.1.1. Save the project

Before proceeding with the next step, which is the meshing of the body, it is convenient to save the simulation.

In the top menu of the program Workbench, display the File option, click the Save As icon and choose the folder of interest. Important: once the folder for the project has been chosen, it is highly recommended not to change the location of the simulation file. This guarantees the correct execution of the simulation and avoids possible errors. Also, the project name cannot contain capital letters or symbols, such as commas, periods, accents, etc. The best option is to give it a lowercase name, for example, semicircle.

3.2. Mesh

Double-click on the **Mesh** option in *Module A* to open another program (it may also take a little while) called **Meshing**, where the number of nodes and elements to be used during model resolution is determined.

Next, the basic meshing data is established: analytical model, element size, etc. In the *Outline* window, choose the Mesh option and in the lower work window, *Details of Mesh*, assure that the **Defaults** section has the following parameters established (see Figure 25):
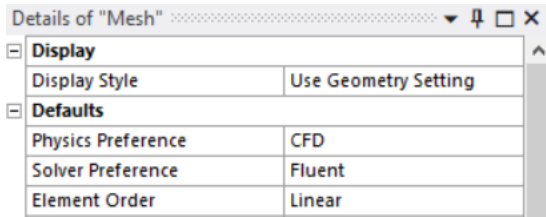
Figure 25. The parameters chosen in the Details of "Mesh" work window.

In the same window, in the **Element Size** field, write down the value of 0,001 m (again, the comma is used for the decimal).

Then, proceed to the separation of the geometry into zones, so the different number of nodes/elements can be used in each area. Also, this step is necessary to define the symmetry later. The areas to be separated are interior, edge, and axis (see Figure 23).
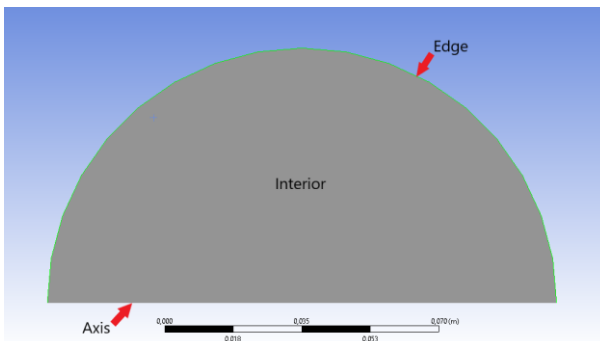

Figure 23. The areas of the semicircle to be separated.

To separate the edge and the axis, the **Edge** command of the top toolbar is used (see Figure 24).

Figure 24. Part of the central work window top bar with mesh commands.

First, click on the **Edge** command and then click on the upper edge of the sketch to select it. The edge of the semicircle should turn green. Once selected, right-click on it and, from the list, choose one of the options: **Create Named Selection**. In the name field, type *edge* and click the **OK** button.

Now, choose the **Edge** command again, but now select the base of the semicircle. Right-click on it and choose the **Create Named Selection** option. In the name field, type *axis* and click the **OK** button. In this case, it is <u>important</u> to give to the zone this exact name in order to simplify the work later on, during the setup of boundary conditions.

In order to select the interior of the figure, choose the **Face** option (a cube icon with the upper face in green) in the top toolbar (see Figure 24) and select the inner part of the semicircle. Once selected, right-click on it and from the pop-up list choose the command: **Create Named Selection** and name the area as *interior*.

After separating the figure into three areas, edge, interior and axis, proceeded to mesh them (fractionate the figure into small portions). The idea is to achieve a nonhomogeneous mesh by having more nodes on the surface of the figure. To do this, in the *Outline* window, right-click on the **Mesh** section, unfold the **Insert** option and choose the **Inflation** function.

Now, return to the top bar of the central window (see Figure 24), click on the **Face** option and then select the interior of the semicircle. In the *Details of "Inflation"* window, within the **Scope** section, there is a **Geometry** field marked in yellow. Click on **No selection** and then, within the same line, on **Apply**. The figure has been selected correctly if the **Geometry** field is no longer marked in yellow and it is annotated **1 Face** there. The semicircle in the central window should be blue at this point.

Then, click on the **Edge** option in the top toolbar and then select the upper edge of the figure. Go back to the *Details of "Inflation"* window and in the **Boundary** field (within **Definition** section) click on the **No selection** and then, within the same field, on **Apply**. The edge of the figure has just been selected. To prove that it has been chosen correctly, in the **Boundary** field, the following text must appear: **1 Edge**. Before proceeding to the next step, check that the **Inflation** function has been completely defined. If so, then the **Inflation** function, which forms a part of the **Mesh** section within the **Outline** window, should have a green tick instead of the question mark.

