Data in Brief 41 (2022) 107987

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

Dataset and mesh of the CFD numerical model for the modelling and simulation of a PEM fuel cell

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ARTICLE INFO

Article history:
Received 17 January 2022
Revised 15 February 2022
Accepted 17 February 2022
Available online 22 February 2022

Keywords:
PEMFC fuel cell
Bipolar plates
CFD
Meshing

ABSTRACT

A CFD mesh corresponding to a Proton Exchange Membrane Fuel Cell (PEMFC) with an active area of 50 cm^2, serpentine channels and cross-flow field distribution is presented. The mesh was developed using ANSYS ICEM CFD hexa (v12.0) and it is divided into 3D regions corresponding to the different components of the fuel cell: bipolar plates (anode and cathode), gas diffusion layers (GDLs), catalytic layers (CLs) and membrane. The mesh was generated following Best Practice Guidelines, and mesh quality parameters are reported including minimum cell angle or maximum aspect ratio amongst others. Mesh independence results were checked in the corresponding CFD model and simulation of an experimental fuel cell ANSYS FLUENT with the PEM Fuel Cell module. Simulation results were also validated with the experimental data available from a fuel cell test bench for a set of different operating conditions. The experimental validation provides credibility to the CFD model and supports the use of the proposed mesh for fuel cell research, ensuring accurate results and enabling further validation works and

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https://doi.org/10.1016/j.dib.2022.107987

comparison of different designs and operating conditions using numerical simulations.

Specifications Table

Subject	Energy
Specific subject area	Meshing for CFD modelling and simulation of a PEM fuel cell
Type of data	Tables Images Mesh files for CFD simulation
How the data were acquired	The mesh was generated using the software ANSYS ICEM CFD version 12.0. The mesh was used for the development of the CFD model whose numerical analyses were performed in ANSYS FLUENT software version 12.0, using an HP Z600 workstation, using quad-core and 4.0 GB RAM, running Windows XP OperatingSystem with SP2.
Data format	Raw (file in .msh format)
Description of data collection	The mesh is based on a fuel cell with an active area of 50 cm^2 and the bipolar plates have been considered with the following elements: serpentine cross-flow channels design, gas diffusion layers (GDLs), catalytic layers (CLs) and membrane. A hexahedral mesh was generated, including a previous mesh independence analysis, finally setting the number of elements to 1.8 million. In addition, the mesh has a minimum cell angle of 19° and a maximum aspect ratio of 2500. The minimum cell angle is appropriate to ensure satisfactory convergence and precision of the solver results. Even though the maximum aspect ratio value is relatively high due to the small dimensions in the perpendicular direction to the plane of the catalytic layers, the solver did not require double precision for convergence.
Data source location	• Institution: University of Seville • City: Seville • Country: Spain
Data accessibility	Repository name: idUS Data identification number: 11,441/129,878 Direct URL to data: https://idus.us.es/handle/11441/129878
Related research article	A. Iranzo, M. Muñoz, F. Rosa, J. Pino, Numerical model for the performance prediction of a PEM fuel cell. Model results and experimental validation, International Journal of Hydrogen Energy 35 (2010) 11,533–11,550. 10.1016/j.ijhydene.2010.04.129

Value of the Data

- This dataset containing the CFD mesh of a validated CFD PEM Fuel Cell model provides a fundamental basis for the numerical modelling of PEMFCs in CFD.
- The proposed mesh can be used by researchers and engineers in the field of PEM Fuel Cell research and development. The mesh can be used in CFD simulations aiming at providing a deeper knowledge, information and understanding of the complex, highly coupled and non-linear physical and chemical phenomena that take place in fuel cells.
- The mesh provided can be used in CFD simulations of PEM Fuel Cells (Low Temperature and also High Temperature PEM). The mesh can be used to model the fuel cell with different operating conditions flow configurations, as well as different properties of the components (BPs, GDLs, CLs, membrane). It provides a basis for further generation of new meshes for modelling novel designs of flow fields and cell dimensions. The mesh can be used as well for the validation of CFD codes involving PEM Fuel Cell modelling and simulation.

