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Journal Computational Simulation

Definition of Journal

Scientific Objectives

Support the international scientific community in its written production Science, Technology and Innovation in the Field of Engineering and Technology, in Subdisciplines of telemetry, diffuse interval, electrical stimulation, diffuse controller, mobile application, communications network, web platform, production control, computer technology, computer electronics, control devices, programming languages and automated production systems.

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The works must be unpublished and refer to topics of telemetry, diffuse interval, electrical stimulation, diffuse controller, mobile application, communications network, web platform, production control, computer technology, computer electronics, control devices, programming languages and automated production systems and other topics related to Engineering and Technology.

Presentation of Content

The first article presents, *Computational simulation a system of waterborne polyurethane matrix by β -C induction with ZnO and CaCO₃ particles*, by AGUILAR-MARURI, Saul, CONTRERAS-LÓPEZ, David, GALINDO-GONZÁLEZ, Rosario and FUENTES-RAMÍREZ, Rosalba, by LÓPEZ-PADILLA, Gilberto, SORIA-GARCÍA, Myriam and SANTOS-POMPA, Diego Marcelo, with a secondment at the Centro de Investigación en Materiales Avanzados and Universidad de Guanajuato, as the next article is *Gravity process foundry simulation*, by CERRITO-TOVAR, Ivan de Jesus, VALDES-MEDRANO, Adriana Paulina, GARCIA-DUARTE, Oscar Enrique and HUERTA-GÁMEZ, Héctor, with a secondment at the Universidad Politécnica de Juventino Rosas and Brovedani Reme, as the next article is *Development of an application for the estimation of vegetation indices using SENTINEL remote sensing data*, by SERVÍN-PRIETO, Alan Joel, TRUCÍOS-CACIANO, Ramón, SIFUENTES-MORÍN, Norma Guadalupe and MONTEMAYOR-TREJO, José Alfredo, on secondment to the Instituto Tecnológico de Torreón, Instituto Nacional de Investigaciones Forestales, Agrícolas y Pecuarias and Instituto Tecnológico Superior de Lerdo, as the next article is *Construction of a PUMA-type robot with 3 degrees of freedom*, by DE ANDA, Rosa, VALLE, Pablo, ACEVEDO, Francisco and LOPEZ, José.

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Computational simulation a system of waterborne polyurethane matrix by β -C induction with ZnO and CaCO₃ particles

Simulación computacional de una matriz de poliuretano base agua, con inducción de β -C y compuestos de ZnO y CaCO₃

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Abstract

This work includes the search for the development of a composite of a WPU (waterborne polyurethane), β -CD (β -Cyclodextrin), PZnO (zinc oxide particles), and the presence of CaCO₃, to obtain new properties such as adhesion to multiple substrates of organic and inorganic origin. Therefore, a development sequence was proposed: Computational development: conformation of the polymeric matrix (with the intermediary polymers) and simulation of the interaction between β -CD and PZnO and Ca⁺² and CO₃⁻² ions, as well as insertions in β -CD, computational simulations were carried out with the help of ACD LABSTM (free version) software and by molecular dynamics with GROMACSTM. With the above, we were able to determine properties such as interfacial tensions, surface tensions, and contact angles, and degrees of solvation and stability in waterborne emulsions. Therefore, it is important to point out that one of the main contributions of this research proposal is that there are no studies that combine these materials.

Resumen

El presente estudio desarrolla la factibilidad teórica computacional de desarrollar un compuesto de una matriz de PUBA (poliuretano base agua), con la inserción de β -CD (β -Ciclodextrina), en la cadena polimérica, PZnO (partículas de óxido de zinc) y CaCO₃. Este material tendrá propiedades de adhesión a múltiples sustratos (orgánicos e inorgánico). La metodología de síntesis considera la simulación computacional: conformación de la matriz polimérica (con sus intermediarios) y simulación de la interacción entre la β -CD y las PZnO e iones Ca⁺² y CO₃⁻², así como las inserciones en la β -CD, se realizaron simulaciones computacionales con ayuda del software ACD LABSTM (versión libre) y por dinámica molecular con GROMACSTM. Con lo anterior, logramos determinar propiedades como tensiones interfaciales, tensiones superficiales, ángulos de contacto y grados de solvatación y estabilidad en emulsiones base agua. Este trabajo presenta un material que combina las interacciones de la β -CD, PZnO y CaCO₃, las cuales no se han conjuntado hasta el momento.

Waterborne polyurethane, ZnO particles, computational simulation

Poliuretano base agua, partículas de ZnO, simulación computacional

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Introduction

Currently, PU's (polyurethanes) are a class of versatile polymers (Christopher *et al.*, 2016) with multiple synthesis routes and applications, which have been affiliated in different utilities such as the manufacture of liquid coatings, elastomers, elastic fibres, etc., (Akindoyo *et al.*, 2016). These types of materials are chosen in the various industrial branches for their superior properties, such as mechanical properties (excellent rigidity, hardness, resistance to abrasion, and flexibility at low temperatures), chemical resistance (corrosion resistance), and resilience (Akindoyo *et al.*, 2016). WPU systems represent non-toxic, non-flammable, and non-air polluting commercial products (Tornero *et al.*, 2018). Booming research is looking for multiple synthesis routes for these materials, where blocks composed of polyols, diisocyanates, neutralizers, hydrophilic extensor chains, and additives will determine the structure of said PU and its properties (Kang *et al.*, 2018). Therefore, there is a tendency to generate PU's with better elasticity, resistance to dry film abrasion, among other properties (Noble, 2018).

Structural modifications to PU's provide specific performance properties to the coating, that has been explored with the addition of nanoparticles or various chain extenders to the polymeric matrix. It has been found that including ZnO nanoparticles (synthesized by sol-gel method) in the matrix of a WPU is an ecological alternative to delay corrosion in AISI 1018 CS substrates due to the increase in the impedance displayed in the EIS (Electrochemical impedance spectroscopy) (Salazar-Bravo *et al.*, 2019). Other analysis by EIS determined that the β -CD/WPU film blocks the corrosive medium to the substrate, especially in the presence of CaCO_3 , which verifies an anti-corrosive system with effective self-healing on metallic substrates (Hua *et al.*, 2019).

Furthermore, the use of computational simulations has allowed economic and risk-free validation, aspects such as experimental synthesis or determination of conformations of new proposed polymeric structures.

This work establishes the computational feasibility of a WPU synthesized by induction via β -CD, and with the addition of CaCO_3 and PZnO , as a precursor of a coating with significant adhesion to polymeric and inorganic materials, it will possess a self-healing mineralization and possible protection against UV radiation. And by means of computational simulation (considering the synthesis conditions, ZnO and CaCO_3 addition sites, and emulsion feasibility of the polymeric matrix in water), some structural and physicochemical characteristics can be predictively analysed.

Methodology

Computational simulation:

1. Using AVOGADRO (optimizing with the following parameters: UFF as Force Field and Steepest Descent as algorithm, 9 optimizations or until obtaining an energy difference between simulations of 0.5%), the structures corresponding to β -CD, ZnO , and Ca^{+2} and CO_3^{-2} ions were drawn, obtaining the corresponding structures in *pdb* files (Brookhaven Protein DataBank format).
2. Subsequently, in GROMACSTM (using the corresponding topology), the effective interaction of β -CD with PZnO and CaCO_3 was established. Molecular dynamics simulations considered one molecule of β -CD, 200 molecules of water, 50 of Ca^{+2} , 50 of CO_3^{-2} , and 100 of ZnO , using a long-range Van der Waals interaction model, which has Lorentz-Berthelot corrections. Nine simulations were carried out to obtain a variation of minimization of total energy of 0.5%, between continuous simulations.
3. The synthesis stages of Hua *et al.*, (2019) were considered for the simulation of the conformation of the polymeric matrix. These stages consider the mole equivalents, with which it was possible to determine some polymeric intermediates that could be expected in the synthesis stage.

4. The formation of the polymer corresponding to each reaction stage was simulated in ACD LABS™ (free version) with the molecular mechanics algorithm based on the parameterization of the force field, CHARMM, with modifications and simplifications to increase the stability and speed of calculation of the model of (Brooks, B. *et al.*, 1983), obtaining the estimation of the surface tension.
5. The final structure of step 4 was transferred to GROMACS™ with which the feasibility of solvation of the proposed system was established, using *gro* files. Fifteen simulations were carried out to obtain a variation of minimization of total energy of 0.5%, between continuous simulations.

Results

The result of the molecular dynamics simulations, for the effective interactions between β -CD, ZnO particles and calcium carbonate ions were successful, is shown in Figure 1.

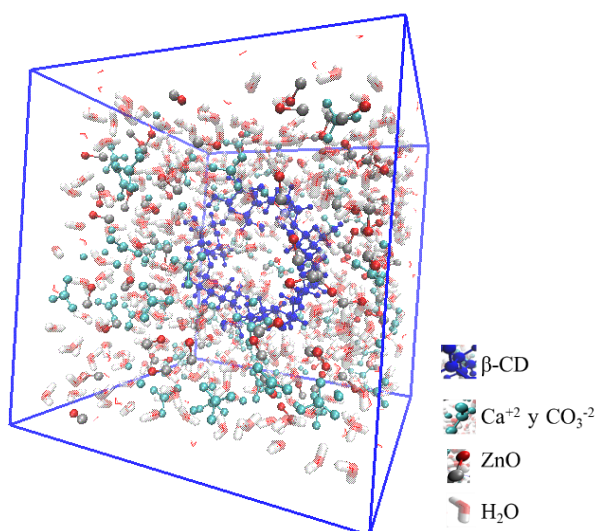


Figure 1 Configuration resulting from the balanced simulation of molecular dynamics of the interaction of ZnO, Ca^{+2} , CO_3^{-2} , and β -CD in aqueous medium, carried out in GROMACS™. Analysis volume of 14.33 nm^3
Source: Own work [VMD (Visual Molecular Dynamics) program]

With concentration calculations and considering the average density obtained from the simulation (1898.23 kg/m^3 , as shown in the Figure 2), it would imply the possibility of an interaction of β -CD with 112073 ppm of Ca^{+2} , 455136 ppm of ZnO and 167807 ppm of CO_3^{-2} .

The optimization leads to a negative value of the total energy of the system at the simulation temperature (300 K), which means that the system is bounded and stable, because the energy that is optimized in a greater proportion is the potential energy and not kinetics, obtaining an average value of -7708.39 kJ/mol , as shown in Figure 3.

