Analysis of the degradation in lithium-ion batteries

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Abstract: The purpose of this project is the application of the discrete element method (DEM) for the realization of a particle model based on the electrode material of the lithium-ion batteries in electric cars, trying to solve the main problems they present during charging and download since these directly affect the lifetime of the same

Keywords: Electrode, batteries, electric vehicle, litio.

Introduction

The aim of this project is to apply the Discrete Element Method (DEM) to create a particle model based on the electrode material of lithium-ion batteries, trying to solve the main problems that these present during charging and discharging, as these directly affect the useful life of the batteries.

It was decided to focus the study on cells with 18650 dimensions as a graphic representation and composed of LiFePO_4, without forgetting that there is a great diversity of batteries with similar chemical composition of which a brief mention is made.

The GiD software and its complement Kratos with the G-DEMPack extension were used for the study and discretisation of the structure to be analysed.

This project is carried out in order to give a guideline for the resolution of the problem of the batteries with respect to the charge and discharge cycles, since these cause problems of physical and mechanical character among which we find: the dilation and contraction which generates a growth of the delamination, local buckling, beginning of the vacuum and loss of the electrical contact with the current collector.

The growing demand for electric vehicles is causing intense development and research in the creation of more efficient batteries to drive these cars for longer distances, with more charge and a longer service life.

Thanks to this need arises the initiative to analyse the components of electric batteries and the problems they present over time, to know why the elements that store electrical energy gradually lose the quality of retaining enough energy for its proper functioning as well as transmitting it in a correct way to the parts of the car that require it.

-Electric battery

A battery is a device capable of storing energy in electrochemical form. There are two types: primary batteries and secondary batteries.

Primary batteries are characterised by the fact that the conversion of chemical energy to chemical to electrical energy is irreversible, i.e. after the battery has been completely discharged it cannot be recharged.

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Secondary batteries: better known as rechargeable batteries. These, when discharged, can be recharged by injecting direct current from an external source.

In general, the operation of a battery is based on an electrochemical cell. Electrochemical cells have two electrodes. The anode and the cathode. The anode is defined as the electrode where oxidation takes place (gives up electrons) and the cathode where reduction takes place (picks up electrons).

Lithium-ion batteries are supposed to solve many of the problems present in the electric car industry, but like all electronic components they are prone to problems caused by the passage of energy.

A feasible way to predict capacity degradation and possible mechanical failures in lithium-ion batteries is the analysis of macroparticles based on the Discrete Element Method (DEM) as this procedure performed correctly in the right software can save calculation time and give us a preview of the physical evidence of the problem we are facing.

Methodology

The Discrete Element Method (DEM) applied to the lithium-ion battery charging and discharging problem is more efficient than applying other types of numerical methods to solve it, as it fits perfectly with the type of problem being analysed in this project, unlike the Finite Element Method (FEM) where you can only do simulations in the elastic zone of a material, with DEM we can work in the elastic-plastic part and even in the plastic zone, that is to say with FEM we apply loads either physical, chemical or electrical and when removing them the material to analyse will recover in its totality its form and properties, this is of great utility when it is wanted to know a point of rupture, the quantity of load that supports a material, the pressure to which a pipe burst, etc. But what happens if we want to know at how many loads a material will break, if we apply a certain pressure on a pipe, at how many times it will have to be replaced to avoid damage.

The need to use the Discrete Element Method arises from what has been investigated in this work as the different contributions in different areas of people or organisations that have applied this method to different problems related to the deformation of a material not only with the passage of time but also with the passage of the loads placed and removed in its useful life, as well as what is already known about lithium-ion batteries and their different characteristics:

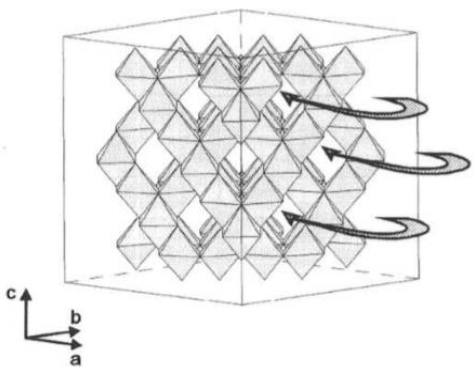

Figure 1. Empty channels defined in the three dimensions of space.