1. Data Description

Data file: fluent_EC_serpentine_05_mesh_BPGpar_crossflowEC_fullBP2.msh

The data presented in this article are based on the generated mesh for the simulation of a PEMFC with serpentine flow field channels. ANSYS FLUENT was used to develop the model with Computational Fluid Dynamics (CFD). The obtained results with CFD simulations under different operating conditions have been verified by experimentation, as explained in the full-length article “Iranzo et al. numerical model for the performance prediction of a PEM fuel cell. Model results and experimental validation” [1]. The mesh was generated following Best Practices Guidelines [2].

The mesh has also been used in the following research works: “Iranzo et al. update on numerical model for the performance prediction of a PEM fuel cell” [3], “Iranzo et al. effect of the membrane thermal conductivity on the performance of a polymer electrolyte membrane fuel cell” [4] and “Iranzo and Rosa validation of a three-dimensional PEM fuel cell CFD model using local liquid water distributions measured with neutron imaging” [5].

The provided dataset is the complete meshing of the fuel cell, including the bipolar plates for anode and cathode with the distribution of channels and manifolds, the gas diffusion layers (GDL), the catalytic layers (CL) and the membrane. The file format is .msh and can be imported into both ANSYS FLUENT and ANSYS ICEM CFD, as well as other CFD modelling and simulation software.

In the following figures, the corresponding areas of the mesh of the different components of the cell are shown. The parts are differentiated with distinct colours. In Fig. 1, the active area of the fuel cell, where the gas exchange takes place, is presented. The dimensions of this area are approximately 50 cm^2 (69.85 x 69.85 mm).

In addition to the active area, another part of the bipolar plates is the external zone to this area. The main function of this area is to structurally support the fuel cell assembly. As shown in Fig. 2, the bipolar plates have dimensions of 101.59 x 101.59 mm, with a thickness of 9.5 mm.

Flow channels distribution are located on the inner surface of the bipolar plates. In this case, the mesh consists of serpentine and cross-flow channels, i.e., the channel distribution in the anode BP was horizontal and the channel distribution in the cathode BP was vertical.

In Fig. 3 the channels dimensions and structure are shown.

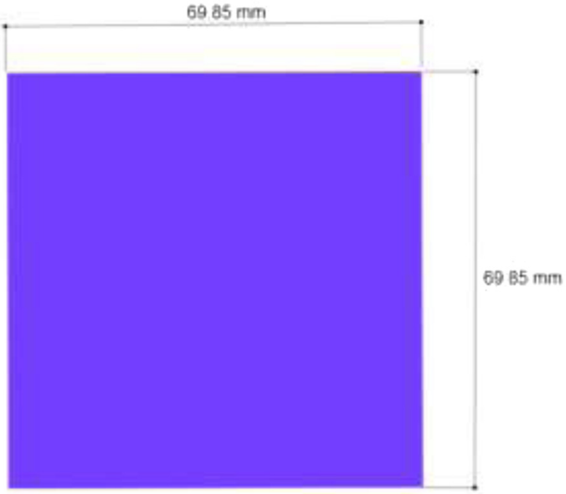

Fig. 1. Dimensions of the active area.

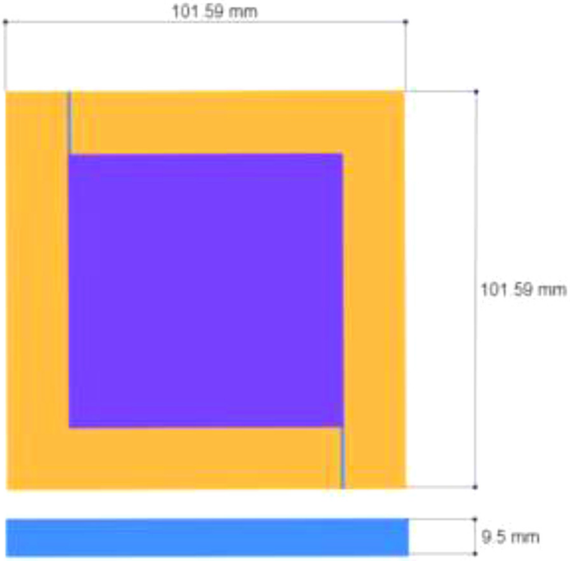

Fig. 2. Dimensions of the bipolar plates for anode and cathode.