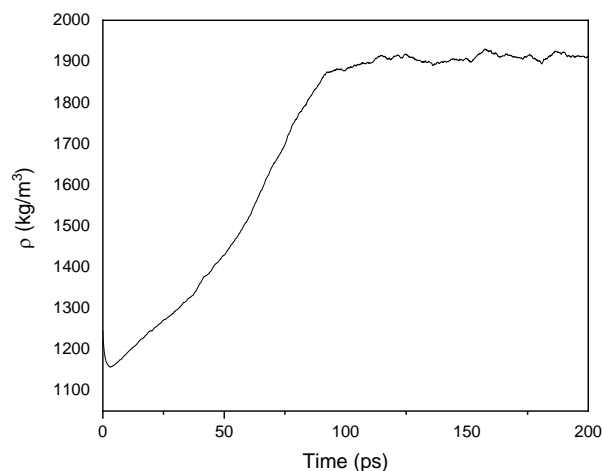


Figure 2 Density of the system balanced by molecular dynamics, in GROMACS™, for the interaction of ZnO, Ca^{+2} , CO_3^{-2} and β -CD in an aqueous medium
Source: Own work [OriginPro 9]

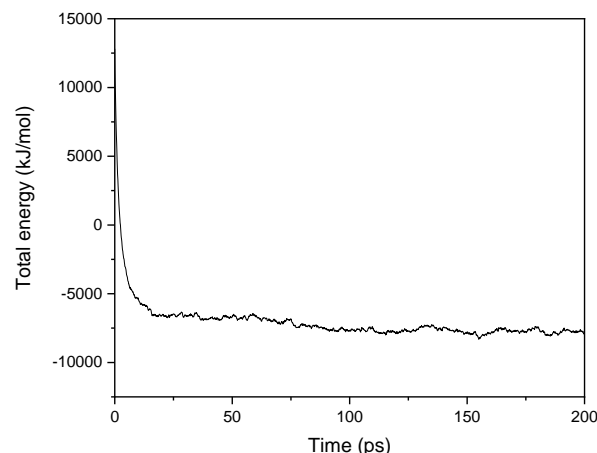


Figure 3 Total energy of the system balanced by molecular dynamics, in GROMACS™, for the interaction of ZnO, Ca^{+2} , CO_3^{-2} and β -CD in an aqueous medium
Source: Own work [OriginPro 9]

The molecular dynamics simulations, Figure 4, estimated a surface tension of 625 bar nm for the system, which is equivalent to 62.5 mN/m. The surface tension of the water is 73 mN/m therefore, the system has a slight variation in the intramolecular cohesion forces that occur.

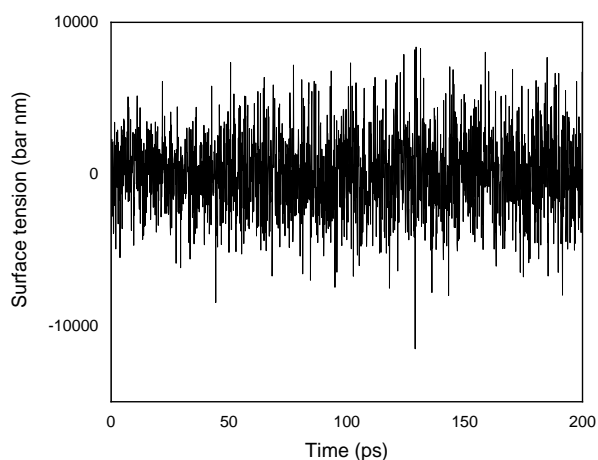


Figure 4 Surface tension of the system balanced by molecular dynamics, in GROMACS, for the interaction of ZnO, Ca^{+2} , CO_3^{-2} and β -CD in aqueous medium
Source: Own work [OriginPro 9]

The analysis of the radial distributions of ZnO, water, Ca^{+2} and CO_3^{-2} , by means of the simulations of molecular dynamics carried out in GROMACSTM, indicate that β -CD was found with the first ZnO species at 0.56 nm (Figure 5), with Ca^{+2} at 1.27 nm (Figure 6), with CO_3^{-2} at 0.25 nm (Figure 7) and with water at 0.52 nm (Figure 8). This indicates a good interaction of β -CD with ZnO and CO_3^{-2} (because β -CD is composed of seven d-glucopyranose residues linked by α -1,4-glycosidic bonds with a structure with a hydrophobic internal cavity and a hydrophilic exterior), and above all a good solvation of the system.

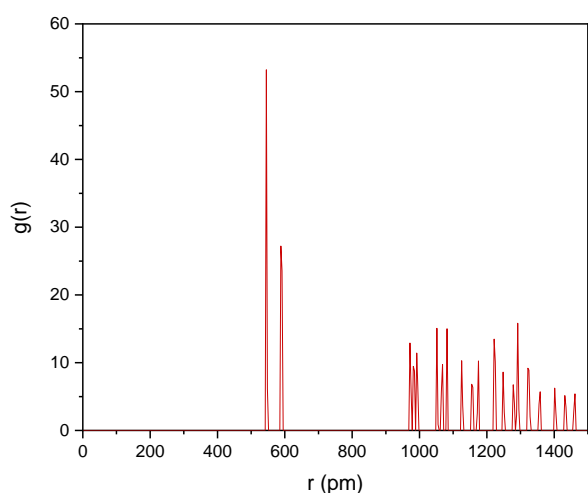


Figure 5 Radial distribution function of ZnO in the system balanced by molecular dynamics, in GROMACSTM, for the interaction of ZnO, Ca^{+2} , CO_3^{-2} and β -CD in aqueous medium
Source: Own work [OriginPro 9]

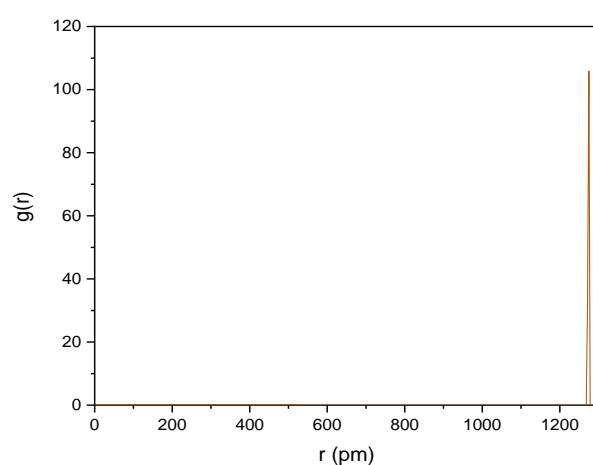


Figure 6 Radial distribution function of Ca^{+2} in the system balanced by molecular dynamics, in GROMACSTM, for the interaction of ZnO, Ca^{+2} , CO_3^{-2} and β -CD in aqueous medium
Source: Own work [OriginPro 9]

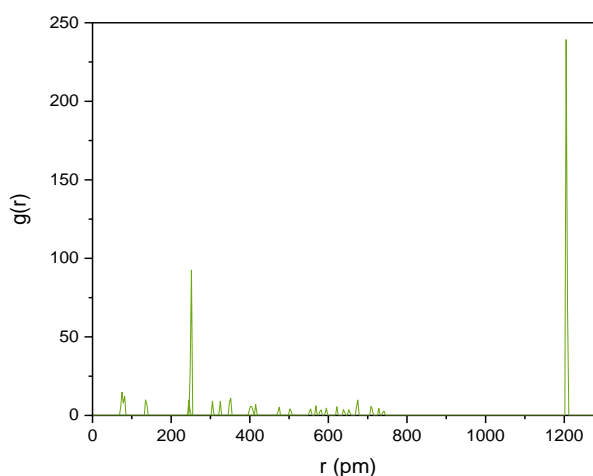


Figure 7 Radial distribution function of CO_3^{-2} in the system balanced by molecular dynamics, in GROMACSTM, for the interaction of ZnO, Ca^{+2} , CO_3^{-2} and β -CD in aqueous medium
Source: Own work [OriginPro 9]

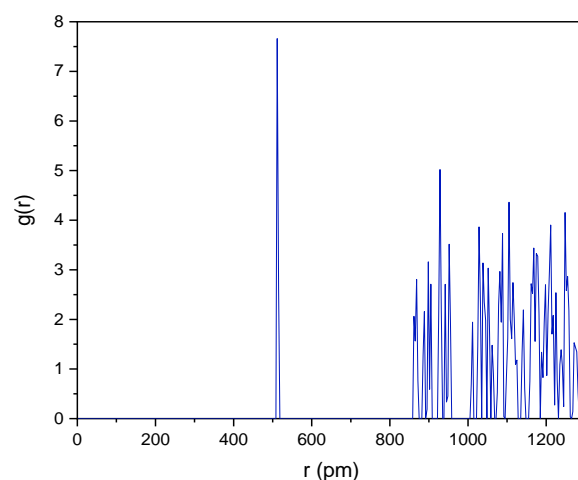


Figure 8 Radial distribution function of water in the system balanced by molecular dynamics, in GROMACSTM, for the interaction of ZnO, Ca^{+2} , CO_3^{-2} and β -CD in aqueous medium
Source: Own work [OriginPro 9]

The radial distribution functions obtained in Figures 5-8 indicate that the system will have a very close interaction with respect to the studied particles (ZnO, CO_3^{-2} and water), especially for the CO_3^{-2} and ZnO particles, with which the β -CD is an interaction-retention site, as other works have already reported for CO_3^{-2} (Hua *et al.*, 2019). And from the correct interaction with PZnO, the polymer matrix is expected to acquire resistance properties from exposure to UV radiation, as has been reported in the bibliography (Hua *et al.*, 2019).

The stages of synthesis of polymer matrix consider the mole equivalents, this indicate someone reagents are in excess and is possible occurrence parallel reactions like show in Figure 9, this polymer resulting from the reaction between 6 molecules of IPDI (Isophorone diisocyanate) and 3 of PD (polycaprolactone diol average $M_n \sim 2000$ g/mol), resulting in an optimized system in AVOGADRO with a final energy of 7817.56 kJ/mol and a molecular weight of 7028.76 g/mol. The result of these simulations was visualized with VMD.

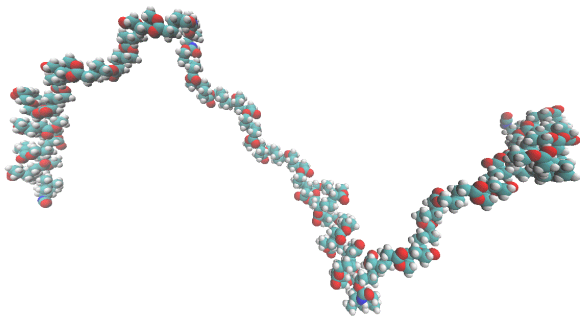


Figure 9 Polymer resulting from the reaction between 6 molecules of IPDI and 3 of PD, hydrogen (white), oxygen (white), carbon (light blue) and nitrogen (navy blue)
Source: Own work [VMD (Visual Molecular Dynamics) program]

The final polymer, Figure 10, in GROMACSTM reports a cell volume of 169.22 nm^3 , with a density of 1005.25 g/L and optimal solvation with 5323 water molecules. The percentage of solids that our water-based coating would have is estimated, which is 6.21%, which is a good percentage for a coating that will be applied by spraying with a pressure of 2.5 kg/cm^2 , although the layer that will be deposited in the surface of the substrate would be very small for which it would arise to apply several layers.

