Present and future of the numerical methods in buildings and infrastructures areas of biosystems engineering

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Abstract

Biosystem engineering is a discipline resulting from the evolution of the traditional agricultural engineering to include new engineering challenges related with biological systems, from the cell to the environment. Modern buildings and infrastructures are needed to satisfy crop and animal production demands. In this paper a review on the status of numerical methods applied to solve engineering problems in the field of buildings and infrastructures in biosystem engineering is presented. The history and basic background of the finite element method is presented. This is the first numerical method implemented and also the more developed one. The history and background of other two more recent methods, with practical applications, the computer fluids dynamics and the discrete element method are also presented. Besides, a review on the scientific and professional applications on the field of buildings and infrastructures for biosystem engineering needs is presented. Today we can simulate engineering problems with solids, engineering problems with fluids and engineering problems with particles and get to practical solutions faster and cheaper than in the past. The paper encourages young engineers and researchers to make progress these tools and their engineering applications. The capacities of all numerical methods in their present development status go beyond the present practical applications. There is a broad field to work on it.

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Introduction

The present paper is a review of the numerical methods at present and their applications in solving engineering problems. The field is too wide to be considered in a single article. This is why the paper focuses on presenting the fundamentals of the most significant numerical methods that can be applied for buildings and infrastructures areas of biosystems engineering. The three next numerical methods will be considered: i) finite element method (FEM); ii) computer fluid dynamics (CFD); iii) discrete element method (DEM).

In the paper the main features of these methods will be presented along with showing some examples in areas of biosystems engineering. Modern engineering can be considered to begin with the industrial revolution in the late eighteenth and early nineteenth century. From the very beginning, it has used the most powerful mathematical tools of the time in order to solve problems arising in practice. It was considered a fact that it was essential acquiring solid mathematical foundations for being a good engineer. The programs of studies from all Universities of the time prove it so. Even great figures on mathematics of the nineteenth and twentieth centuries were formally engineers. This symbiosis has produced good results for society. In the second half of XX Century, the fast development of computer science produced a great advance in numerical methods applied to physics and engineering.

Based on this premise, the predictable future is that calculation and structural analysis in all fields of engineering will be based on modern numerical methods. This powerful mathematical tool has now applications in almost every field of engineering, but its development and first applications are linked to structural engineering. Its evolution and development has been linked in the second half of the twentieth century to the development of computer capabilities. The generalisation of its use is still today limited in some applications by the power of computers. This aspect will be discussed afterwards.

Numerical methods are the result of the different working procedure of the human brain and computers. While our brain seeks relationships that explain the phenomena occurring in reality and allows us to simulate them, computers are not able to perform more than simple logic operations, but at enormous speed. Thus, with appropriate algorithms, we can build those relationships that our brain think, decomposing them in these simple operations that can be performed by the computer.

The scientific and mathematical foundations of numerical analysis are already well established, but the field of practical applications is still open. It could even be said that this powerful tool is still underutilised. In many engineering firms and Universities there is still a worrying lack of applications of these methods and many engineers lack capabilities on them.

Today there is a great variety of methods that could be considered *numerical methods*: finite differences, finite elements, computational fluid dynamics, discrete elements, fuzzy logic, genetic algorithms, neural networks, system dynamics etc. from all of them this paper will deepen on FEM, CFD and DEM representing, respectively, the origin of the numerical calculation in engineering, a development and expansion of the technique and the modern development of numerical methods. Besides, the paper will focus on applications to the particular areas of buildings and infrastructures in biosystems engineering. There are a number of topics under the general term *buildings and infrastructures areas of biosystems engineering*: animal housing building structures, food and fibre processing building structures, greenhouses structures, storage and handling of food and fibre products, indoor environment in animal houses, industries and greenhouses, rural buildings and landscape, wastes from agricultural buildings, irrigation devices, rural roads, etc. The paper will present examples from literature of applications of numerical methods to some of these topics.

Finite element method

The finite element method was first formulated as used today by Turner *et al.* (1956) although from 1940 engineers and mathematicians were proposing computing systems that can be considered its predecessors and the term *finite element* was first used by Clough (1960). In the sixties, only a few research articles mentioned the term *finite elements*, but in the early seventies, there were more than a thousand. Soon it was seen the need to have specific publications and it began to appear the first books on the topic and the first specific journals. Among the first books, now considered classics, it should be cited those of Zienkiewicz (1967) and Bathe and Wilson (1976).

Although FEM was born under the field of engineering, it was soon incorporated into the science of mathematics and it was generalised as an approximate method for solving differential and integral equations. There are numerous definitions of the method, however, in this paper it is defined as a technique used by scientists and engineers to obtain an approximate solution to many physical problems by dividing an object into small elements that allow the resolution of the problem over this element and it can be assembled afterwards in order to obtain the global solution. Typically at first the method began to be used with solid objects subjected to external forces and the physical problem to be solved was the state of stresses and strains that caused these forces to the solid object. But the method subsequently expanded to liquid, gaseous or even electromagnetic fields to solve problems that were not only mechanical but also thermal, electrical, etc.