Finally, create the mesh by clicking on the button **Generate** (the one with the lightning bolt, see Figure 25).
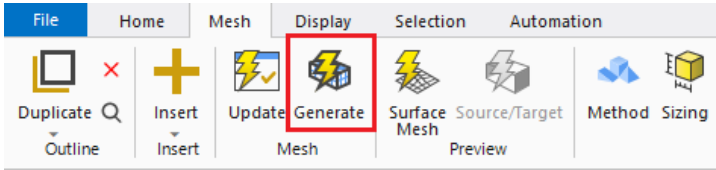
Figure 25. Generate function of the Meshing application.

The meshing process takes less than a minute. Once generated, the semicircle should be grey and have a net all over its surface (see Figure 26). If in the central window, the figure is still blue or green, simply click on the **Mesh** option of the *Outline* window.
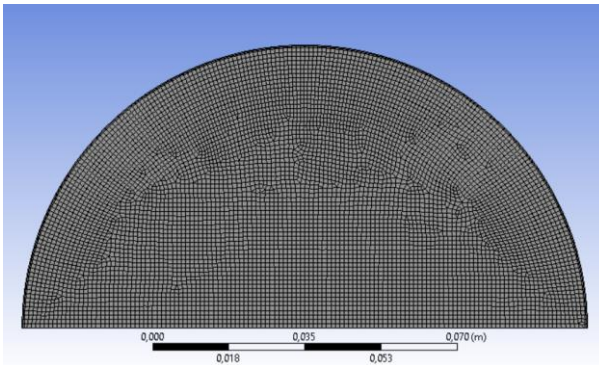

Figure 26. Meshing of the semicircle with a node size of 0.001 m.

To see the total number of nodes and elements involved in the generated mesh, once the **Mesh** option of the *Outline* window has been selected, in the lower window, *Details of "Mesh"*, open the **Statistics** section. Considering the size of the element that had been chosen previously, the mesh should exceed 7000 elements, which in this case is enough to obtain reliable results.

Now close the *Meshing* program and return to the main program: *Workbench*. If a lightning bolt appears in the **Mesh** section of the *Module A*, then right-click on it and choose the **Update** command from the list. Once the mesh section has a green tick, proceed to the next step of the simulation: **Setup**.

3.3. Setup

Double-click on the **Setup** option of *Module A* to launch the program *Fluent*. In the pop-up window, *Fluent Launcher*, in the **Options** section, active the **Double Precision** option. The rest of the default **Solver** options and variables are left by default. Reassure that the in the **Dimension** section **2D** appears. Click the **Start** button.

Once the work window of the *Fluent* is open, click the **OK** button of the pop-up *Key Behavioural Changes* window. In the bottom window *Console* appear some warnings (yellow triangle and red circle with the exclamation mark in it) related to the absence of one of the licenses, which the academic version does not have. This notification can be ignored as it does not have any influence on this simulation.

The next step consists of establishing the series of conditions for the simulation. The underlined commands in Figure 27 are the ones that are used to set up the desired simulation. The rest of the commands of the *Outline View* window are left unchanged.
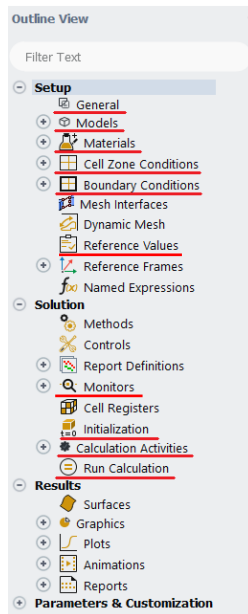

Figure 27. The Outline View window with the parameters to be defined.

Select the command **General** and in the *Task Page* window, active the non-stationary state of the system by choosing the **Transient** option in the **Time** section and choose the **Axisymmetric** option in the **2D Space** section (see Figure 28).
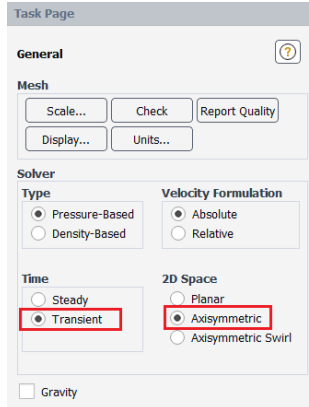
Figure 28. Configuration of the General parameters to be set.