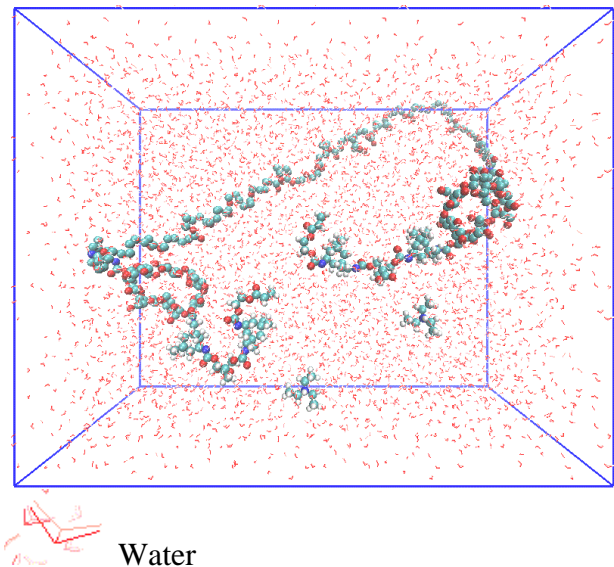


Figure 10 Configuration resulting from WPU final in solvation, in GROMACSTM, hydrogen (white), oxygen (white), carbon (light blue) and nitrogen (navy blue)
Source: Own work [VMD (Visual Molecular Dynamics) program]

Making an analysis of the results obtained in the simulations with ACD LABS/ChemSketchTM (free version) and considering equations 4 and 5 of the work of (Good, R. J., & Girifalco, L. A., 1960), Figure 16 is obtained. The program cannot estimate properties of the final polymer because it does not have a continuous structure.

$$\theta = \cos^{-1} \left[2\Phi \left(\frac{\gamma_{Prepolymer}}{\gamma_{water}} \right)^{\frac{1}{2}} - 1 \right] \quad (1)$$

$$\gamma_{Prepolymer-water} = \gamma_{Prepolymer} + \gamma_{water} - 2\Phi(\gamma_{Prepolymer}\gamma_{water})^{\frac{1}{2}} \quad (2)$$

Where:

- θ is the contact angle between the prepolymer and the water.
- γ surface tension in mN/m.
- $$\Phi = \frac{4(V_{prepolymer}V_{water})^{\frac{1}{3}}}{\left[(V_{prepolymer})^{\frac{1}{3}} + (V_{water})^{\frac{1}{3}} \right]^2}$$
- V is the molecular weight (g/mol) of the species divided by its density (g/cm^3).

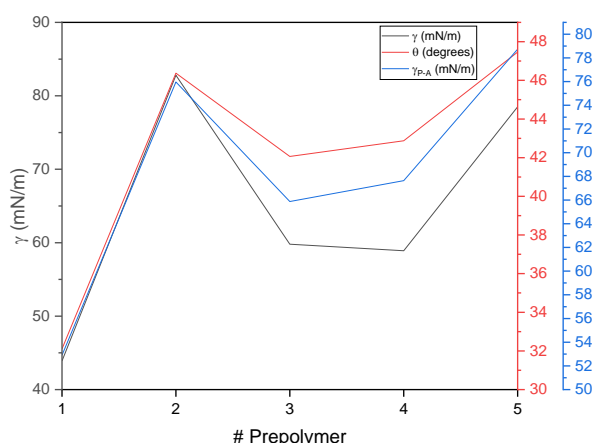


Figure 11 Variation of γ , θ and γ_{P-A} (Prepolymer-water) of the prepolymers generated by computational simulations and 3-D CHARMM-type of force field optimization in ACD LABS/ChemSketch™ (free version)

Source: Own work [OriginPro 9]

The θ found for each prepolymer analyzed indicates that there is an interface between water and the polymeric matrix and suggests a measure of the wettability of the polymer by water. When carrying out the analysis of the variability of γ_{P-A} we found values between 52 and 79 mN/m, which indicates dispersed systems with a larger particle size and a reduction in interfacial tension favours the formation of a dispersed system from the point from an energetic point of view. The evaluation of θ and γ with substrates of different chemical origin with prepolymer 5 (m-P5) is summarized in Table 2.

Material	$\gamma_{material}$ [$\frac{mN}{m}$]*	θ_{m-P5} [°]	γ_{m-P5} [$\frac{mN}{m}$]
Polyethylene	30-32	57.13	63.25
Polypropylene	30-35	56.60	63.43
Steel	40-55	58.87	84.03
Glass	70-73	48.30	80.54

* Data extracted from (Pye, 2016)

Table 2 Evaluation of $\gamma_{material}$, γ_{m-P5} and θ for the generated prepolymer 5 and proposed materials

Source: Own work [Microsoft Office Word]

For all the θ shown in Table 2, we can infer that there is a polymer with a medium degree of wettability, which favours the mass transfer mechanism within the roughness of the proposed substrates, benefiting an interfacial adhesion between two immiscible systems. Although based on the results of γ_{m-P5} we can consider that the polymeric system will have a higher interfacial resistance for substrates such as steel and glass.

Conclusions

The polymerization process between IPDI and PD was studied, and as chain extenders β -CD, dimethylolpropionic acid and ethyl acrylate, and from the polymers formed laterally with the minimization of energies by the conjugate gradient in the AVOGADRO software.

The theoretical feasibility of the formation of the polymeric matrix and the insertion of $PZnO$, Ca^{+2} and CO_3^{-2} ions, with the formation of an emulsion (in a waterborne system) of the polymeric matrix and the adhesion to organic and inorganic substrates (polyethylene, polypropylene, steel, and glass), and an equilibrium model with long-range Van der Waals interactions, using molecular dynamics with GROMACS™ software.

The simulations carried out of the polymeric matrix, in GROMACS™, demonstrate its viability as a coating that can be applied by spraying, under standard industrial operability conditions, due to the feasibility of creating a system with a 5% total solids percentage.

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Gravity process foundry simulation

Simulación del proceso de fundición a gravedad

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Abstract

In this work, they going to use a foundry simulation software to compare the virtual vs real results and try to reduce the time of the real process in the foundry area. In the real process they work with the re-engineering process of the pistons, first they take the original element and take the physical properties (length, width, thicknesses, etc.), after make a cast design and is assigned some parameters for the process, planning the process to make a test, after the casting process it goes to the machining process and finally the final inspection says if all the process during the tests is correct, if not, we need to take others parameters or casting design. With this project is going to be possible to save time in the foundry area and make a virtual process to see the result and change all the necessary things to have a perfect process

Resumen

Éste trabajo utilizará un software de simulación de fundición para hacer una comparación entre resultado virtual y real del proceso de fundición para tratar de reducir los tiempos del proceso en el área. En el proceso real se realiza a través de la reingeniería en la fabricación de pistones, primeramente se es tomado el pistón original con sus respectivas propiedades físicas (longitudes, espesores, ancho, etc.), después se realiza un proceso de diseño del molde y se le son asignados parámetros para su proceso en piso, se planea el proceso para realizar una prueba en producción, después de que se lleva a cabo dicha prueba, pasa al área de maquinado para después ser inspeccionado en la línea y determinar si las condiciones del diseño contra las reales en piso fueron correctas, si no, se necesita tomar nuevos parámetros basándose en los resultados para una nueva prueba. Con éste proyecto será posible ahorrar tiempo en fundición ya que el proceso virtual ayudará a saber el resultado antes de que se lleve a cabo en piso y así de ese modo poder trabajar con los parámetros correctos para tener un producto sin defectos.

Foundry, Piston, Simulation process

Fundición, Pistón, Proceso de simulación

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Introduction

The pistons are manufactured mostly through the aluminum gravity casting process, for that reason, you must have correct parameters in your process and avoid defects that can be caused by a misallocation of the same, the defects are divided in 2 branches, natural variations and parameter variations, the former are difficult to control externally, but can have immediate corrections in the process. Parameter variations are entirely the responsibility of the process and mold design, therefore, a correct assignment of them will eliminate this variation.

With the process that was proposed for the design prior to the launch of a new product, the process will be simulated in a virtual way with the first parameters that are thought to help the process correctly, if they are not favorable, the software will indicate its results. In this way, we will be able to assign or adjust the parameters previously proposed, in such a way that the process will be simulated as many times as necessary until the expected result is reached.

The defects that appear have their possible causes and if any defect of this type appears, new parameters will have to be assigned (time, temperatures, internal design, etc.) to carry out the process and obtain a piece free of imperfections, this type of arrangement the process can take from 2 weeks to 6 months. Consequently, time and material are wasted in what is reached a suitable time or more approximate to what would be a successful process, which ideally consists of the shortest possible time to carry out solidification and at the end of this that the piece is free of blemishes.

By using the software it is intended to understand and analyze how it will behave in the conditions with which it is worked when it is molded, in this way to know and predict areas of porosity and correct filling times to obtain a clean molded part.

Establishment of the Project

In the first part of the project, it was to carry out a simulation test on an existing part number within the company, which already has a bad history in terms of defects, that is, it is already a product that is made on the floor but always had scrap complications, based on any number of defects that had occurred and due to having derived from the casting process, a defect that was considered the most recurrent in this part number was the pores in the piston head, this defect, for more that they moved and changed parameters on the floor, it was never successful in correcting such a defect, therefore, it is a litmus test for the reliability of the software, that is, the piston will be analyzed in such software and the result we need obtain will be a piston with the most reminiscent defect in the mechanical element, if the result in this case is favorable, that is, it comes out with the defect shown, the parameters will be changed virtually until a result is obtained favorable casting, that is, without defects.

Afterwards, a test will be carried out on the floor to compare and verify virtual vs real, in such a way the reliability of the program will be demonstrated and verified and if this turns out as planned, it will be passed to a second stage that will be with a new product to establish to its new conditions before doing the process on the floor. For this, companies in the automotive sector have worked to improve casting processes [1]. The aforementioned process is represented in figure 1.



Figure 1 Re-engineering process in the company

The defects in casting are infinite, but with their respective reason for being, therefore, each defect is different from each other as much as its solution [2], the piston of the so-called reliability test for the most part or the most critical defect it is "head pore" as it sounds it is a hole in the head of the element as shown in Figure 2.



Figure 2 Pore in the head of a piston

From a production of 2000 pieces of such part number, a description was made of its defects and their percentages which are shown in table 1.

Default	N. Pieces	Percentage
Gas	250	25%
Pore in head	500	50%
Cold junction	100	10%
Not filled	50	5%
Metallic inclusion	100	10%

Table 1 Description of the defects of a production run

The part number used for its demonstration has a performance of 50%, that is, of the manufactured parts derived from its low performance, half will always be considered scrap as shown in the production identified in the previous Table.

Development of the methodology to obtain parameters

As described at the beginning, to obtain the parameters to work on the floor, the current process is to compare a piston that has similar characteristics (size, alloy, model, etc.) in order to copy and adjust the parameters and obtain similar results to a product with a high yield (greater than 85%), therefore, the parameters shown in Table 2 are the ones with which the part number is currently being worked on the floor and even so there is a very high yield. low (50%), in such a way that they have been modified several times and it has not been possible to reduce the scrpa of said product.