In the practical application of the finite element method, elaborate computer programs are often used, which consist of three distinct blocks: pre-processing, calculation and post-processing. The first and last blocks often require the direct intervention of the user, either interacting with the program or by undertaking specific programs. These specific programs are linked to the main one, but all peculiarities of the problem, the main data and the selection and presentation of results are defined on them (Guedes and Kikuchi, 1990).

Pre-processing usually consists in dividing the object into a mesh of finite elements, boundary conditions definition, contacts, definition and properties of materials that constitute the object or objects, the external loads and the initial conditions.

The process of dividing an object into elements is called discretisation or meshing, because the object is divided into a number of elements as small as you like, but considering the processing capabilities of the computer, because the greater the number of elements in the discretisation, the more computing time is needed (which is usually called computational cost). These elements are composed of nodes and rods. The nodes are at the bars intersection, but can also be in its midpoint. The elements have different forms but usually tetrahedral, penthaedral (wedges) and hexahedral forms. The discretisation is adapted to the object geometry, many times a non-uniform mesh is needed or even the combination of different types of elements. Today meshing process is highly automated with internal optimisation algorithms incorporated into programs (Ho-Le, 1988). Another important FEM analysis process is the boundary conditions definition of the problem. The object is analysed with its environment connections (support, contacts, flows, etc.). In many cases the best approximation to the actual results of the analysis depends on a correct definition of these conditions. In addition, these edges can become the contacts between different materials and both are discretised by finite elements which further complicates the simulation, but also increases the ability to analyse complex problems with this procedure (Zhong and Mackerle, 1992).

Once geometrically defined the solid, the boundary conditions and contacts, the next step is pre-processing of materials. Today these materials can be solid, liquid, gas and even electric or magnetic fields. According to the problem to be analysed, it will be needed to define the material behaviour model (mechanical, fluid, etc.), and its parameters or relationships. Most current commercial programs have an important library of materials behaviour, so, it is only necessary to choose and define the parameters of the behaviour model accurately. Also most programs allow you to define new behaviour models according to user needs. All these developments greatly facilitate the practical applications of the models and their adjustment to reality (Nayak and Zienkiewicz, 1972; Weber and Ananda, 1990; Mahnken and Stein 1996; Mishnaevsky and Schmauder, 2001).

Pre-processing ends with the definition of the initial conditions of the model, *e.g.* in the case of solids it consists in external load conditions. The current situation also allows a wide variety of these loads (point, surface, mobile etc.), which facilitates the work of the user and extends the capability of analysis (Schwlizerhof and Ramm, 1984).

The calculation module of the finite element program (the program kernel) is usually not open to the user, although some commercial programs allow some interaction. In general the calculation process comprises the following steps: i) definition of tensor equations on each element in local axes; ii) change to global axes; iii) overall tensor assembly; iv) tensor inversion; v) resolution for each load case considered; vi) incremental resolution in cases of non-linearity or transient problems.

The main equations governing this process are derived from the first structural applications of the method that were afterwards extended and generalised to other fields. The fundamental tensor equation relates the stress and strain through a stiffness tensor D and considering the initial stresses and deformations σ_0, ε_0:

$$\sigma = D\,(\varepsilon - \varepsilon_0) + \sigma_0 \qquad (1)$$

In a non-linear problem, the tensor D will have two components, but basically you can keep the same scheme.

The deformations are related to the nodes displacements of each element by one tensor, B, constituting another fundamental equation:

$$\varepsilon = B u^e \qquad (2)$$

Finally the equation of virtual work completes the picture of basic needs in structural problems:

$$\delta u e^T q^e = \delta u^{eT} \left(\int_\Omega e\, B^T \sigma d\Omega - \int_\Omega e\, N^T b d\Omega\right) \qquad (3)$$

where q^e is the tensor of external forces applied to the nodes (obtained from all the forces in the solid), δu^e the nodal displacement tensor, b the gravitational forces tensor (or body forces in general), N

the element shape tensor and Ω_e the element volume. With these three equations it is possible to compose the fundamental tensorial equation of equilibrium in the element:

$$q^e = K^e u^e + f^e \quad (4)$$

where K^e is the element stiffness tensor (this tensor can be known from the shape and orientation of the element and the material properties) and f^e the tensor which includes the internal forces caused by distributed forces and the initial solid conditions of stress and deformation (this tensor is also known if these initial conditions and distributed forces in the solid, such as gravitational forces, are known).

Once these tensor relationships for each element are established then the analysis proceeds to what is called the elements assembly, gathering all of them by changing global axes to local axes and blurring the nodal forces, which are internally compensated. The resulting global equation is:

$$Ku + f = 0 \quad (5)$$

where K is the overall stiffness tensor and f the initial force tensor (external and body forces). Thus the problem becomes solving this tensorial equation and find out the displacement tensor. Once the displacements are known it is obvious to obtain the solid deformations and stresses using Equations (1) and (2). This resolution involves inverting tensor K, which is the main mathematical problem of the method. Great advances have been made on the efficiency of this process of inverting the tensor (Bank and Dupont, 1981; Taylor, 1985). It should be considered that every discretisation process implies adding nine rows and columns to the K tensor for each element, so a dense discretisation, such as those currently used for getting accurate results, implies tensors with thousands of rows and columns, which requires special algorithms to get the tensor inverted within a reasonable time taking into account the computing power of modern computers.