Discrete Element Method

The discrete element method is the decomposition of a physical model into smaller particles, which can be of different shapes such as circles, squares, triangles, etc., which are part of the analysis of the 2D method, or spheres, cylinders and tetrahedrons applying the 3D model. The purpose of this is to carry out a more detailed study of movement and fracture, by decomposing the element into smaller shapes we can analyse in particular how the body is affected at particle level according to the problem to be solved.

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The figure below shows a solid drawn and discretised in the GiD software creating a total of 89,279 spheres and the same number of nodes.

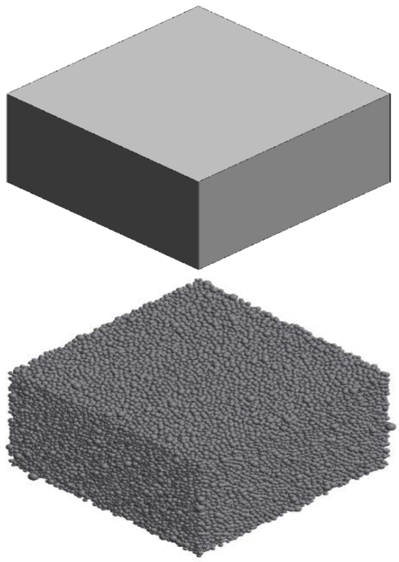


Figure 2. Representative cube in solid and discretised GiD

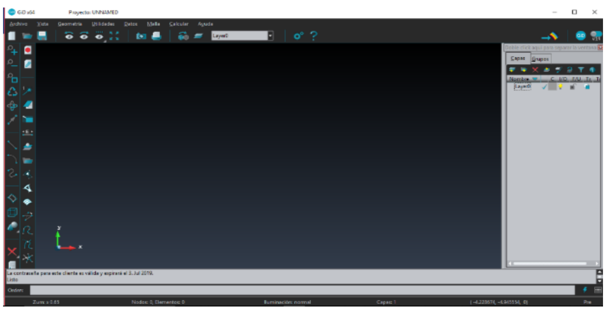
Software

For the implementation of the method, the GiD software with its Kratos extension was used, this is a framework for multidisciplinary problem solving. Within this branch of solution it was decided to work with the G-DEMPack complement as it has the necessary tools to establish the indispensable parameters both in the properties of the materials and in the solution strategy.

GiD is a pre and post processor for numerical simulation in science and engineering, designed to cover common needs in the field of numerical simulations from pre to post process such as:

- - Geometric Modelling (CAD)
- - Mesh generation.
- - Definition of data analysis.
- - Data transfer to analysis software.
- - Post-processing operations.
- - Visualisation of results.

Figure 3. GiD user interface



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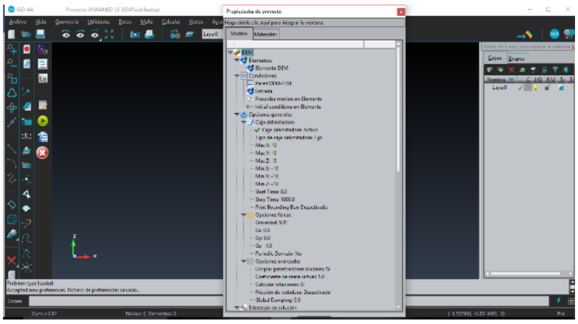

Figura 4. Window of the G-DEMPack Kratos extension

The use of this software was chosen because it requires less computing power compared to other programmes offered, as well as having a free licence for a period of one month, allowing us to use all the tools available in the paid version.