Solidification parameters	
Mold temperature	430°C
Metal temperature	750°C
Outside temperature	25°C
RH	25%
Solidification time	85 s
Cooling fluid	Water

Table 2 Solidification parameters

Based on these parameters, we will proceed to simulate in the software using the CAD models of the piston and the mold, to later use these parameters and obtain the desired results.

Obtaining the CAD model and assembly of the mold

Due to the current technological conditions for the standards of the companies, there are constant changes on the pieces, these changes must be reflected in the documents that support the elements, for that reason the way of working is through CAD software with which they make the 3D pieces and after that they generate the plans that will later support their manufacture, therefore, when making a modification or improvement of it, it is carried out directly on the 3D piece and automatically a change is generated in the plane [3], now logically this will be the new plane already with the modification. Therefore, the CAD parts of the part and the mold were obtained as the complete part was designed (piston and casting mold) as can be seen in Figure 3.

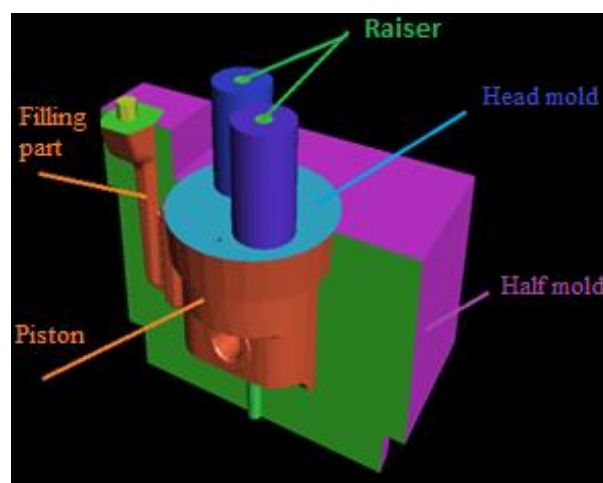


Figure 3 Piston and mold for casting (assembly)

Once the assembly is finished, it must be checked that the export of the CAD model does not have out of place geometries, that is, the virtual assembly must remain as the real one, for this there is a tool in the software that is responsible for detecting some geometry irregular or something that could affect us in the simulation.

If they do exist, the same software gives you the option to correct automatically as shown in Figure 4, if there are no discrepancies in the software, it sends you a message that the simulation can be started.

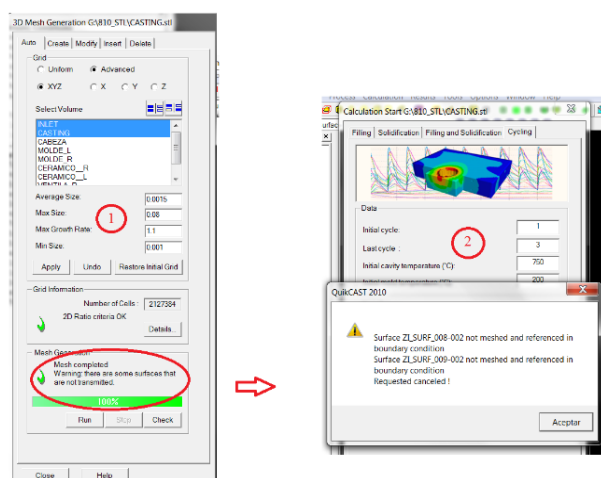


Figure 4 Export problems message

Piston alloy to simulate

In the company 3 types of alloys are used, derived from this, the mechanical and thermal properties change depending on it, for that reason, it is necessary to place the percentages within the software so that the results are the most approximate to reality depending on their chemical composition elements as shown in Table 2.

The elements that make up the alloy to be oxidized are shown in Table 2 in which the alloy contains 8.5 - 10.5% silicon.

Element	M-124	F-132	AS-17
%Si	11.00 - 13.00	8.5 - 10.5	15 - 16
%Fe	0.7 max	1.00 max	0.7 max
%Cu	0.8-1.3	2.0 - 4.0	2.0 - 3.0
%Mn	0.3 max	0.5 max	0.4 max
%Mg	0.8 - 1.3	0.5 - 1.50	0.5 - 1.0
%Ni	0.8 - 1.3	0.5 max	0.35 - 0.80
%Zn	0.3 max	1.00 max	0.030 max
%Ti	0.2 max	0.25 max	0.2
%Ca	0.007 max	0.007 max	0.007 max

Table 2 F-132 alloy elements

According to these elements, the alloy is registered with its different percentages within the program as shown in figure 5, it is only the alloy to be cast, because the molds are made of cast iron and the same software it already has the parameters established in its memory, therefore, its effect within the similar foundry is already taken into account for its possible effects.

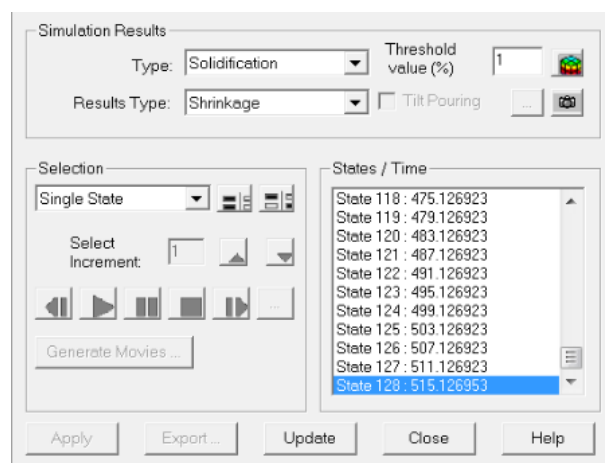


Figure 5 Alloy to be used in simulation

Once the base parameters have been established within the program, we proceed to indicate each of the elements and place their boundary condition (Figure 6).

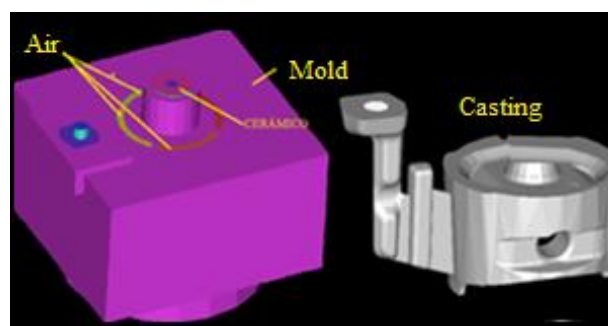


Figure 6 Selection of parts for material assignment

Simulation and results (Software)

Once the data has been emptied into the software and having the assembly free of imperfections within its export [4], the simulation is run with the established parameters (Figure 7).

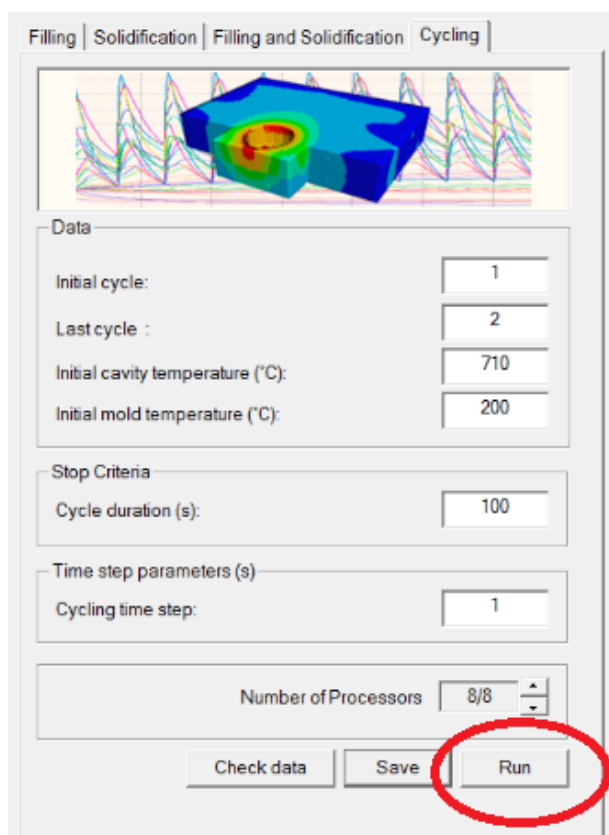


Figure 7 Simulation start

As a result, a transparent part is shown with possible defects in another color to make a contrast and identify possible defects more clearly as shown in Figure 8.

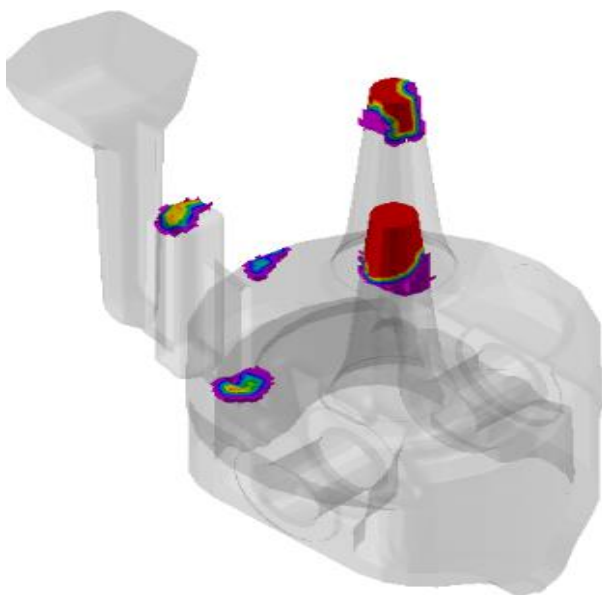


Figure 8 Simulation result with initial parameters

The defects, as previously explained, are shown in another color and are the result of virtual casting with the parameters established on the floor. As indicated with this part number, there were 50% defects due to "pore in the head" as the simulation showed it and is shown in Figure 9.

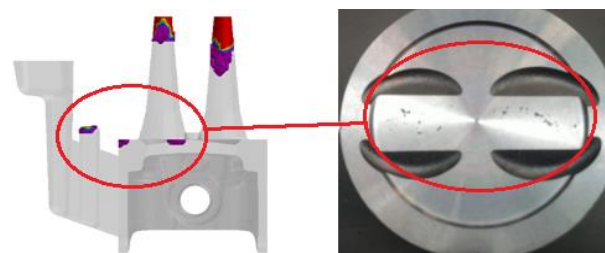


Figure 9 Piston with defective head

Once it has been demonstrated that the software is throwing us the problem that is supposed to be greater in our performance of the element, we have to analyze the design of the mold for the piston, because it can clearly be seen that the defect is due to the variation of the piston design of the process and not of external functions, since the software encapsulates the conditions by design in the results.