Now, display the **Materials** command menu. Two options appear: **Fluid** and **Solid**, which by default are air and aluminium. It is not essential to change the fluid that surrounds the sphere, but it is important to establish that it is made of nylon. To do this, right-click on the **Solid** option and then click on the **New** button. In the pop-up window, **Create/Edit Materials**, enter the following data:

- Name: nylon
- Chemical Formula: c12h20n2o2
- Material Type: solid
- Density (kg/m3): constant; 1165
- Cp (Specific Heat) (j/kg-k): constant; 1557 (mean integral between To and the last experimental temperature)
- Thermal Conductivity (w/m-k): constant; 0.3 (average value for practice temperature)

To save the material, click on the **Create/Generate** button and close the window. Now there are two materials in the list: aluminium and nylon. At this point, the aluminium cannot be removed because it is selected in some settings of the program. Once the boundary conditions have been established, which is the next step, it will be possible to delete the aluminium from the Materials.

Then go back to the *Outline View* window and expand the **Cell Zone Conditions** command and right-click on the **Fluid** option. In the pop-up list in the **Type** select **Solid**. In the *Solid* window, which opens immediately, before clicking the **Apply** button, confirm that in the **Material Name** field **nylon** is chosen and then close the window.

Now, open (in the same way as above) the following command: **Boundary Conditions**. Assure it consists of three sections: axis, internal and wall (see Figure 29).
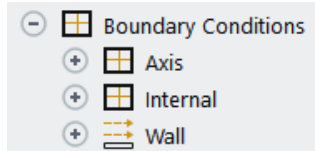

Figure 29. The Boundary Conditions displayed command.

Each section corresponds to the separated area during the mesh process. In case the created zone that corresponds to the axis of the semicircle does not appear in the **Boundary Condition** command, display the **Wall** option and right-click on the name that was given to the axis area, open the **Type** parameter and choose the **Axis** option.

Now, display the **Wall** option and double-click on the **Edge**. In the pop-up window, *Wall*, open the **Thermal tab** and choose the **Temperature** option in the *Thermal Conditions* section, as shown in Figure 30. The temperature in the **Temperature field** corresponds to the T_e (stirred bath temperature) of the CTS practice, introduce it or use the one from Figure 30. Before closing the window, check that in the **Material Name** field the chosen material is nylon.
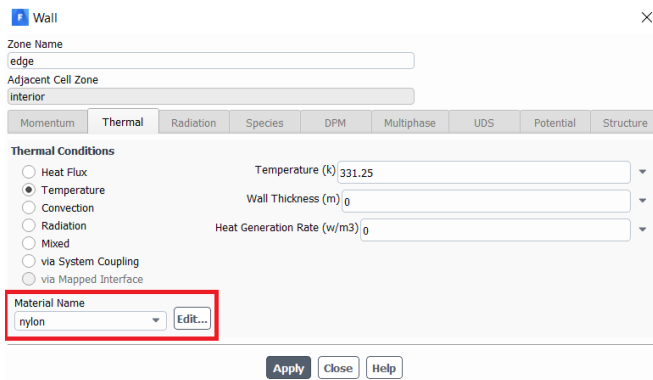

Figure 30. Configured Wall window.

To avoid possible confusions, go back to the **Materials** command and delete the aluminium from the list.

Now, open the **Reference Values** command by double clicking on it. In the *Task Page* window, display the **Compute from** option and choose the edge of the semicircle. Repeat the same with the last line of the menu, the **Reference Zone**, but in this case choose the interior of the figure. It is not necessary to change the rest of the reference values.

In the *Outline View* window, in the **Solution** section, there are many parameters that can be left at their default values. However, it should be noted that in the **Monitors** section, when displayed, the **Residuals** parameter of the **Energy** Balance is set to 10^{-6}.

Then double-click on the **Initialization** command. In the neighbouring *Task Page* window, set the following parameters:

- Initialization Method: **Standard Initialization**

- Compute from: **Edge**

- Initial Values. Temperature (k): Initial temperature value of the solid in laboratory practice, T_o. For example: 298.75 (a point is used to separate decimals).

The rest of the fields are left as they are. Click the **Initialize** button (the parameters have been saved, but the simulation has not started yet).

Then, click twice on the **Calculation Activities** command in the *Outline View* window and, in the *Task Page* window, edit the first line, **Autosave Every (Time Steps)**, by clicking on the **Edit** button. Choose the parameters shown in Figure 31:
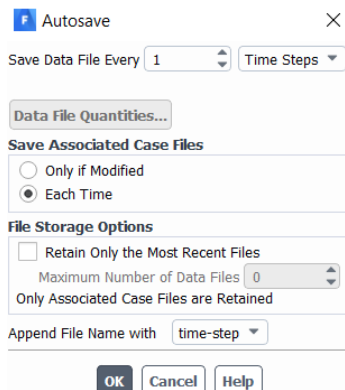

Figure 31. Calculation Activities Autosave window with set parameters.

As the last step, click on the **Run Calculation** command in the *Outline View* window. In the *Task Page* window, in the **Parameters** section, enter the same as shown in Figure 32:

Figure 32. The parameters of the Run Calculation command to be set.