The last step in the method is post-processing, which mainly consists on selecting the results relevant for the problem analysis and the presentation of these results in a friendly and useful way. Most current programs have graphical capabilities to help in this step and the possibility of user interaction. In most cases this post-processing phase can be automated by means of a program or subprogram (Babuska and Miller, 1984a, 1984b, 1984c; Forde *et al.*, 1990).

The use of FEM in engineering is now a common practice, and the fields of application are not only structures in static situation but also structural dynamic analysis, heat transfer analysis, fluid behaviour analysis, electromagnetic and electronics analysis, etc.

Finite element method in buildings and infrastructures areas of biosystems engineering

During the development of the finite elements method, practical applications to many engineering problems were made, and also to rural engineering and even more specifically in the field of rural buildings and infrastructures. However the range of applications is still very open and it is expected that in the future this tool will be essential in the daily practice of engineers. In this section a review of the last publications made by research groups, which are doing work in these fields, is presented. There are much more, but only a few have been selected to show the different things that can be analysed.

Some of the earliest applications were in the design and calculation of agricultural silos (Jofriet *et al.*, 1977), a field in which continuously there have been research groups working since then. Silos research is a topic in which engineers of various branches have made improvements during more than one century and the power of FEM models cannot be set aside. The first papers were about the interactions between the stored material and the silo structure and then there were a progress in structural analysis direction, considering buckling and construction details (Figure 1). Both tower silos and trench silos were studied. Today the effects of discharging, asymmetric loads, the internal elements and others are analysed. Just to cite some of the contributions, those of the groups leaded by Jofriet *et al.* (1997), Ge and Zhang (2009) and Ayuga (Guaita *et al.*, 2003; Gallego *et al.*, 2011) in the field of agricultural engineering, and Rotter (Topkaya and Rotter, 2014), Tejchman (Iwicki *et al.*, 2011) and Enstad (Ding *et al.*, 2013) in the field of civil engineering.

Another FEM application is in wooden structures. Such structures are very common in many countries for rural buildings and their behaviour is so complex that has been the subject of interest to many researchers. FEM has been proved well suited to their characteristics.

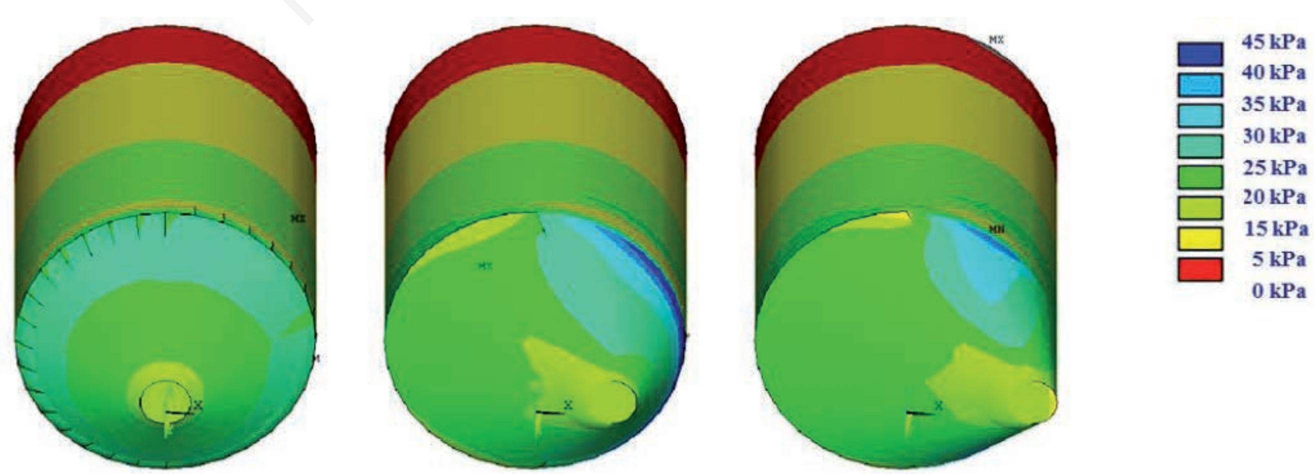

Figure 1. Finite element method analysis of pressures over eccentric hoppers in silos (from Couto *et al.*, 2001; open access).

Researchers have studied the structural behaviour of the individual elements, the whole structures, wooden panels or joints with both wood and metal parts. One of the first papers that considered simultaneously wooden structures and calculation by FEM in rural constructions is that of Wright and Manbeck (1992). Other groups that have worked on this subject are those leaded by Gebremedhin (Cabrero and Gebremedhin, 2009), Lam (He *et al.*, 2001), Gupta (van de Lindt *et al.*, 2009) or Guaita (Baño *et al.*, 2011).

FEM has been used in studying greenhouse structures, analysing both the support elements and flexible plastic coverings or the foundations (their special problem of being on traction). Heat transfer problems in greenhouses have also been studied applying FEM. In this field the main research teams are those leaded by Briassoulis (Briassoulis, 2004), Varela (Molina-Aiz *et al.*, 2010), Fernández *et al.* (2007) and Callejón (Vázquez *et al.*, 2011). Obviously, in the field of the greenhouses the computational fluid dynamics (CFD) has further application, as it will be explained later.