New piston design and simulation

Derived from the result that the simulation yielded and when corroborating the defect that was presented above on the floor, the design was analyzed and it was decided to change the design of the piston feed (riser) since it was deduced that having 2 risers kept too much heat. As a result of this, there was a bad distribution of the metal in the piston head, for that reason the "pore" was having, therefore, a piston with a single riser was designed and placed at the beginning of the piston, to help its distribution and help its solidification as shown in Figure 10.

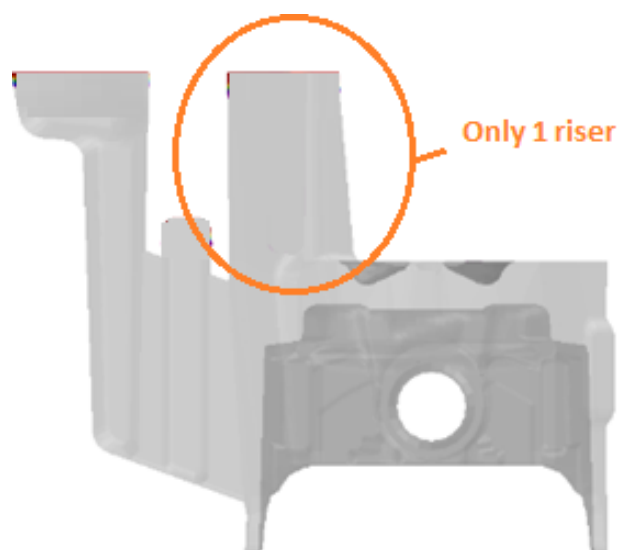


Figure 10 Piston riser 3D modification

Simulation with proposed modification

Using the same process parameters, but with the change in the design, the simulation is run again and thus be able to detect with the change in the design eliminate the main defect [5].

The results are shown in Figure 11.

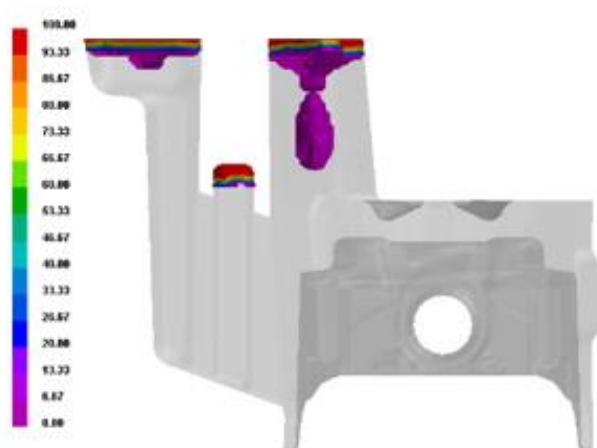


Figure 11 Simulation result with new riser

As can be seen in the simulation result, the defects disappear due to the change in the design of the piston feed during its casting process, so far it is satisfactory as the result is shown, eliminating the defects, but as previously done. , now the change must be made in physics and run a test on the floor to corroborate the result in the real process and demonstrate the reliability of the software in reverse.

The change in the mold and part is carried out in the company's workshop, eliminating the two central risers and leaving only one placed near the main power supply.

Casting process results (modified)

With the change made in physics based on the simulation and the CAD model, we proceed to program a run of 100 pistons on the floor to be able to take a significant sample that helps us to generate a panorama of correct piston conditions, with the same parameters of process but with the change in its design, the floor test is run as shown in Figure 12.



Figure 12 Piston free of imperfections

The piston can be seen that its main defect was eliminated within the main defects of the 100 piston run, therefore, it can be deduced so far that the software has had a high reliability. Therefore, stopping from the second stage is to carry out a larger run to corroborate the data and modifications.

Table 3 shows of the 100 test pistons which were the results and their defects.

Description	N. Pieces
Good parts	78
Pore in head	5
Cold junction	4
Gas	10
Metallic inclusion	3

Table 3

Within this run it can be quickly said that its performance is 78%, that is, 78% of the pieces produced were classified as "acceptable pieces", therefore, it is necessary to corroborate and compare with a larger run, the which will be established as part of the second stage of the Project.

Conclusions

It was possible to find a relationship between the software and the process on the floor, in tests considered as quick the result has been favorable, but a larger test has to be carried out and to be able to have the exact reliability of the software and to be able to make decisions in the future. I respect its use and application as part of the company process.

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Development of an application for the estimation of vegetation indices using SENTINEL remote sensing data

Desarrollo de una aplicación para la estimación de índices de vegetación en imágenes del sensor SENTINEL

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Abstract

Geomatics is an application that covers various topics; sustainable land use, identification and monitoring of crops, production estimation, marketing, evaluation of other lands, environmental impact analysis, among. It groups techniques related to data collection using remote and proximal sensors which allow determining wavelengths and spectral responses to estimate variables that allow quantification of statistical data. Vegetation indices are combinations of spectral bands recorded by the different remote sensing satellites, their basic function is to enhance the vegetation based on its spectral response and thus attenuate the details. The objective of this research was to provide the user with a tool developed by means of GIS that allows to execute complex processes in an automated way and with optimal results whose impact is mainly focused on optimizing production time and obtaining variables whose application can have an impact on the optimal use of fertilizers in agricultural activities. The results obtained are a total of 21 automated vegetation indices having as input the scenes obtained through the SENTINEL 2A and 2B sensor.

SENTINEL, Vegetation index, Python

Resumen

La geomática es una aplicación que comprende temas diversos; el uso sostenible de la tierra, la identificación y monitoreo de cultivos, estimación de la producción, el mercadeo, la evaluación de tierras, análisis de impacto ambiental, entre otros. Agrupa técnicas relacionadas con el levantamiento de datos mediante sensores remotos y proximales los cuales que permiten determinar longitudes de onda y respuestas espectrales para estimar variables que permitan la cuantificación de datos estadísticos. Los índices de vegetación son combinaciones de bandas espectrales registradas por los diferentes satélites de teledetección, su función básica es realzar la vegetación en función de su respuesta espectral y así atenuar los detalles. El objetivo de esta investigación fue el de facilitar al usuario una herramienta desarrollada mediante programación SIG que permite ejecutar procesos complejos de manera automatizada y con resultados óptimos cuyo impacto principalmente va enfocado a la optimización de tiempo de producción y la obtención de variables cuya aplicación puede repercutir en el uso óptimo de fertilizantes en actividades agrícolas. Los resultados obtenidos son un total de 21 índices de vegetación automatizados teniendo como insumo las escenas obtenidas mediante el sensor SENTINEL 2A y 2B.

SENTINEL, Índice de vegetación, Python

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Introduction

In recent years, Geographic Information Systems (GIS) have undergone significant development since their origins. The popularity of these technologies and the development efforts carried out by a large number of sciences that benefit from the use of this tool have contributed to redefining the discipline and integrating elements that were unthinkable at the time (Chuvienco, 2007).

However, the main components that identify the main core of a GIS have been maintained throughout this evolution, and it is their appearance that defines the initial moment in which we can situate their origins.

GIS as a tool emerged in the 1960s as a result of the conjugation of some factors that converged to give rise to the development of the first information systems, these factors are mainly two: the growing need for geographic information, its management and optimal use, and the appearance of the first computers (Calvo, 2012).

These factors are those that have continued to drive the advancement of GIS as a tool since its inception, since interest in the study and conservation of the environment is also gradually increasing today, and this creates an ideal situation for techniques and tools such as GIS to remain in constant evolution.

At present, and as part of this evolution, we can find the emergence and development of some aspects of GIS such as: GIS programming languages (Chuvienco, *et al.*, 2005).

These are a formal language, designed to perform processes in an automated way that can be carried out by computers. They can be used to create desktop applications that control physical and logical behaviour, to express algorithms with precision or as a mode of human communication.

The application of Geomatics is varied, ranging from sustainable land use, crop identification and monitoring, production estimation, marketing, land evaluation, to environmental impact analysis of land uses, among others (FAO, 1995; 1996; Beek, Bie & Driessen 1996).

It groups some techniques such as remote sensing and proximal sensing data relationships, which allow determining appropriate wavelengths and spectral responses to estimate variables for the quantification of vegetation indices.

Materials and methods

GIS programming language

A program is a set of instructions to carry out a task, and is composed of four essential parts:

- Code. This is the actual set of instructions. Normally, the code is written in a way that is easy for a person to understand and manipulate.
- Memory. Provides space for the program to store data for later retrieval.
- Input. This is the set of data that the program receives as it executes and that conditions the actions it performs and, consequently, the results it provides. Generally, the data comes from the user, but it can also come from other programs. In the latter case we have, for example, data sent by a web server or stored in a database.
- Output. This is the set of data generated in the form of a result during the execution of the programme. This data can be perceived as actions from the user's point of view.

The results can be various: a number, a new file, an image, etc. In computer science, programs were written in the form of holes in special cards. These holes were used to represent the data and the code, but going from the programmer's will to the holes and vice versa was not an easy task.

Fortunately, years later, so-called programming languages appeared, which used a syntax very similar to that of a conventional language to describe the actions to be performed by the computer. These programs were then interpreted by another program called a compiler, which was responsible for translating all these sentences into something lighter for the computer.

This way of programming, with few changes, is the one that has survived to the present day.

In the GIS environment, programming has become a very useful tool for users as it helps in the automation of processes, this minimises operating costs by reducing the time to obtain results from complex processes. Among the most popular GIS programming languages are: SQL, Java, Python, JavaScript, CSS, Ruby, PHP, C++, C, C#, Visual Basic NET, R, Flex, Silverlight, Avenue, AML and VBA for ArcObjects.

Graphical user interface

The Graphical User Interface (GUI) is a computer program that operates using a set of images and graphical objects to represent the actions and information available in the interface.

Using a set of images and graphical objects to represent the actions and information available on the interface. Its main function is to provide a simple visual environment that allows communication with a computer's operating system.

Qt Designer is part of the Qt Framework suite of application development software, which designs multilingual graphical user interfaces; it generates XML files whose content is the GUI format, which can be converted with the relevant language-specific software. This is free and open source software, which uses the C++ programming language natively and can additionally be used in other programming languages through bindings.

It works on all major platforms, and is widely supported. The library's API has methods for accessing databases via SQL commands, as well as XML usage, thread management, network support, a unified cross-platform API for file manipulation and a multitude of other file handling and traditional data structures. (Ecu Red, 2010)

Copernicus programme

Copernicus is an Earth observation programme developed by the European Space Agency (ESA), one of the most ambitious programmes of its kind, designed to provide accurate, up-to-date and easily accessible information to improve environmental management, understand and mitigate the effects of climate change and ensure public safety.

SENTINEL-2 Multispectral

The Sentinel-2 mission aims to capture multispectral images of the earth at medium resolution, its main objective is to monitor the variability of the earth's surface. It consists of the MSI (Multi Spectral Instrument), which captures information of the Earth's surface in 13 spectral bands, with different spatial resolutions, four 10 m bands, six 20 m bands and three 60 m bands. Sensor 2A was launched on 23 June 2015, while its twin, sensor 2B, was launched into orbit on 7 March 2017. The revisit time between the two sensors is 5 days.