Finally, the simulation can be started by clicking the **Calculate** button at the bottom of the *Task Page* window. The process can take up to 5 minutes. Once the calculation has been finished, close the *Fluent* work window and save the project. Now proceed to the final step of the simulation, results treatment.

4. Results treatment

4.1. 2D and 3D simulation comparative

Comparison of the results of the two simulations will be made by plotting the temperature profiles of each one.

The steps described below are used to obtain the contour graphics of the temperature of profiles in both 2D and 3D simulations.

From the *Workbench* program, open the last section of the *Module A*, **Results**. Once loaded, the unfilled semicircle should appear in the central window *View 1* in case of the 2D simulation. In 3D simulation the *View 1* window is empty. Nevertheless, the creation of the plane and the contour graph can be executed.

In order to create the plane in the top toolbar (see Figure 33) click on the **Location** button and in the pop-up list choose the **Plane** option.
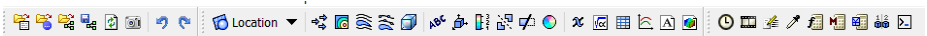

Figure 33. The Results program command bar.

The default name of the plane, *Plane 1*, can be left. In the *Details of (plane name)* window, confirm that the **XY plane** is set in the **Method** parameter and that the **Z** axis is set to 0,0 m. After checking these parameters, click on the **Apply** button. In the case of the 2D, the plane has been created correctly if the previously empty semicircle now has a grey plane, the same size as the original figure (see Figure 34). A grey circle should appear in the *View 1* window in case of the sphere simulation.
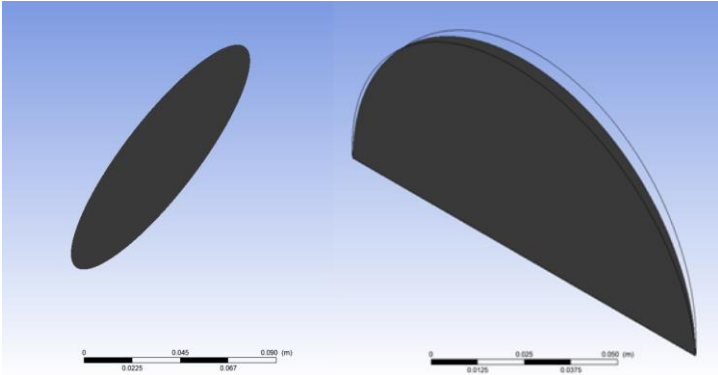

Figure 34. The plan created through the Location command: a) 3D simulation; b) 2D simulation.

In the top toolbar (see Figure 33) click on the **Contour** button (a square with several circles inside) and give it a name, for example, *2d* or *3d*, depends on the simulation. In the *Details of 2d / 3d* window, in the Location parameter, choose the previously created plane, *Plane 1*, and in the next parameter, **Variable**, choose the temperature option, **Temperature**. Then click on the **Apply** button. After a few seconds, the grey plane is divided into different zones (semicircles of smaller radius) of different colours that represent the temperature profiles at a certain time. By default, ANSYS® displays the temperature distribution of the last iteration. To view the temperature profiles at different instants, find the **Timestep Selector** button (a clock icon) in the top toolbar (see Figure 33). In the pop-up window, choose the time of interest (see Figure 35).
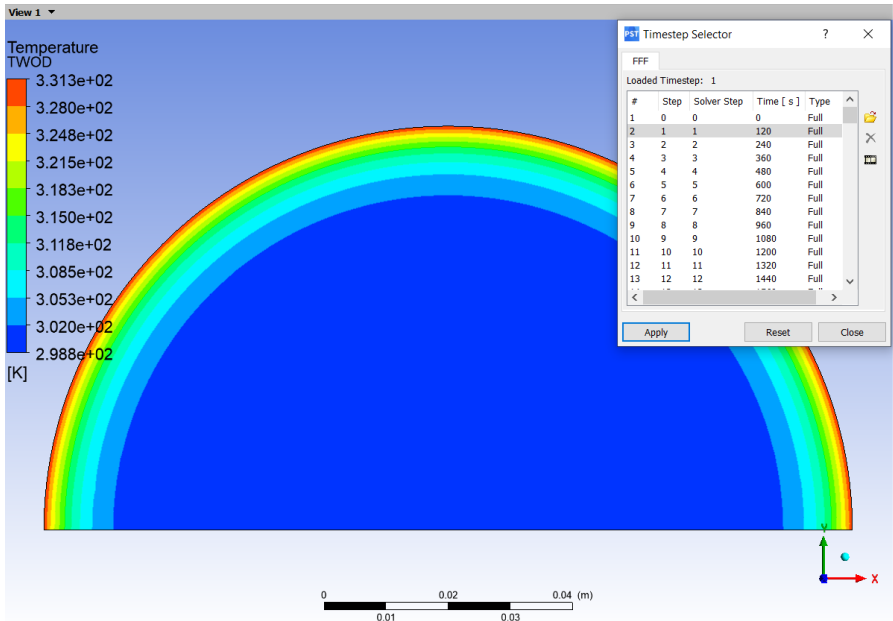
Figure 35. The distribution of temperatures at the second 120 and Timestep Selector parameter window, 2D simulation.