In the field of animal housing, apart from light structure analysis (Kanvinde *et al.*, 2013; Basaglia *et al.*, 2013), the FEM has been used primarily to analyse the suitability of the different animal beds and the damage to animals' hooves. In this field have been working the groups of Tierney (Tierney and Thomson, 2003), Belie (Franck *et al.*, 2008), Jofriet (Thomason *et al.*, 2005; Salo *et al.*, 2010) and Hinterhofer (Hinterhofer *et al.*, 2009).

There are some applications in the design of building elements for livestock housing and industries for processing agricultural products (Mohtar *et al.*, 1995; Estrada-Flores *et al.*, 2001; Idriss *et al*., 2001; Moazed *et al.*, 2012; Shahbazian and Wang, 2013).

There are also applications in rural infrastructures such as small dams (Huisman *et al.*, 2010), buried pipes (Garg and Abolmaali, 2009; Krushelnitzky and Brachman, 2009), rural roads (Yan *et al.*, 2008; Mohsenimanesh *et al.*, 2009), infrastructures for aquaculture (Suhey *et al.*, 2005; Jensen *et al.*, 2007) and even on landscape infrastructure (Rahardjo *et al.*, 2009; Niu and Xing, 2013).

Obviously in addition to these directly related to buildings and infrastructures areas of biosystems engineering applications, there are many others in various fields (building structures, food engineering, agricultural implements and machinery, surface and groundwater hydrology, soil and wind erosion, road engineering, heat and mass transfer, etc.) that may be indirectly in relation with buildings and infrastructures areas of biosystems engineering that are not cited in this paper due to lack of space.

Computational fluid dynamics

A century and a half ago the French engineer Claude Navier and the Irish mathematician George Stokes get to the equations of velocity and fluid pressure at any point of a space, since then known as Navier-Stokes equations. They based their findings on Newton's laws of motion, deriving partial differential equations after introducing viscous transport into the Euler equations. These equations are complex enough to get analytical solution only in elementary cases such as steady flows.

The possibility of numerical solution of the Navier-Stokes equations using computers is the origin of CFD and it was developed along the 60s and 70s of the past century, by using both finite difference and finite element methods. In the 80s most of the commercial codes for computing CFDs were developed.

The general expression of the Navier-Stokes equation can be written as follows:

$$\rho\,(\partial v/\partial t + v\cdot\nabla v) = -\nabla p + \nabla\cdot \mathrm{T} + f \tag{6}$$

where;
v is the velocity;
ρ is the fluid density;
p is the pressure;
T is the stress tensor;
f are the forces (per unit volume) acting on the fluid.
As well as solving the Navier-Stokes equations CFDs models must satisfy the classical fluid mechanics conservation equations:

Conservation of mass equation

$$\frac{\partial \rho}{\partial t} + \nabla(\rho\ \vec{v}) = 0 \tag{7}$$

Conservation of momentum equation

$$\frac{\partial}{\partial t}(\rho\ \vec{v}) + \nabla(\rho\ \vec{v})\vec{v} = \rho\vec{F} - \nabla p + \mu\nabla^2\vec{v} + \frac{\mu}{3}\nabla(\nabla\vec{v}) \tag{8}$$

Conservation of energy equation

$$\frac{\partial}{\partial t}(\rho c_p T) + \nabla(T\,\vec{v}) = \nabla(\lambda\nabla T) + q + \tau \tag{9}$$

All these equations can be solved by ordinary FEM and the structure of the first programs were pretty similar to those described in the previous section, but in the 90s a new finite volume method (FVM) was fully developed, more efficient and powerful for fluid (and flux) analysis (Cai, 1991). FVM is a special finite difference formulation. In this method volumes around the nodes are used, and volume integrals are transformed in surface integrals considering the flux through the volume. A local balance of the fluxes on each discretisation cell (control volume) is established, instead of the static equilibrium as in FEM. This way, the flux phenomena (convection, diffusion and sources and sinks) can be adequately discretised.

Regarding post-processing capabilities, CFDs programs goes beyond FEM programs, because in this case the video production is essential to accurately reflect the simulation results.

Computational fluid dynamics in buildings and infrastructures areas of biosystems engineering

CFD models have multiple applications on buildings for both animal production and crop production. Several years ago a paper was published on the use of CFDs for ventilation of animal houses and greenhouses, proving the fast increase of its applications (Norton *et al.*, 2007; Torre-Gea *et al.*, 2011). This increase has maintained since then. At present it is common to find international workshops or conferences only on this topic proving the importance and extension of this application.

In the field of animal housing these models have been used for ventilation and thermal analysis in different kind of buildings and animal species. For example, in dairy cattle there are interesting papers on ventilation from the Aarhus University (Wu *et al.*, 2012; Shen *et al.*, 2013) or research on ammonia emissions (Sun *et al.*, 2002; Bjerg *et al.*, 2013). Similar approaches have been made in other species such as swine (Predicala and Maghirang, 2003; Mossad, 2009; Tong *et al.*, 2013), poultry (Pawar *et al.*, 2010; Zajicek and Kic, 2012; Bustamante *et al.*, 2013) or rabbit (Flores-Velázquez *et al.*, 2013). A paper on trends regarding research on livestock pollutant emissions, including CFDs, has been recently published (Takai *et al.*, 2013) (Figure 2).