SENTINEL-2 bands	Central wavelength (μm)	Spatial resolution
Band 1 Coast	0.443	60
Band 2 Blue	0.490	10
Band 3 Green	0.560	10
Band 4 Red	0.665	10
Band 5 Edge of red	0.705	20
Band 6 Edge of red	0.740	20
Band 7 Red edge	0.783	20
Band 8 Near infrared	0.842	10
Band 8 Band 8a	0.865	20
Band 9 Water vapour	0.945	60
Band 10 SWIR - Cirrus	1.375	60
Band 11 SWIR	1.610	20
Band 12 SWIR	2.190	20

Table 1 List of spectral bands and their respective spectral and spatial resolutions

Source: Own elaboration

The products acquired by the mission are divided into 100 x 100 km tesserae.

Image processing

Sentinel-2 imagery, available for download, has two processing levels; Level 1C imagery and Level 2A imagery.

Level 1C images are ortho-rectified and have reflectance levels above atmospheric (TOA). That is, they correspond to atmospherically corrected images and provide reflectance data closer to reality.

On the other hand, the level 2A images are ortho-rectified with reflectance levels below the atmosphere (BOA).

Vegetation indices

Vegetation indices are used to highlight the characteristics of healthy, developed vegetation in relation to the soil.

The most common are Normalised Vegetation Index (NDVI), Soil Adjusted Vegetation Index (SAVI) and Leaf Area Index (LAI).

The application developed has a focus and application in the area of agriculture, so the indices studied and selected are focused on the estimation of chlorophyll content in crops.

Vegetation indices	Formula	Reference
Normalized difference vegetation index	NDVI (NIR - R) / (NIR + R)	Rouse <i>et al.</i> (1974)
Soil adjusted vegetation index	SAVI (1 + L) (NIR - R) / (L + NIR + R)	Huete (1988)
Green normalized difference vegetation index	GNDVI (NIR - G) / (NIR + G)	Gitelson and Merzlyak (1996)
Normalized difference red edge index	NDRE (NIR - RE) / (NIR + RE)	Fitzgerald <i>et al.</i> (2010)
Red edge chlorophyll index	CIred edge NIR / RE - 1	Gitelson <i>et al.</i> (2005)
Green chlorophyll index	CIgreen NIR / G-1	Gitelson <i>et al.</i> (2005)
Ratio vegetation index	RVI NIR / R	Jordan (1969)
MERIS terrestrial chlorophyll index	MTCI (NIR - RE) / (RE - R)	Dash and Curran (2004)
Canopy chlorophyll content index	CCCI (NDRE - NDREMIN) / (NDREMAX - NDREMIN)	Fitzgerald <i>et al.</i> (2010)
Transformed chlorophyll	TCARI / OSAVI 3*[(RE - R) - 0.2*(RE - G) (RE/R)]	Haboudane <i>et al.</i> (2002)

absorption in reflectance index/Optimized soil-adjusted vegetation index		/ [(1 + 0.16) (NIR - R) / (NIR + R + 0.16)]	
Modified chlorophyll absorption in reflectance index/Optimized soil-adjusted vegetation index	TCARI / OSAVI	/ [(RE - R) - 0.2*(RE - G)](RE/R) / [(1 + 0.16) (NIR - R) / (NIR + R + 0.16)]	Haboudane <i>et al.</i> (2002)
Red edge-based transformed chlorophyll absorption in reflectance index/Optimized soil-adjusted vegetation index	TCARI / OSAVI RE	/ 3*[(NIR - RE) - 0.2*(NIR - G) (NIR/RE)] / [(1 + 0.16) (NIR - RE) / (NIR + RE + 0.16)]	Wu <i>et al.</i> (2008)
Red edge-based modified chlorophyll absorption in reflectance index/Optimized soil-adjusted vegetation index	MCARI / OSAVI RE	/ [(NIR - RE) - 0.2*(NIR - G)](NIR/RE) / [(1 + 0.16) (NIR - RE) / (NIR + RE + 0.16)]	Wu <i>et al.</i> (2008)

Table 2 List of the main selected indices
Source: Own elaboration

Obtaining vegetation index values

In order to obtain the normalised difference vegetation index (NDVI) values, it was necessary to use the following expression proposed by (Rouse *et al.*, 1974):

$$NDVI = \frac{(IRC - R)}{(IRC + R)} \tag{1}$$

Where:

NIR: is the reflectivity measured in the near infrared.

R: is the reflectivity measured in the red region.

On the other hand, the SAVI index (Huete, 1988) was used in order to reduce the alterations presented in the NDVI values in sparsely vegetated areas and is obtained by means of:

$$SAVI = \frac{(1+L)(IRC - R)}{L + IRC + R} \tag{2}$$

Where:

IRC = corresponds to the reflectivity in the near infrared band, while.

R = refers to the reflectivity in the red band.

L = is a constant for SAVI, if L is 0 the SAVI index becomes equal to NDVI, a value of 0.5 appears frequently in the literature for this variable (Allen *et al.*, 2002).

Processing

The pre-processing phase comprises two parts: the cropping of the study area and the conversion of the digital numbers of the image to reflectance values.

For the cropping of the study area, the user must check the "shapefile" option and indicate which file will be the cropping file.

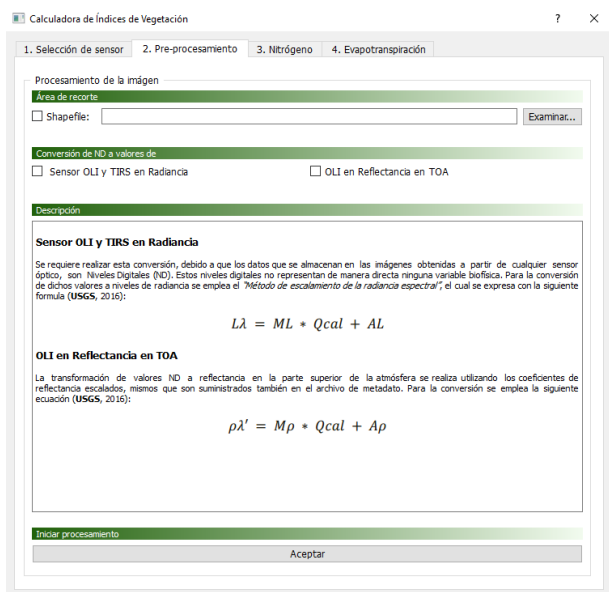


Figure 1 Graphical interface of the application, preprocessing section

Source: Own elaboration

The conversion of digital numbers is performed by selecting the corresponding option, whose results (reflectance) are stored in a folder called: "Processing", located within a specific path and where the products requested by the user are stored.

Obtaining indices

Finally, in the last stage, the user marks the option of those indices he/she wishes to obtain, the results of which are also stored in the folder mentioned in the previous step (Processing).

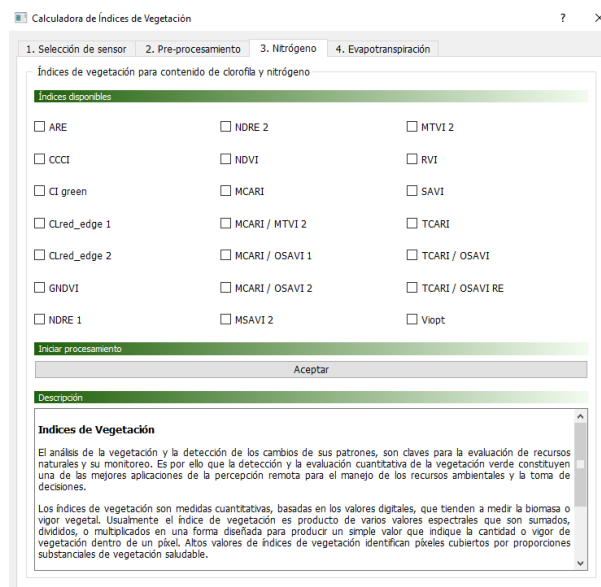


Figure 2 Indices available to the user and that the calculator performs in an automated way

Source: Own elaboration

PyQT4 – QT Designer

Using QtDesigner, a development tool, the graphical interface ("etcalculator.ui") is created and the template and functionalities available to the user are designed. The initial procedure is based on a form without buttons (Dialog without Buttons):

Once the template has been selected, the next step consists of dragging the components to be used (widgets) from the toolbar (Widget Box):

For the design of the application it has been considered to use various elements (widgets) that allow to give the desired functionality to the interface.

The elements considered are:

- Tags.
- Line Edit.
- Check Box.
- Radio Buttons.
- Combo box.
- Push Buttons.
- QHBox Layout.

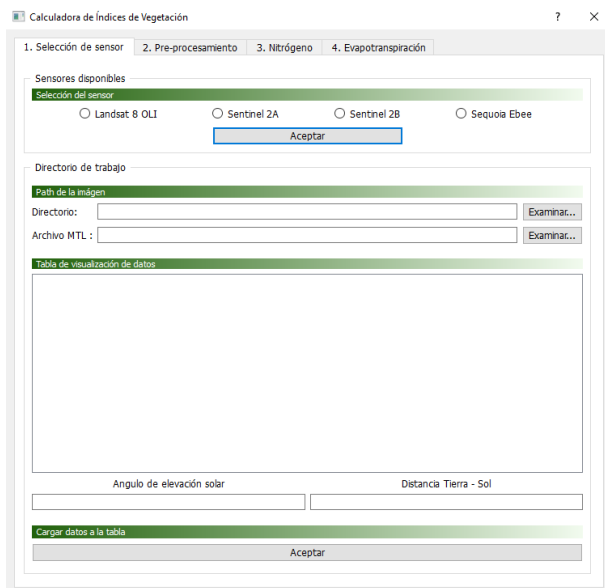


Figure 3 Graphical interface of the application, sensor selection section

Source: Own elaboration

What each of them does is described below:

Tags (QLabel)

A QLabel object acts as a placeholder to display non-editable text or image, or an animated GIF movie. It can also be used as a mnemonic key for other widgets. Plain text, hyperlinked rich text can be displayed in the label.

Line Edit (QLineEdit)

The QLineEdit object is the most commonly used input field. It provides a box in which one line of text can be entered. To enter multi-line text, the QTextEdit object is required.

CheckBox (QCheckBox)

A rectangular box before the text label appears when a QCheckBox object is added to the main window.

Like QRadioButton, it is also a selectable button. Its common use is in a scenario when the user is asked to choose one or more of the available options. Unlike radio buttons, checkboxes are not mutually exclusive by default. To restrict the choice to one of the available items, checkboxes must be added to QButtonGroup.

Radio Button (QRadioButton)

An object of class QRadioButton presents a selectable button with a text label. The user can select one of the many options presented in the form. This class is derived from the QAbstractButton class.