Graphical representation

Currently there are different types of electric battery arrangements, as already mentioned this depends on the needs of these, in this particular case we will talk about the batteries of electric vehicles.

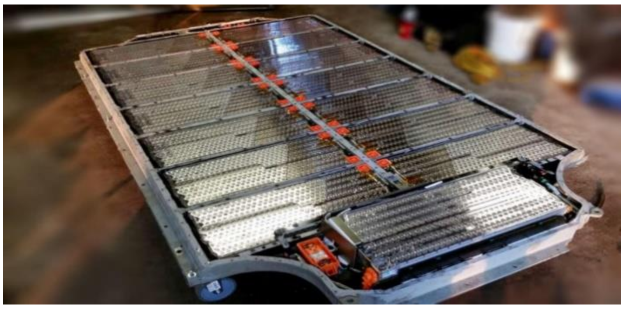

Figure 5. Tesla Model S Battery.

Simulations

The standard dimensions of the layers composing the electrode were taken into account, ranging in the order of 100-300 µm as a whole and each individual layer between 20 and 35 µm.

Three representative plates were drawn for each of the materials (graphite, polypropylene and lithium iron phosphate) with the above mentioned units. They were then decomposed into particles as shown in the following pictures.

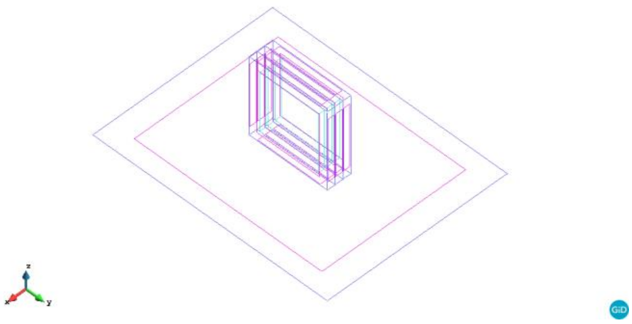

Figure 6. Drawing of the plates.

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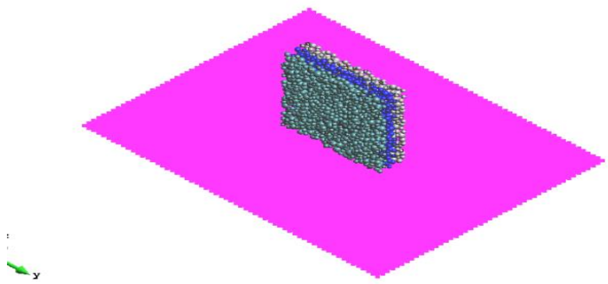

Figura 7. **Discretised plates in spheres.**

The simulation below shows the passage of smaller particles representing the release of lithium ions (smaller blue particles) from the cathode (LiFePO_4) to the anode (graphite) through the separator (polypropylene).

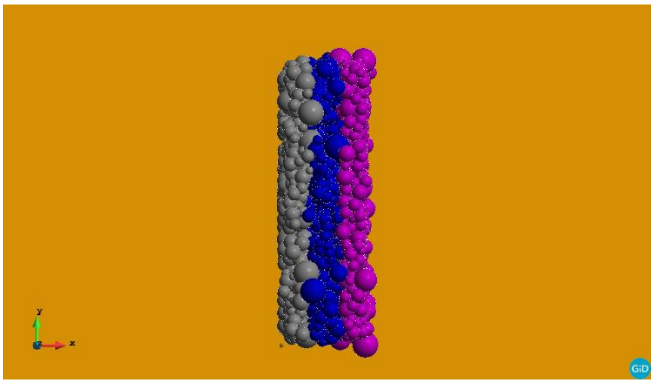

Figura 8. Starting position.

Failure mechanism

Taking into account the simulation in figures 7 and 8, we can use the post-processing tool offered by the software for displacement analysis.