There are also some other papers focusing on thermal aspects of the livestock buildings (Zhang *et al*., 1999; Gebremedhin and Wu, 2003; Norton *et al.*, 2010; Mondaca *et al.*, 2013; Mostafa *et al.*, 2013) or odour problems (Li and Guo, 2006; Lin *et al.*, 2009; Hong *et al.*, 2011).

The second interesting topic under this section is greenhouses. Ventilation is one of the major problems in greenhouse technology. Greenhouses' designers tend to minimise the building volume to cut structure costs, but the plants need a minimum air volume and air renovation. A good balance is critical along with airflow and air speed inside the building knowledge. CFDs can help designers in this task. A lot of papers have been recently published on this issue, many of them based on international research projects with collaboration of the countries with larger surfaces devoted to greenhouses such as Spain, Italy, Greece, the Netherlands, Israel or USA (Majdoubi *et al.*, 2009; Molina-Aiz *et al.*, 2010).

Airflow outside greenhouses is also important to a proper design of the structure, some authors focus on this aspect (Mistriotis and Briassoulis, 2002; Dados *et al.*, 2011).

Besides airflow, microclimate, temperatures and humidity can also been simulated using CFDs. A number of papers have been produced taken into account these aspects (Fatnassi *et al.*, 2003; Molina-Aiz *et al.*, 2004; Rouboa and Monteiro, 2007; Kim *et al.*, 2008; Franco *et al.*, 2011). A recent review on other aspects of crop production and greenhouses can be found in Bartzanas *et al.* (2013).

Another emerging field of application of CFD is bioenergy facilities (Fletcher *et al.*, 2000; Rosendahl *et al.*, 2007; Shiehnejadhesar *et al.*, 2013; Wu, 2013), it is expected a publications increase in this field in the near future.

Only to finish this section, it must be pointed out that there are many other applications apart from those listed before in buildings and infrastructures areas of biosystems engineering. An interesting paper can be consulted on other applications in the general field of biosystems engineering (Lee *et al.*, 2013).

Discrete element method

Dealing with engineering problems in which particles are involved, FEM, and other numerical methods derived from it, cannot provide the right solution in most cases. Discretisation of continuum solids has been applied to granular materials in some geotechnical problems and can be useful to explain certain phenomena in which the granular materials remain at rest. But it is not possible to consider particulate solids as a continuum when great deformations or movements are involved. This is a common problem in many real cases, both in soils and in agricultural products such as grains and powders. For this reason Cundall and Strack (1979) proposed a new method to study fracture in rocks. This method should be capable of simulating the movement, collision and contact between particles. This procedure was known as DEM and since then it has been improved till became essential in all physical problems involving particle movement whatever their size, from big rocks of several tons (Psycharis *et al.*, 2011) to microscopic nanoparticles (Peng *et al.*, 2010).

At this moment there is enough literature on the topic to consider DEM as a consolidated engineering tool. Some technical books have been written (Radjaï and Dubois, 2011), hundreds of papers have been