To make the comparison, the contour is saved at 600 s (10 min), 3600 s (60 min) and 8040 s (134 min). To save the image, click on the camera icon, **Save Picture**, and in the pop-up window choose the folder and give it a clear name mentioning the chosen time and the figure you are working with to avoid possible confusion.

Once the images are created, close the *Results* program and save the project.

4.2. ANSYS® and experimental results comparative using 3D simulation

The following section explains how to obtain time-dependent core temperature data and verify the reliability of the experimental data obtained.

Reopen the sphere simulation and launch the *Results* program.

In the top toolbar click the **Location** button and this time choose the first option, **Point**, in the pop-up window give it a name, for example, *centre*. In the *Details of centre* window, confirm that the parameters set in the **Geometry** section coincide with those in Figure 36.
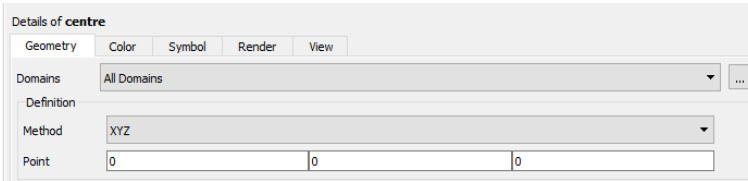
Figure 36. The Details of centre window with point parameters set.

In the tabs **Colour** and **Symbol** it is possible to change the colour and the image of the point, which will appear in the *View 1* window once it has been created. These two parameters are optional, as they have no influence on the results. Once the parameters of the point have been set, the point is generated by clicking on the **Apply** button. The created point should appear in the *View 1* window.

Next, proceed to the creation of a chart which represents the temperature at the centre of the sphere in function of time. In the command bar, click on the **Chart** button (icon with the image of a graph) and give it a name, for example, *Chart centre*. In the *Details of Chart centre* window, in the **Type** parameter, choose the following option, **XY - Transient or Sequence**. In the next tab of the window, **Data Series**, in the **Data Source** parameter, the **Location line** menu is displayed and the previously created point is chosen. In the **X Axis** tab, confirm that **Time** is selected in the **Data Selection** field, and in the **Y Axis** tab, select the **Temperature** variable in the same field. Now proceed to the creation of the graph by clicking on the **Apply** button. It may take a few minutes to generate the graph.

Once the chart has been made, the obtained data are saved[9] by clicking on the **Export** button in the *Details of Chart* centre window. Important: in the pop-up window, confirm that the file format is a text file (txt). To do this, in the **Files of type** field, choose the Text format (*.dat *.txt), and in the **File name** field, at the end of the file name, add .txt to be able to open it in *Excel*.

After the data are recorded, the text file is opened through *Excel* and compared with the experimental data, obtained in the CTS practice. The relative error is calculated to evaluate the accuracy of the experimental temperature values. A graph of the theoretical (ANSYS®) and experimental temperatures throughout time is also plotted and the obtained curves are compared.

4.3. Questions

1. Are there differences between 2D and 3D temperature profiles? Why?
2. What are the advantages of creating the simulation in 2D versus 3D? Is it possible to create a 2D simulation of any figure and obtain the same results? Why?
3. After comparing the theoretical and analytical data and calculating the relative error, if there is considerable deviation between the temperatures, why does this happen?
4. Why, in both the 2D and 3D simulations, is a non-homogeneous mesh created, generating more nodes on the surface than inside the figure?
5. Why is it that in the configuration of the simulations, both in 2D and 3D, in the section on materials it is not essential to change the fluid and air is left, while the fluid that surrounds the body in practice is water?
6. Would it be possible to simulate a sphere that was partially submerged? What should change in the model?