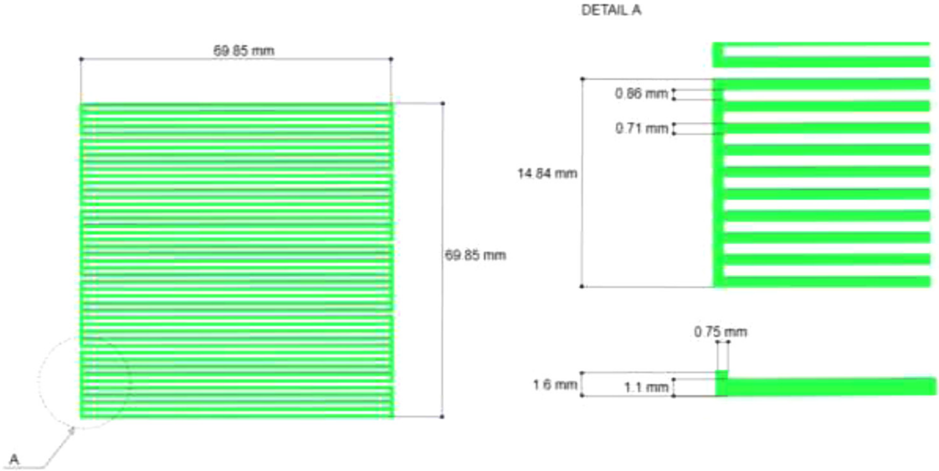

Fig. 3. Dimensions of the BP channels and manifolds.

The channel surface has the same dimension as the active zone (50 cm^2) and it is composed of 5 groups. The distance between channels is 0.86 mm and the width of the inside of the channel is 0.71 mm, with a height of 1.1 mm. The manifold, which is the area where the channels converge and depart, have a width of 0.75 mm and a height of 1.6 mm.

The GDL and CL have thicknesses of 0.42 mm (Fig. 4) and 0.012 mm (Fig. 5), respectively.

The last fuel cell component is the membrane, which is differentiated between an anode membrane and cathode membrane, as shown in Fig. 6. Both membranes have a thickness of 0.0875 mm, giving a total thickness of 0.175 mm.

Once the different elements and their dimensions have been defined, the mesh can be carried out using the aforementioned methodology. In Fig. 7, the complete fuel cell mesh is shown.

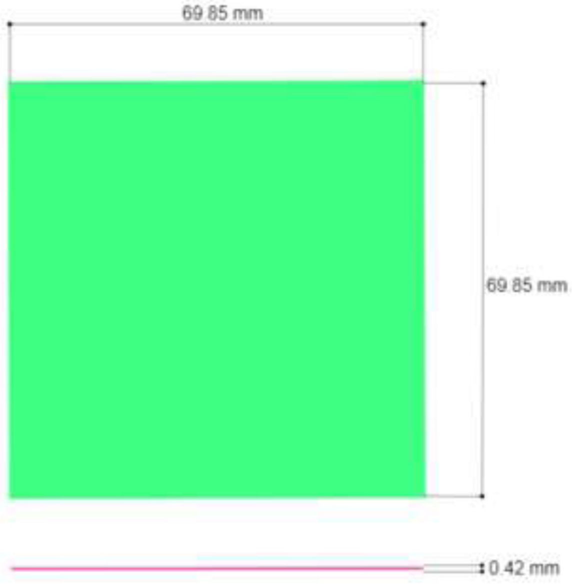

Fig. 4. Dimensions of the GDL.

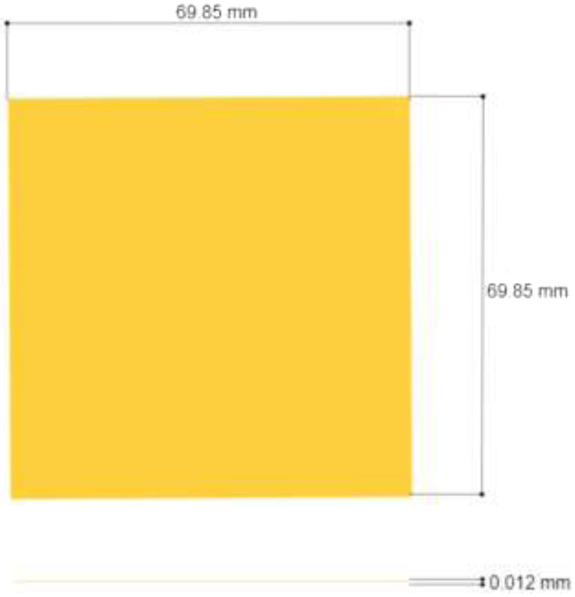

Fig. 5. Dimensions of the CL.