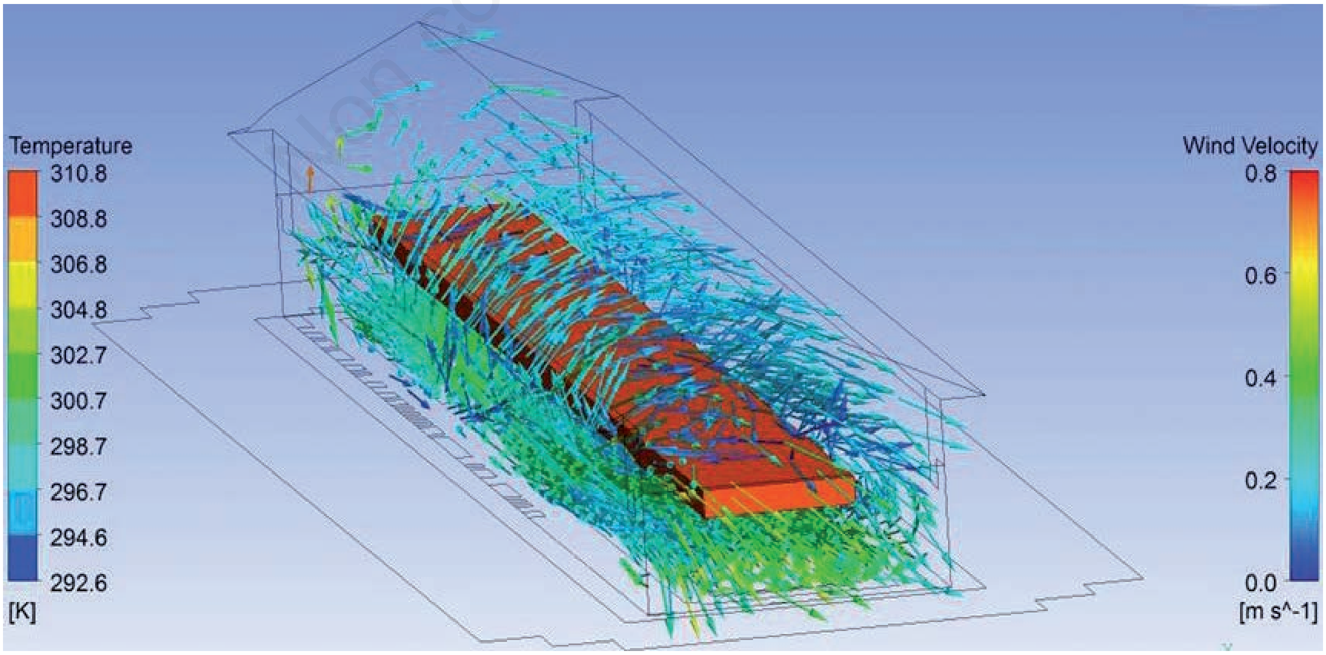

Figure 2. Computer fluid dynamics of a rabbit house (from Flores-Velázquez *et al.*, 2013; used with permission).

published and even commercial software is now of common use in research and engineering companies. The possibilities of new applications development using this tool in all engineering fields are really important. But we are interested in applications to buildings and infrastructures areas of biosystems engineering.

The limitations of DEM refer mainly to hardware needs and computing time. FEM presented some limitations of this type when the problem required very fine meshes. In the case of DEM, the number of particles that can be analysed in a reasonable time is clearly a limiting factor. Yet there are procedures to isolate parts of a larger problem, or some models that make use of combinations of DEM and FEM *e.g.* simulating mobile individual particles inside the whole granular material considered as a continuum solid. These procedures can ease computing time problems.

The DEM mathematical foundation begins with a time discretisation, evaluating for each time step, the particle position, its speed and trajectory and the particle-particle contacts (Džiugys and Peters, 2001).

The position of a particle is determined by the classical equations of motion:

$$\left(\mathbf{F}_i^{[\Phi]}\right)^t = m\left(\ddot{\mathbf{x}}_i^{[\Phi]}\right)^t \tag{10}$$

$$\left(\mathbf{M}_i^{[\Phi]}\right)^t = I\left(\ddot{\theta}_i^{[\Phi]}\right)^t \tag{11}$$

$$\left(\ddot{\mathbf{x}}_i^{[\Phi]}\right)^{(t)} \approx \frac{\left(\dot{\mathbf{x}}_i^{[\Phi]}\right)^{(t+\Delta t)} - \left(\dot{\mathbf{x}}_i^{[\Phi]}\right)^{(t)}}{\Delta t} \tag{12}$$

$$\left(\dot{\mathbf{x}}_i^{[\Phi]}\right)^{(t+\Delta t)} = \left(\dot{\mathbf{x}}_i^{[\Phi]}\right)^{(t)} + \left(\frac{\left(\mathbf{F}_i^{[\Phi]}\right)^t}{m} + \mathbf{g}_i\right)\Delta t \tag{13}$$

$$\left(\dot{\theta}_i^{[\Phi]}\right)^{(t+\Delta t)} = \left(\dot{\theta}_i^{[\Phi]}\right)^{(t)} + \left(\frac{\left(\mathbf{M}_i^{[\Phi]}\right)^t}{m} + \mathbf{g}_i\right)\Delta t \tag{14}$$

$$\left(\mathbf{x}_i^{[\Phi]}\right)^{(t+\Delta t)} = \left(\mathbf{x}_i^{[\Phi]}\right)^{(t)} + \left(\dot{\mathbf{x}}_i^{[\Phi]}\right)^{(t+\Delta t)}\Delta t \tag{15}$$

where Φ is the particle number, x is the particle position vector, θ is the inclination angle, F is the contact force vector, M the moment vector, t the time step, m the particle mass and g the gravity acceleration vector.

For the kind of analysis performed in DEM it is considered a valid simplification to substitute the particle deformation in the moment of particle contact by some virtual overlapping of particles. This overlapping is related with the contact force and should be of the same magnitude of the equivalent deformation of the particle. The calculation algorithms are easier with this simplification without lacking of accuracy in the results.

At the time of contact, the particles suffer certain deformation (overlapping), a normal rebound, a tangential rebound and friction (slip-stick). These phenomena can be mathematically expressed by means of three equations, two of them using springs and dashpots (normal and tangential) and the third one being the classical equation of particle friction (González-Montellano, 2010) (Figure 3):

$$\left(\mathbf{F}_i^n\right)^j = K^n U_n^j \mathbf{n}_i^j + C^n\left(V_i^n\right)^j \tag{16}$$

$$\left(\mathbf{F}_i^s\right)^j = K^s U_s^j \mathbf{t}_i^j + C^s\left(V_i^s\right)^j \tag{17}$$