Annex

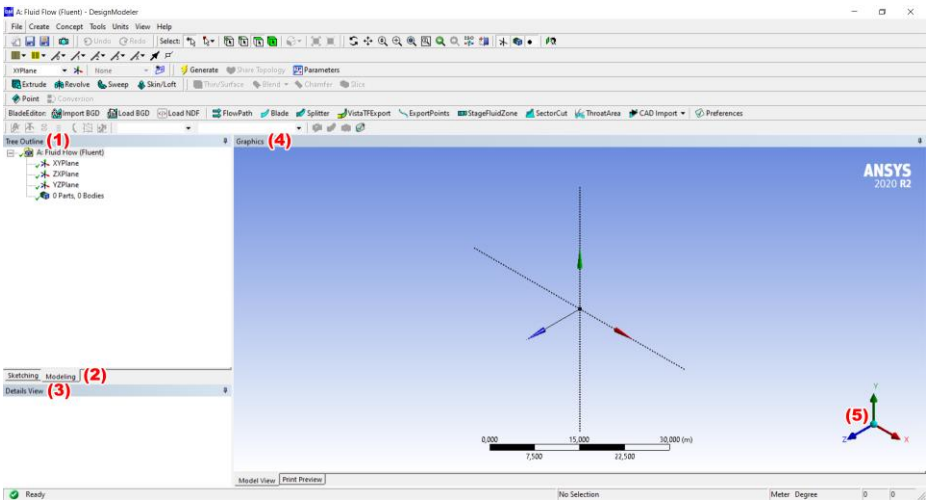### *Workbench* program
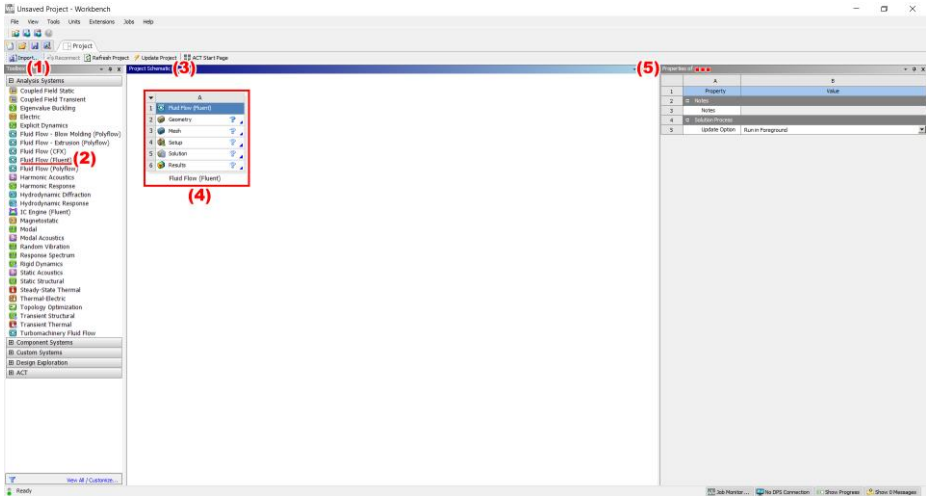
1. *Toolbox* window
2. *Fluent Flow (Fluent)* analysis system
3. *Project Schematic* window
4. Work module
5. *Properties of …* * window

   *varies depending on the chosen command/option

Geometry program

1. *Tree Outline* window
2. *Sketching* and *Modelling* tabs
3. *Details View* window
4. *Graphics* window
5. Plane controller