The layout of the different layers that constitute the fuel cell is illustrated in Fig. 8. From top to bottom it consisted of the following elements: anode BP, GDL, anode catalytic layer, anode membrane, membrane interface surface, cathode membrane, cathode catalytic layer, GDL and cathode BP. Note the splitting of the membrane in two to handle the non-conformal mesh,

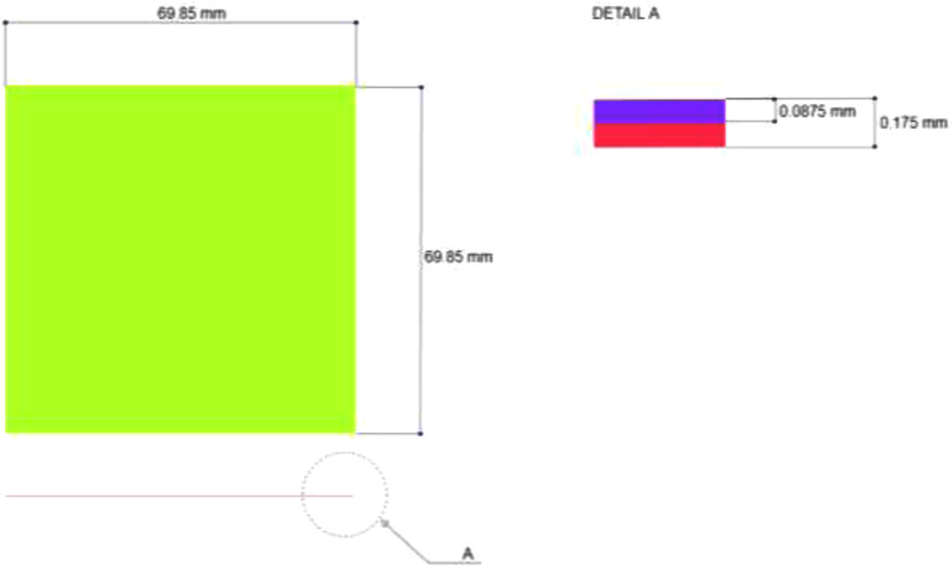

Fig. 6. Dimensions of the membrane.

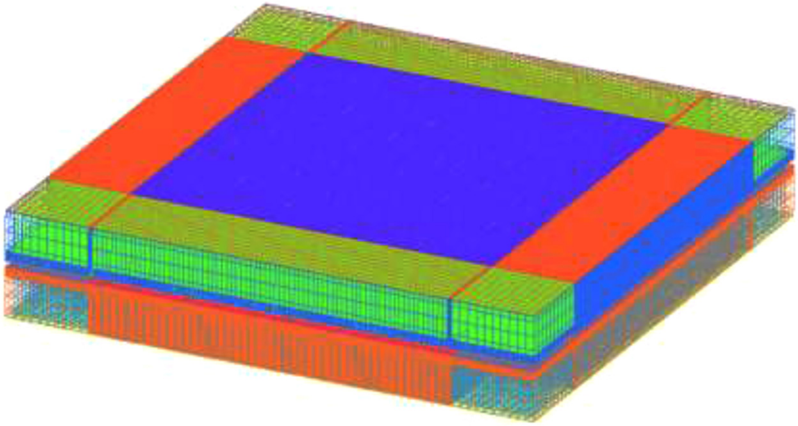

Fig. 7. Complete mesh of the PEMFC fuel cell.

because the anode side is equal to the cathode side, but rotated 90° to satisfy the cross-flow condition. Thus, there is an interface at the midplane of the membrane.

In Table 1, the nomenclature used for the different parts of which the complete mesh is composed is shown, including a brief description of the mesh elements with the aim of assisting the future user of this dataset.

Finally, in Table 2 relevant meshing parameters are shown, useful to check the mesh quality and therefore important to ensure convergence and quality of the subsequent CFD simulation results.

Table 1
Description of the parts of the mesh.