Radio buttons are self-exclusive by default. Therefore, only one of the radio buttons in the parent window can be selected at a time. If one is selected, the previously selected button is automatically deselected. Radio buttons can also be put in a QGroupBox or QButtonGroup to create more than one selectable field in the parent window.

Combo Box (QComboBox)

A QComboBox object presents a drop-down list of items to select. It takes minimal screen space on the required form to display only the currently selected item.

Push Button (QPushButton)

In any GUI design, the command button is the most important and most used control. Buttons with Save, Open, OK, Yes, No and Cancel etc. as captions are familiar to any computer user.

In PyQt API, the QPushButton class object presents a button that when clicked can be programmed to invoke a certain function. The QPushButton class inherits its core functionality from the QAbstractButton class. It is rectangular in shape and a text title or icon can be displayed on its face.

QHBoxLayout

The QHBoxLayout class aligns widgets vertically or horizontally. Its derived classes are QVBoxLayout (for arranging widgets vertically) and QHBoxLayout (for arranging widgets horizontally). (The Qt Company Ltd, 2021).

Lenguaje Python

Python is a high-level, object-oriented, scripting language. Python is also the language of choice for QGIS to automate GIS tasks, using PyQGIS. First, uic.py was used to convert the .ui file created in QTDesigner into a .py file that we will use as the project file.

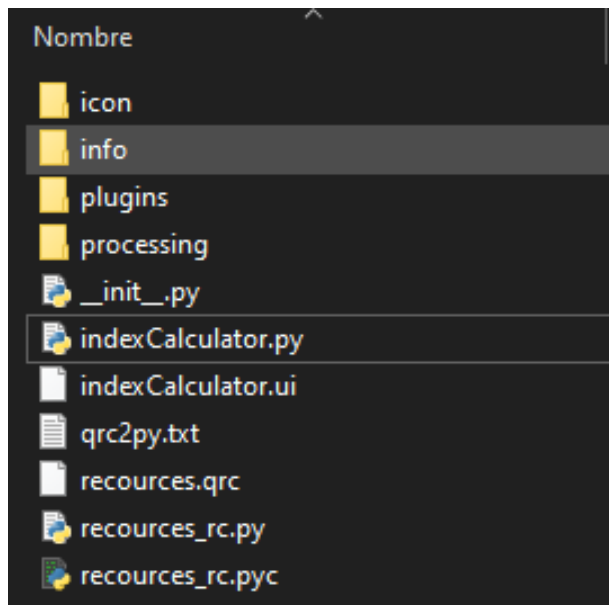


Figure 4 Resources of the application
Source: Own elaboration

Inside the plugins folder (work folder) there is a Python module called processing which contains a script called process, in which the functions for calculating radiation, reflectance and the different vegetation indices available for the user to execute are defined.

There is also a folder called icon, which contains the graphics used in the design and presentation of the graphic interface.

On the other hand, the file indexCalculator.py is the script that gives functionality to the graphical interface.

```

        QtGui.QFileDialog.ShowDirsOnly
    )
    self.lineEdit1.setText(str(imgDir)) ## Introducimos la ruta como
    global imagen ## Creamos una variable global
    imagen = self.lineEdit1.text() ## A la variable le indicamos que
    return self.lineEdit1.setText ## Esta función devuelve el acceso

def mtlPath(self):
    """Selecciona la ruta donde se encuentra el archivo MTL"""
    ## Se abre una ventana de diálogo para indicar la ruta del archivo
    mtlDir = QtGui.QFileDialog.getOpenFileName(
        None, 'Test Dialog', os.getcwd(), '*.txt')
    self.lineEdit2.setText(str(mtlDir)) ## Introducimos la ruta como
    global MTL ## Creamos una variable global
    MTL = self.lineEdit2.text() ## A la variable le indicamos que es

def shpPath(self):
    """Selecciona el archivo shapefile que servirá de área de recorte
    if self.checkBoxShapefile.isChecked(): ## En el caso de que SI se in
    shpDir = QtGui.QFileDialog.getOpenFileName(
        None, 'Test Dialog', os.getcwd(), '*.shp') ## Se abre una
    self.lineEdit5.setText(str(shpDir)) ## Se introduce la ruta de
    else: ## En el caso de que NO se introduzca shp de área de recorte
    QtGui.QMessageBox.information(self, "Alerta", '''Para cargar
        QtGui.QMessageBox.OK) ## Si se dete

def openMTL_LANDSAT(self):
    """Agregamos los encabezados de la tabla de visualización"""
    self.tableWidget.insertRow(1)
    headers = ['Banda', 'Rad_MULT', 'Rad_ADD', 'Ref_MULT', 'Ref_ADD']
    self.tableWidget.setColumnCount(len(headers))
    print 'listo'
    for c in range(len(headers)):
        item = QtGui.QTableWidgetItem(headers[c])
        #print item
        self.tableWidget.setHorizontalHeaderItem(c, item)

```

Figure 5 Example of the Python code of the calculator
Source: Own elaboration

Results

In the field of remote sensing there are studies that have currently been developed for the automation of the calculation of vegetation indices, one of them was carried out by Castellanos, Moreno and Maldonado, whose objective was to obtain vegetation indices by applying the techniques for the calculation of the SAVI and NDVI, from multispectral images with reflectance values.

The images used in the application are LANDSAT 8 from the OLI sensor and the software used is QGIS 2.8.3. The technique starts with the radiometric calibration of the images and the calculation of the metadata file parameters using the QGIS GeoSudTOA add-on.

The results obtained are very similar to those obtained with the application proposed here, the difference lies basically in the input, considering the specific characteristics of both sensors.

The main factor to consider is the temporal resolution and spatial resolution; that is, while the LANDSAT sensor has 15 days and 30 m per pixel respectively, the SENTINEL 2A and 2B sensors have 5 days of temporality and 10 m per pixel.

It is important to mention that, although the results have been very satisfactory, due to its recent development, it is recommended to continue validating the data obtained through the script developed in order to control if any possible error arises in the process, detect it and therefore correct it. It is hoped that this will not be the case.

The processing time of the images was reduced considerably, obtaining a total of 21 vegetation indices in a time of less than 5 minutes, ready to be analysed and interpreted by the user.

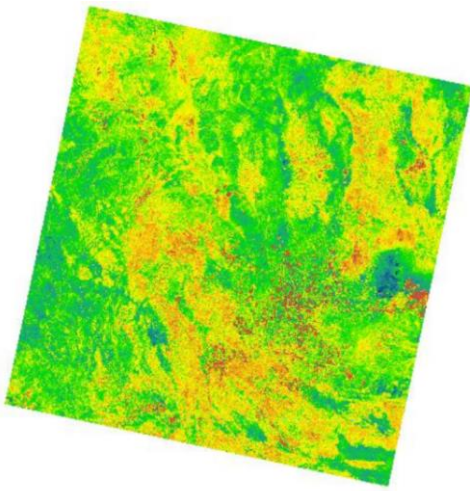


Figure 6 NDVI obtained with the use of the calculator
Source: Own elaboration

ARE.TIF	14/10/2020 10:55 a. m.	Archivo TIF	473,461 KB
CCCI.TIF	14/10/2020 10:55 a. m.	Archivo TIF	473,461 KB
Clgreen.TIF	14/10/2020 10:55 a. m.	Archivo TIF	473,461 KB
CLredE1.TIF	14/10/2020 10:55 a. m.	Archivo TIF	473,461 KB
CLredE2.TIF	14/10/2020 10:56 a. m.	Archivo TIF	473,461 KB
MCARI.TIF	14/10/2020 10:57 a. m.	Archivo TIF	473,461 KB
MCARI_OSAVI1.TIF	14/10/2020 10:58 a. m.	Archivo TIF	473,461 KB
MCARI_OSAVI2.TIF	14/10/2020 10:59 a. m.	Archivo TIF	473,461 KB
MSAVI2.TIF	14/10/2020 11:00 a. m.	Archivo TIF	473,461 KB
MTVI2.TIF	14/10/2020 11:00 a. m.	Archivo TIF	473,461 KB
NDRE1.TIF	14/10/2020 10:56 a. m.	Archivo TIF	473,461 KB
NDVI.TIF	14/10/2020 10:57 a. m.	Archivo TIF	473,461 KB
RVI.TIF	14/10/2020 11:01 a. m.	Archivo TIF	473,461 KB
SAVI.TIF	14/10/2020 11:02 a. m.	Archivo TIF	473,461 KB
TCARI_OSAVI.TIF	14/10/2020 11:02 a. m.	Archivo TIF	473,461 KB
TCARI_OSAVI_RE.TIF	14/10/2020 11:03 a. m.	Archivo TIF	473,461 KB
Viopt.TIF	14/10/2020 11:04 a. m.	Archivo TIF	473,461 KB

Figure 7 Results obtained with the application
Source: Own elaboration

It should be mentioned that it is expected to continue working with the application, so that the application not only generates the products but also provides the user with an interpretation of the values obtained, which would make the development more complete and would have an immediate application.

Would be more complete and would have an immediate application.

Currently the application already has three modules, it is capable of processing images from LANDSAT and SENTINEL sensors and images obtained by Unmanned Aerial Vehicles (UAVs), as well as including a module for obtaining useful variables in the estimation of crop evapotranspiration.

Conclusions

GIS programming languages allow the estimation of vegetation indices with a fairly acceptable accuracy. The application is very user-friendly, which allows the user to obtain the different indices without major inconvenience.

The development of the graphic interface reduces the processing time of satellite images and also automates the processes and also automate complex calculation processes for the generation of vegetation indices, which implies great benefits within the working reality.

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Construction of a PUMA-type robot with 3 degrees of freedom

Construcción de un robot tipo PUMA de 3 grados de libertad

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Abstract

Construction of a PUMA robot type 3 degrees of as technology has improved, specialized machines have been developed to perform various tasks. Most existing robots today are those which are used in the industry, so-called industrial robots, which are constituted by one or more arms. The robotic arm, PUMA (Programmable Universal Machine for Assembly, or Programmable Universal Manipulation Arm), for its acronym in English, which is presented below consists of three axes to move, 3GDL (degree of freedom), where it was considered essentially for teaching purposes, purchase an industrial type robot is very expensive, so it becomes viable development and make it available to the lab, so that students achieve their associated practices. To construct specialized software was used for design SolidsWorks , and linked with Matlab SimMechanics. LabView, for virtual and physical communication, arduino one card was used to provide the link between engines and software, currently tests are done with the Compaq Rio NI card to improve communication. The relevance of this project is the dynamic analysis, design, manufacturing and programming, and the whole process was conducted within the premises of the University.