$$\left(F^s\right)_{\max}^j = \mu\left|\mathbf{F}_i^n\right|^j \tag{18}$$

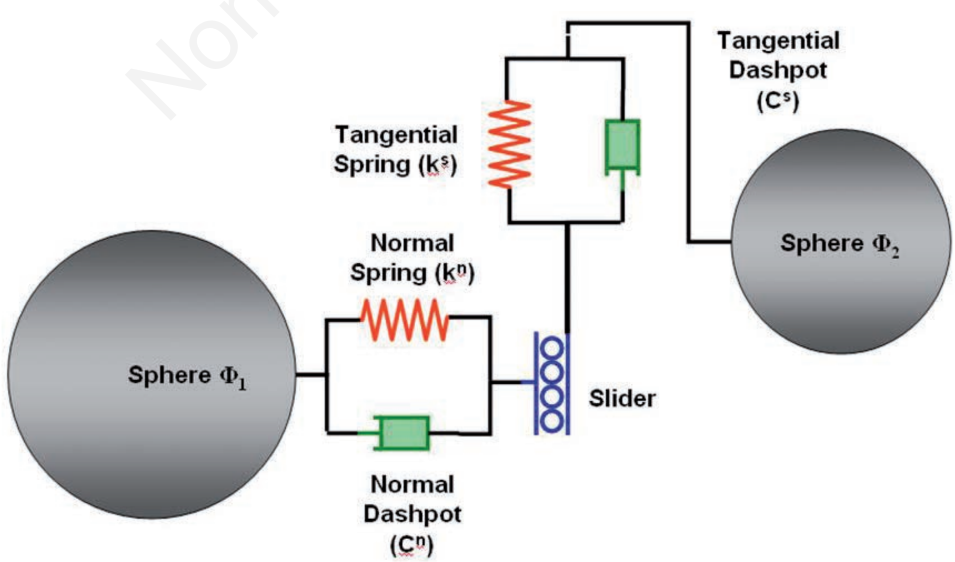

Figure 3. Contact between particles (from González-Montellano, 2010).

where K^n and K^s are the secant stiffness and the tangent stiffness of the normal and tangential springs, U_n is the total overlap in the normal direction, U_s is the tangential overlap, n_i and t_i are unit vectors in the normal and tangential directions of the contact, C^n and C^s are the contact damping coefficients for the normal and tangential directions, V_i^n and V_i^s are the relative normal and tangential velocities at the contact and μ the friction coefficient.

All constants and parameters on these equations depend on the physic-chemical characteristics of the particles, their shape and dimensions.

The flowchart of the calculation process begins with the initial values of position, speed (translational and rotational), forces and moments in each particle. For each step (time increment) positions and velocities are refreshed by means of the motion equations. New contacts can appear, others can disappear or modify their situation. To all these positions and contacts, the equations of force-displacement are applied, starting a new cycle.

Of course all the processes, equations and algorithms are described in a simplified way. Many other factors have influence, like the problem boundaries, the particle shape, etc. It is also important to correctly select the time step, being small enough to get the desirable accuracy and not so much that makes unstable the calculation process or the calculation time too long. There is a critical value that should not be surpassed, but it is common to use smaller values (Kruggel-Emden *et al.*, 2008). To get an idea of the time step magnitude it is enough to say that the unit used is microsecond.

As it was said before, there are some commercial software based on DEM, but they are not as well developed as the FEM software. New versions and important updates are very common every so often, incorporating the last research developments. These commercial programs work in a similar way to the FEM programs on the way they interact with the user. There are three parts, the pre-processor, the resolution module and the postprocessor, in this case not only with graphical capacities but also with video capacities, because of motion on these models is very important.

It is under development FEM and DEM combination in a commercial software, and DEM and CDF combination to analyse the behaviour of solid particles inside a liquid flow or a gas flow (Brosh *et al.*, 2011).