Part	Description
CC_TOP	Outer surface of the active area of the anode BP
CC_TOP_0	Outer surface of the active area of the cathode BP
CC_TOP_HT	Outer surface (out of the active area) of the anode BP
CC_TOP_HT_0	Outer surface (out of the active area) of the cathode BP
CC_SIDES	Lateral surface of the anode BP
CC_SIDES_0	Lateral surface of cathode BP
CC_CHANNELS_INT	Inner surface of the anode BP including channels and manifolds
CC_CHANNELS_INT_0	Inner surface of the cathode BP including channels and manifolds
CC_TOP_HT_INTERNAL	Inner surface (out of the active area) of the anode BP
CC_TOP_HT_INTERNAL_0	Inner surface (out of the active area) of the cathode BP
INOUT_01	Inlet/outlet surface of gases of anode area
INOUT_01_0	Inlet/outlet surface of gases of anode area
INOUT_02	Inlet/outlet surface of gases of cathode area
INOUT_02_0	Inlet/outlet surface of gases of cathode area
CHANNELS_GDL_INT	Interface surface between the inside of the channels/ manifolds and the GDL in the anode area
CHANNELS_GDL_INT_0	Interface surface between the inside of the channels/ manifolds and the GDL in the cathode area
CC_GDL_INT	Interface surface between the outside of the channels/ manifolds and the GDL in the anode area
CC_GDL_INT_0	Interface surface between the outside of the channels/ manifolds and the GDL in the cathode area
GDL_SIDES	Lateral surface of the GDL in the anode area
GDL_SIDES_0	Lateral surface of the GDL in the cathode area
GDL_CL_INT	Interface surface between the GDL and the CL in the anode area
GDL_CL_INT_0	Interface surface between the GDL and the CL in the cathode area
CL_SIDES	Lateral surface of the CL in the anode area
CL_SIDES_0	Lateral surface of the CL in the cathode area
CL_MEM_INT	Interface surface between the CL and the membrane in the anode area
CL_MEM_INT_0	Interface surface between the CL and the membrane in the cathode area
MEM_SIDES	Lateral surface of the membrane in the anode area
MEM_SIDES_0	Lateral surface of the membrane in the cathode area
MEM_SYM	Interface surface between the anode zone membrane and the cathode zone membrane
MEM_SYM_0	Equal to MEM_SYM
CC_3D	3D mesh volume of anode BP
CC_3D_0	3D mesh volume of cathode BP
CHANNELS_3D	3D mesh volume of the anode BP channels/manifolds
CHANNELS_3D_0	3D mesh volume of the cathode BP channels/manifolds
GDL_3D	3D mesh volume of the GDL of the anode area
GDL_3D_0	3D mesh volume of the GDL of the cathode area
CL_3D	3D mesh volume of the CL of the anode area
CL_3D_0	3D mesh volume of the CL of the cathode area
MEM_3D	3D mesh volume of the membrane of the anode area
MEM_3D_0	3D mesh volume of the membrane of the cathode area

Table 2
Characteristics of the mesh.

Description	Value
Nodes	1,378,918
Elements	1,746,952
Determinant	Min. = 0.9935, Max. = 1
Skewness	Min. = 0.9916, Max. = 1
Aspect ratio	Min. = 1.4142, Max. = 2582

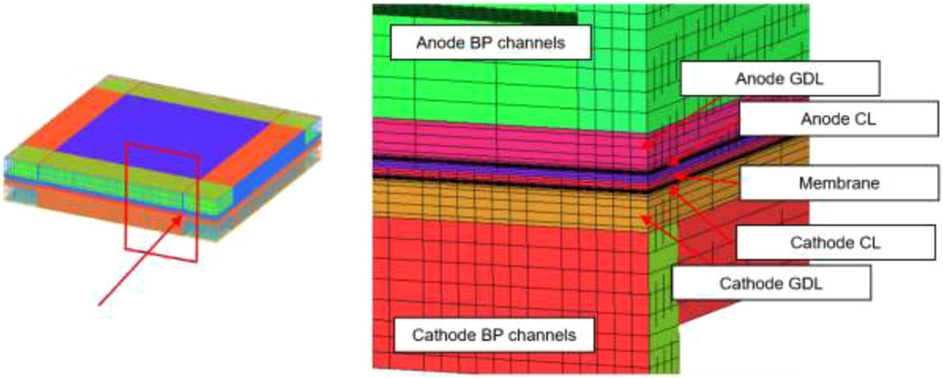

Fig. 8. Details of meshing and the composition of the parts.