Robot, GDL, Programming, Design, Communication

Resumen

A medida que se ha mejorado la tecnología, se han desarrollado máquinas especializadas para ejecutar diversas tareas. La mayoría de los robots existentes en nuestros días son aquellos que son utilizados en la industria, llamados robots industriales, los cuales están constituidos por uno o más brazos. El brazo robótico presentado a continuación consta de tres ejes para movilizarse, 3GDL, y utilizarlo para una aplicación industrial o ya sea para una aplicación especial, especialmente para aspectos didácticos. Para su construcción se utiliza software especializado, SolidsWorks para el diseño, y vinculado con Matlab y SimMechanics. LabView, para la comunicación virtual y física, se utilizó una tarjeta Arduino para proporcionar el enlace entre los motores y el software, en la actualidad se realizan pruebas con la tarjeta Compaq Rio NI para mejorar la comunicación. La relevancia de este proyecto es el análisis dinámico, diseño, fabricación y programación, todo el proceso se llevó a cabo dentro de las instalaciones de la Universidad.

Robot, GDL, Programación, Diseño, Comunicación

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Introduction

When we hear the word Robot, we think of those movies that have surprised us by presenting us with robots that perform actions superior to the capabilities of the human being. Perhaps the most famous robot models have been those created by George Lucas in his movie Stars Wars whom we knew as C₃PO and R₂D₂. However, the idea that the films present to us is quite far from the industrial application of robots, which are considered as a type of machine-tools (Ogata, 2003). The eighteenth century is the time of the birth of industrial robotics. More than two hundred years ago, mechanical dolls were built, the size of a human being, that played musical pieces. Undoubtedly, today it can be said that the development of machine tools has been extremely accelerated.

An industrial robot is a reprogrammable multifunctional manipulator, capable of moving materials, parts, tools, or special devices, according to variable trajectories, programmed to perform various tasks (Barrientos, Peñín, alaguer, & Aracil, 1997).

A PUMA-type robot (Programmable Universal Machine for Assembly, or Programmable Universal Manipulation Arm) is an industrial robot arm developed by Victor Scheinman at the robotics pioneer Animation. Initially developed for General Motors, the PUMA robot arm grew out of initial designs invented by Scheinman while he was at MIT and Stanford University.

Animation produced PUMAs for a few years until it was absorbed by Westinghouse (ca. 1980), and later by the Swiss company Stäubli (1988) (Barrientos, Peñín, alaguer, & Aracil, 1997).

The Technological University currently has a robotic arm, Motorman brand, with six degrees of freedom, the great disadvantage with which it works is that commercial models have a specific work environment, a programming model and specific types of controllers by the manufacturer.

This situation impoverishes the learning process, the study program requires students to develop the design of a robot, from its conceptual design, its manufacture, its manufacture and the design and development of the control part.

The objective of this work is to generate the design and construction of a PUMA-type robot with 3 DOFs, which allows for versatility in the control stage and programming environments, which is didactic, placing it in the robotics laboratory of the institution so that be used by students of the subject.

In the methodology section, the techniques used to solve the problem are presented. It is important to note that the important part of the work is the development of skills in control and design techniques, which although they are not new in the field, they are for the University.

The results section shows the mechanism and control designs that were built by the researchers.

And the part of conclusions, the achievement obtained is presented, as well as future works and their applications.

Methodology to develop

A robot is mainly composed of three parts: the mechanical part (shape and size of the casing), the electronic part (composed of the robot's control circuit and sensors), and the power part (control of the robot's servo motors). The casing constitutes the mechanical part, its shape is one of the determining factors in the success of the development of a certain task. The electronic part is constituted by the control circuit that in turn contains a microcontroller which is programmed using a certain algorithm, in said algorithm lies all the decisions that the robot is going to make in certain given cases according to the problem (Hutchinson, Vidyasagar, & Mark, 2001).

Model of the robot

The structure to be used is based on a PUMA robot with 3 rotational degrees of freedom (DOF), so that the dynamic model of the robot is simpler and more manipulable to carry out the control and redundancy is avoided as far as possible.

Same the following and specifications, shown in table 1:

Estructura mecánica	Especificaciones
Número de ejes	3
Rango de movimiento en los ejes. Eje 1: cintura Eje 2: hombro Eje 3: codo	310° 310° 310°
Máximo radio de operación	340 mm
Home físico	Por posición fija de cada eje, determinado por microswitchs
Actuadores	Motores PITTMAN a 24VCC (GM9234C212-R3)
Características de motores	45 oz-in @ 1090 rpm 2.5 A

Table 1 DOF PUMA Robot Specifications

The robot model was obtained in 2 ways, using the Biomechanics application of MATLAB, and through the Lagrange mathematical model.

A model was obtained through the MATLAB calculation tool, working on the mechanical design made by Solidworks, obtaining the following diagram, which considers each of the robot's joints, as shown in figure 1.

Characterization

Knowing the variables of the joints, the position of the end of the forearm in the PUMA will be determined. The variables of the joints are the angles between the links in the case of rotational joints, and the extension of the link in the case of prismatic or sliding joints, the Denavit-Hartenverg analysis proposal will be used.

Dynamic Model

The Lagrange equations of motion will be used to obtain the dynamic model of the manipulator (Kelly & Santibáñez, 2003).

Results

The meaning of the various constants as well as their numerical values are summarized in Table 2.

Descripción	Notación	Valor	Unidades
Longitud del eslabón 1		0.350	
Longitud del eslabón 2		0.150	
Longitud del eslabón 3		0.150	
Distancia del centro de masa de eslabón 1		0.003	
Distancia del centro de masa de eslabón 2		0.024	
Distancia del centro de masa de eslabón 3		0.033	
Masa eslabón 1		2.010	
Masa eslabón 2		2.450	
Masa eslabón 3		0.675	
Inercia eslabón 1 respecto al centro de masa			
Inercia eslabón 2 respecto al centro de masa			
Inercia eslabón 3 respecto al centro de masa			
Aceleración de la gravedad		9.81	—
Offset		0.14	

Table 2 PUMA parameters

It is important to note that the design was made using the Solid Works software, to link it with Biomechanics and Mat lab, to perform the kinematic, direct and inverse analysis, as well as the dynamics.

The robot design can be seen in figure 1.



Figure 1 CAD design of robot type PUMA BY 3GDL

Derived from the dynamic analysis of the arm, the following results were obtained, as shown in figure 2, the analysis was performed in MATLAB and Biomechanics:

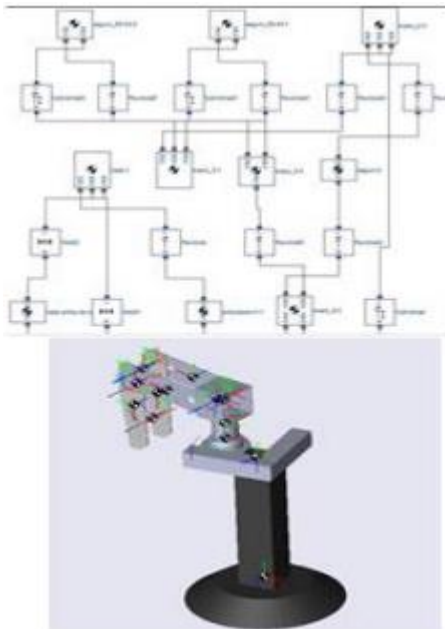


Figure 2 And dynamic analysis of the arm

The movement that was obtained in the joints is shown in table 3, in figure 3 the range of operation of the designed arm is shown.

Número de eje	Articulación	Movimiento	Número de motor
1	Cintura	Rota el cuerpo	1
2	Hombro	Sube y baja el brazo	2
3	Codo	Sube y baja el antebrazo	3

Table 3 Joint movement specifications

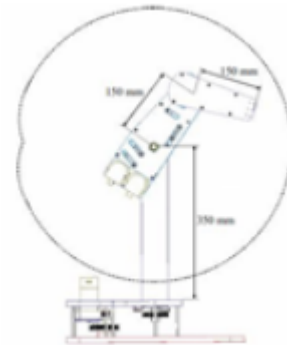


Figure 3 Operating Range

Transmission system

Figure 4 shows the high-torque toothed pulleys that transmit the movement of the motors to the waist, shoulder, and elbow joints. For the three movements, toothed pulleys are used in two stages to increase the reductions and their respective tensioners. The choice of the bands was made considering the criteria proposed by the manufacturer (FACE, 2001).

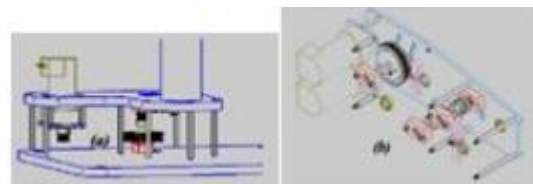


Figure 4 Powiats pulleys, shoulder pulleys

Electronic and control system

In the electronics part, an external power card was designed, since the selected card, which was the Arduino UNO, did not support the torque required by the servomotors. For the control part, an Arduino card and Lab View control software are used, it is important to mention that a power stage was required, since the Arduino card did not support the power required by the servomotors, as shown in figure 5.



Figure 5 Robot control and power for a servomotor

Figure 6 shows the work prototype, which was designed, manufactured, and to which the control systems are applied, using a personal computer as a work tool.



Figure 6 Robot prototype PUMA type of 3GDL

Gratitude

The work was supported by PROMEP to strengthen key academic bodies: UTSEM-CA-2, IDCA: 9786, for which we express our most sincere gratitude.

Conclusions

It was possible to carry out the design and manufacture of the 3GDL PUMA-type robotic arm, likewise tests are being carried out to identify which is the best control that can be had, the physical and virtual control interface is being developed.

The mass-length relationship for each element-link must always be taken into account and thus not require too much torque from the base links. Currently, the communication platform with Lab View is still being developed.

It is important to mention that currently the tenth semester students are already working with this model, they have developed a programming platform, communication, and communication using USB is currently being developed, it is expected to generate communication using Wi-Fi.

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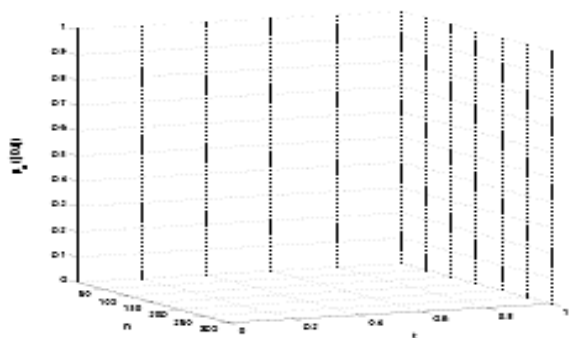
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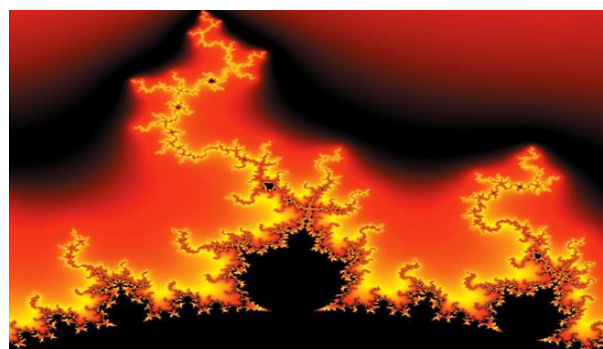


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