Mesh program
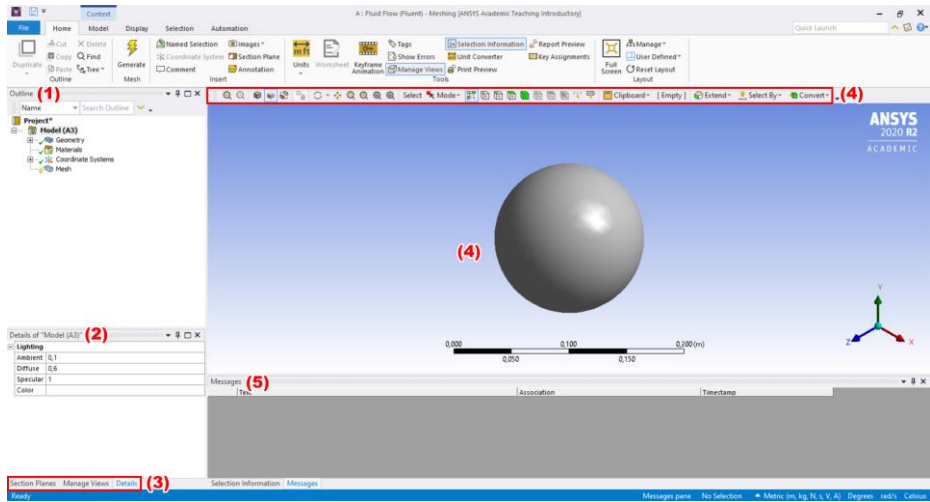
1. *Outline* window

2. *Details of … * * window

3. *Section Planes, Manage Views, Details* tabs

4. Main commands bar

5. *Message* window

   *varies depending on the chosen command/option

Setup/Fluent program
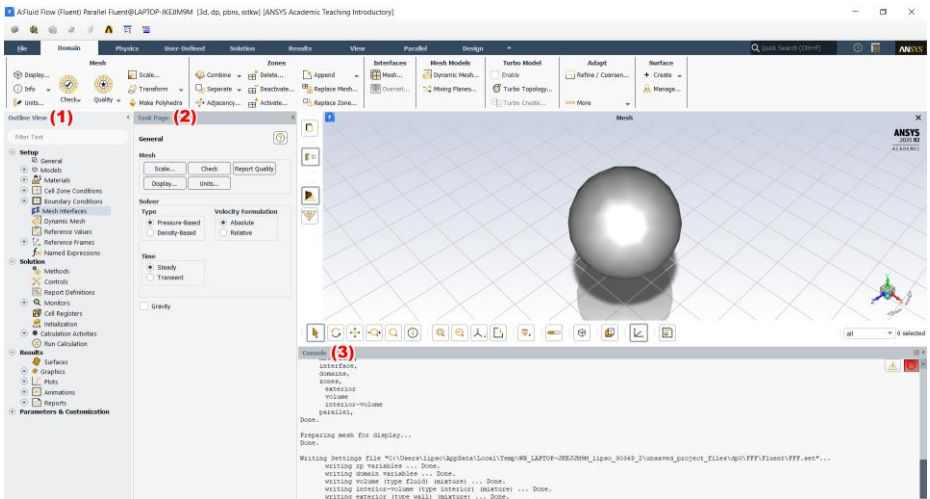
1. *Outline View* window
2. *Task Page* window
3. *Console* window

Results program
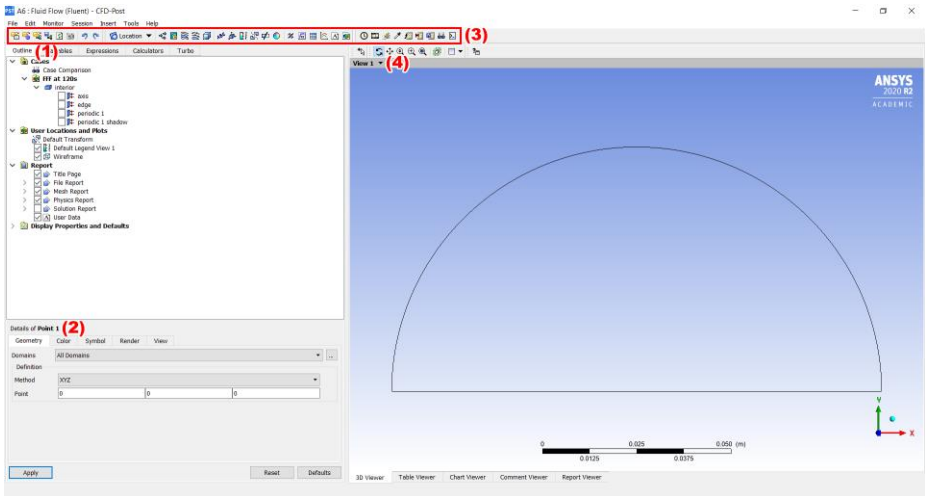
1. *Outline* window

2. *Details of … * window

3. Main commands bar

4. *Geometry/View 1* window

   *varies depending on the chosen command/option

5. CONCLUSIONS

After project realization it can be concluded that:

- Sufficient knowledge of ANSYS® was obtained to simulate the temperature variation within the nylon sphere through 3D and 2D models and elaborate a final script that students have been able to understand and follow.

- It is proved that the academic version of ANSYS® is eligible to create a simulation of the "*Thermal Conductivity of Solid*" laboratory practice after comparing the analytical values with the ones obtained within the software. Moreover, it is not mandatory to use the total number of elements available in the academic version to obtain trustworthy simulation results. Accurate data are obtained with a total number of 411 900 elements in case of the sphere (3D) simulation and with 7 758 elements in the semicircle (2D) simulation.

- The results obtained through the simulations can be treated differently, more visually, through graphs and contours, or more analytically, by exporting the values and comparing these with another type of data, for example, an experimental one. Also, comparing the 3D and 2D simulation results, it was demonstrated that it is always better to optimize the problem whenever possible. In this study, it took 25 minutes to execute the 3D simulation and only 4 minutes to obtain the 2D simulation results having almost equal accuracy.

- The script is written so that it can be followed from beginning to end, or the sections of interest can be chosen and carried out independently of the rest.

- The proposed methodology did work successfully since the obtained feedback from students after the first script testing was positive.

- The implemented improvements after the first group of students were necessary as, after the second testing of the script, the realization time dropped by approximately 23 minutes, as well as the total number of inquiries.