2. Experimental Design, Materials and Methods

Computer simulations represent a very helpful tool in developing models under different operating conditions. In this article, the PEMFC module of ANSYS FLUENT software was used to develop the mesh used in the original paper [1] and validate the design and the operating conditions of the fuel cells in CFD.

In the first part of the process, geometrical dimensions and channels design were defined. In a review of the existing literature, Li and Sabir [6] summarised the different channel designs and their main advantages and disadvantages, serving as a basis for the development of the bipolar plates under study. Furthermore, a study was carried out comparing two bipolar plate designs, with serpentine flow field channels and with parallel flow field channels [7]. The dimensions used in the bipolar plates are shown in Figs. 1-3. GDL, CL and membrane thicknesses are defined in Figs. 4–5 and 6, respectively.

Once the geometry has been created, it was possible to mesh the set of elements. Computational domain must be discretised to provide adequate resolution of both the geometry and the results. There are two types of meshing: structured and unstructured meshing. The proposed mesh is structured as it provides better convergence and accuracy in the results than the unstructured mesh.

The thermophysical properties of the flow are calculated along the nodes of the mesh, so as the number of nodes and therefore the number of elements increases, the accuracy of the result will be better and closer to reality. However, there must be a compromise between increasing the number of elements and the computational cost, as there is a technical limitation in the required computing power. Meshes with several million cells are required to obtain a detailed model, making parallel computing necessary in many cases.

The Best Practice Guidelines for CFD [2], was used for the mesh. Due to the fact that the mentioned best practice guidelines were not fully developed for use in fuel cells, a previous validation of the CFD model was performed, and CFD results were tested by comparing the obtained numerical results with experimentation.

To ensure mesh quality, a mesh independence analysis was developed. In this case, three meshes were taken, one mesh with 0.5 million elements, another mesh with 1 million elements and finally, a third mesh with 1.8 million elements. The reported cell voltage results for the two lower number of elements differed less than 5%.

In addition to the mesh density, the quality of the mesh depends on other factors such as aspect ratio, skew angle or mesh deformation. For hexahedral meshing, the angle between the edges of the cells should be approximately 90° As illustrated in Table 2, the obtained skewness values were very close to 1, so the cell is very close to being ideal and therefore, the hexahedrons have angles of approximately 90°. The value of the determinant refers to the determinant of the Jacobian matrix. This value gives information about the behaviour of the function at a point. Non-zero values are required to be invertible, so it was found that on the study mesh with a value close to 1 (Table 2), the solver is able to solve the Navier-Stokes equations correctly. On meshes with a high aspect ratio, rounding errors can be relevant for the final result. Therefore, the Best Practice Guidelines [2] recommend checking the influence of these errors by performing the same calculation with single and double precision and comparing the objective result. It is recommended to use double precision solvers, although in the case study the same behaviour and convergence solution was obtained, deciding to use the single precision solver.

For all the above reasons the high quality of the proposed mesh illustrated in Fig. 7 is verified.

Ethics Statements

This work does not contain any studies with humans, animals from protected areas, or endangered animals. The authors declare that they have followed the general ethics rules for scientific research and publishing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT Author Statement

Alfredo Iranzo: Conceptualization, Data curation, Methodology, Investigation, Software, Supervision, Validation, Writing – review & editing; **Baltasar Toharias:** Data curation, Methodology, Investigation, Writing – original draft, Writing – review & editing; **Christian Suárez:** Investigation, Writing – review & editing; **Felipe Rosa:** Methodology, Project administration, Resources, Supervision; **Javier Pino:** Project administration, Resources.

Acknowledgements

This publication has been possible thanks to the following grants: Grant PID2019–104441RB-I00 funded by MCIN/AEI/10.13039/501100011033, co-funded with ERDF funds. Grant PY20 RE 026 AICIA funded by S.G. de Universidades, Investigación y Tecnología, PAIDI 2020 program by Junta de Andalucía, co-funded with ERDF funds. General Secretariat of Universities, Research and Technology, Junta de Andalucía, project P08-TEP-4309, co-funded with ERDF funds.

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