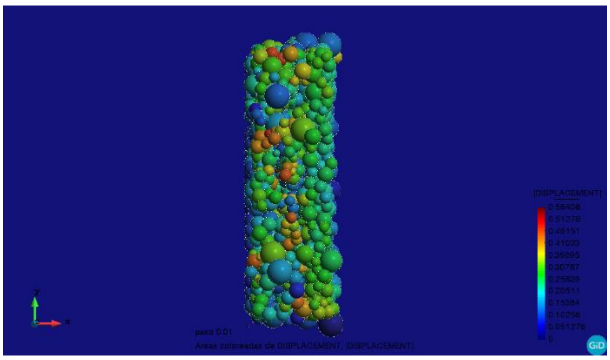

Figura 9. Post-processing starting position.

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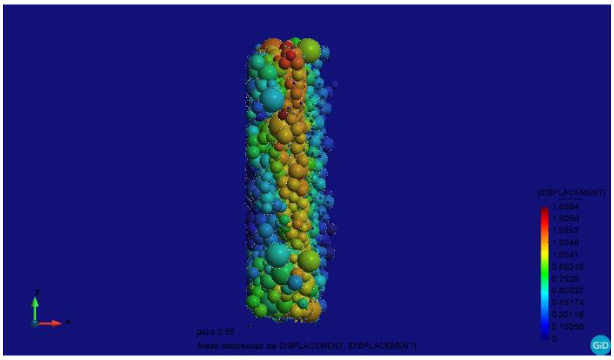
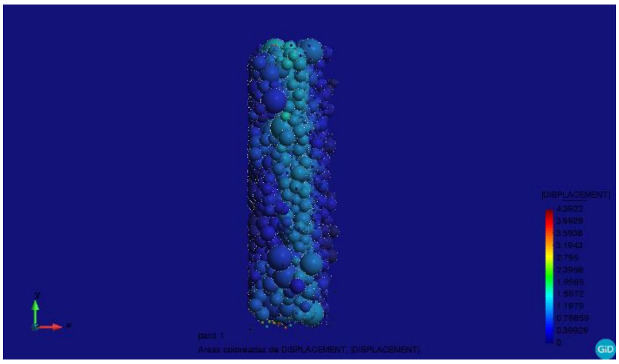


Figura 10. Position at the passage of half the time

Figura 11. Final post-processing position.



We can see in the previous images that the part with the greatest displacement is the intermediate plate, which corresponds to the separator material, in which red, yellow and green particles can be seen according to their degree of displacement, thus affirming that one of the main failures will be generated by wear in this part.

Local buckling.

As we already know, local buckling will generate a very noticeable change in the structure with the appearance of bending points. To appreciate this failure, one plate was taken into account, hiding the other two in a lateral view. The figure of the final position represents this phenomenon, buckling at the bottom of it.

Figura 12. Starting position.

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Figura 13. Final position.

Conclusion

As seen so far, this project was primarily based on the collection of information about the problem to be solved. We found advances regarding the failures and lifespan of lithium-ion batteries. However, none of them included a graphical representation for understanding the problem, which was what was done in the presented work. The existence of these internal and microstructural phenomena, leading to mechanical failures such as the aforementioned: local buckling, vacuum onset, delamination, and loss of contact with the current collector, was verified.

Referring to the simulations section, the main cause of failures in these batteries is the change in the structure of the separator between the anode and cathode, generating direct contact between these two materials, which produces a short circuit, directly affecting their lifespan.

This project can be used as a basis for solving the problem of the lifespan of electric car batteries by optimizing the composition and manufacture of their electrodes. The results obtained in other works along the same lines of research were also verified. We can conclude that the model created has reliable bases that can be implemented and improved to obtain more accurate results.

Availability of data and materials

The articles used within the table and important points to support the information of this project are available.

The data used are those found through a literature search.

Abbreviations

1.- **CAD** - Computer-Aided Design

2.- **DEM** - Discrete Element Method

3.- **FEM** - Finit Element Methot

4.- **MED** - Método de Elementos Discretos

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