6. FUTURE WORK

- To revise and update the original script of the "*Thermal Conductivity of Solids*" laboratory practice.
- To script the simulation of the cylinder or parallelepiped bodies.
- To simulate and script the experiment in case the solid-liquid heat transfer coefficient, *h*, is not infinite.

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8. *ANSYS Fluent Tutorial: Natural Convection Heat Transfer 2D Transient Analysis on a Solid Cylinder*. **30.06.2019**. https://www.youtube.com/watch?v=XBwDa2YsIeY. 06.03.2021

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APPENDICES

APPENDIX 1: EXPERIMENTAL AND ANSYS® TEMPERATURE VALUES

Time (min)	Experimental T (K)	ANSYS® T (K) 3D e = 2,000 · 10⁻³ m	ANSYS® T (K) 2D e = 1,000 · 10⁻³ m	Time (min)	Experimental T (K)	ANSYS® T (K) 3D e = 2,000 · 10⁻³ m	ANSYS® T (K) 2D e = 1,000 · 10⁻³ m
0	298,75	298,75	298,75	38	311,45	306,35	306,26
2	300,75	298,75	298,75	40	312,25	307,20	307,10
4	301,65	298,75	298,75	42	312,95	308,04	307,94
6	302,25	298,77	298,76	44	313,65	308,88	308,78
8	302,65	298,80	298,79	46	314,25	309,70	309,61
10	303,05	298,86	298,85	48	314,95	310,52	310,43
12	303,45	298,97	298,95	50	315,55	311,32	311,23
14	303,85	299,13	299,11	52	316,15	312,11	312,02
16	304,25	299,37	299,34	54	316,85	312,87	312,78
18	304,75	299,69	299,65	56	317,35	313,61	313,53
20	305,25	300,09	300,04	58	317,95	314,33	314,25
22	305,85	300,56	300,51	60	318,45	315,03	314,95
24	306,55	301,11	301,05	62	318,95	315,71	315,63
26	307,15	301,73	301,66	64	319,45	316,36	316,29
28	307,85	302,41	302,33	66	319,95	316,99	316,92
30	308,55	303,14	303,05	68	320,45	317,60	317,53
32	309,35	303,90	303,82	70	320,85	318,18	318,11
34	310,05	304,70	304,61	72	321,25	318,74	318,68
36	310,75	305,52	305,43	74	321,75	319,28	319,22

APPENDIX 2: PART OF THE LABORATORY PRACTICE SCRIPT

Experimental device

The experimental device consists of the following elements:

a) stirred thermostatic bath

b) temperature sensor and digital temperature readout of the liquid in the thermostatic bath

c) temperature probe and digital temperature readout of the solid core temperature

d) a set of nylon bodies (cylinder, sphere and parallelepiped with square base) with a hole in the geometric centre of the body for the insertion of the probe

Dimensions of the nylon bodies:

- Cylinder: $x_o = L = 6{,}5$ cm.

- Parallelepiped: $x_1 = 8{,}5$ cm, $x_2 = 5{,}6$ cm.

- Sphere: $x_o = 6{,}5$ cm.

The density of nylon, ρ, is 1 165 kg/m³, while the heat capacity is given by the following equation:

$$c_p = 1\,287 \ + \ 7\,267 \cdot T$$

The equation is valid between 25 and 100 °C and when T is expressed in °C, c_p is obtained in kJ/(kg·K).

For the calculations, the value of c_p resulting from the mean integral between T_o and the last experimental temperature T can be taken:

$$(c_p)_m = \frac{\int_{T_o}^{T} c_p \cdot dT}{\int_{T_o}^{T} dT}$$

Experimental procedure

Nylon solids

a) Fill the bath with water to about 2-3 cm below the top edge.

b) Connect the stirrer-heater and set the bath temperature to 60 °C.

c) Wait for the temperature of the bath to be constant. It is recommended to cover the top of the bath to avoid loss due to evaporation.

d) Note down the temperature of the bath (T_e) measured with the probe and its digital reader.

e) Choose a solid or solids to experiment with (consult the teacher).

f) Insert, if it is not already, the dry probe into the hole of the solid up to the bottom, making sure that the hole is perfectly sealed with Teflon to prevent water from entering and falsifying the measurements (if it does not fit well, consult the teacher).

g) Note down the initial temperature of the solid (T_o).

h) Immerse the solid in the bath and start timing. It is necessary to ensure that, throughout the experiment, the water level is at least 2 cm above the solid.

i) Record the solid temperature (T) every 2 minutes until a temperature is reached that gives a value of Y less than or equal to 0,3.

$$Y = \frac{T_e - T}{T_e - T_o}$$

j) Remove the solid from the bath and disconnect the heating-stirring system.