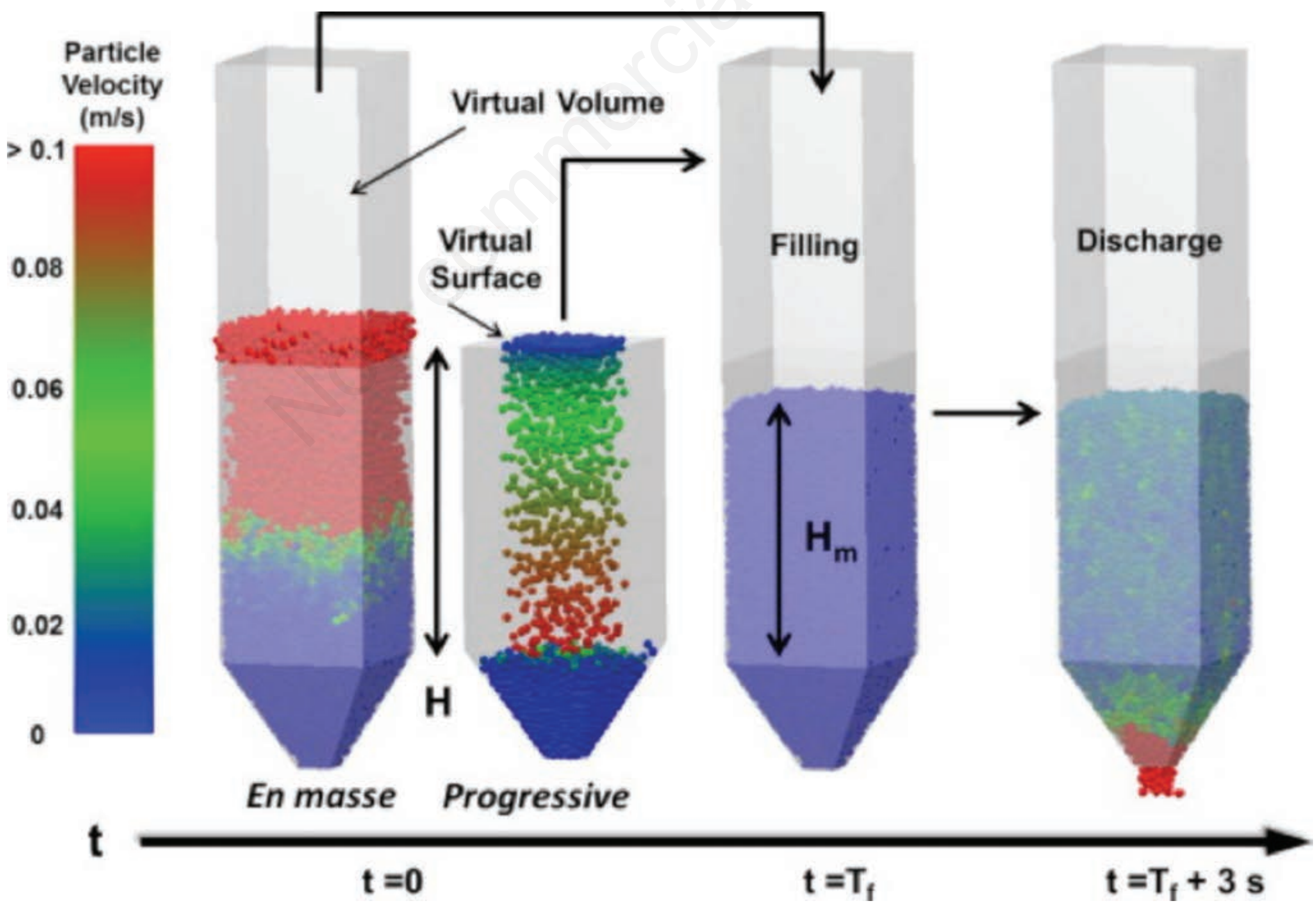

Figure 4. Silo filling and discharge. Discrete element method simulation (from González-Montellano *et al.*, 2012b).

Discrete element method in buildings and infrastructures areas of biosystems engineering

There are a great variety of fields under buildings and infrastructures areas of biosystems engineering in which DEM can be applied (Tijskens *et al.*, 2003), mainly in food engineering where handling of particles is so common. Food processing requires conveying, handling and storage of particles, and the design of the equipment for these processes can be better achieved by using DEM.

Another important field is the design of storage infrastructures for agricultural grains and powders (including fibre or biomass), in the field, in intermediate structures or at processing industries.

Combined with CFD, DEM can be used to simulate particle dispersion inside the buildings, pneumatic transport and other engineering problems.

Many other areas of biosystems engineering can benefit from DEM such as the design of machinery for seeds, harvesters, fertilisers and others or the soil erosion simulations.

DEM was firstly used to study granular materials flow in silos, hoppers and storehouses, to help in the structural design of these industrial elements.

As in the FEM case the research team led by Jofriet in Canada was pioneer in the use of DEM for these purposes (Rong *et al.*, 1995). Besides, this group introduced a very important concept for later developments, the hybrid models. These models combine the use of FEM for the static parts of the grain mass with DEM in those parts in which particle movement and interaction with the structural elements are more important. This way, important improvements in computing time can be achieved and some problems that could not be solved because of the great number of particles become affordable (Lu *et al.*, 1997). Some other research groups developed applications to agricultural silos and hoppers such as Horabik (Sykut *et al.*, 2008; Parafiniuk *et al*., 2013), Ayuga (González-Montellano *et al.*, 2011, 2012b), Coetzee (Coetzee and Els, 2009). Other researchers have made applications to silos and hoppers in other engineering fields like Ooi (Holst *et al.*, 1999; Chung and Ooi, 2008, 2012), Martínez (Masson *et al.*, 2003) or Sielamowicz (Balevičius *et al.*, 2011) (Figure 4).

DEM has also been used in other fields besides silos and hoppers, such as some infrastructure problems involving handling of soils or rocks. This is the case of slope protection (Kim *et al.*, 1997; Plassiard and Donze, 2010), geotextiles (Bhandari and Han, 2010), buried pipes (Kuwata *et al.*, 2010), or rural road pavements (Mahmoud and Masad, 2010; Shen and Yu, 2011).

Validation and calibration of all these models require knowing some mechanical parameters at particle level. These parameters are usually unknown because previous mathematical or numerical models did not use them. Some recent researchers focused on the determination of these values, designing specific tests or calibration procedures. Just to cite some of them working mainly in agricultural or biomass products: the Molenda group (Stasiak *et al.*, 2007, 2013), the Boac group (Boac *et al.*, 2010), the Ayuga group (González-Montellano *et al.*, 2012a; Ramírez-Gómez *et al.*, 2014), the Ooi group (Chung and Ooi, 2011; Härtl and Ooi, 2011) or the Tijskens group (Vanstreels *et al.*, 2005; Van Liedekerke *et al.*, 2008).

Conclusions

Numerical methods to solve physical problems are a powerful tool for engineering applications, which has already penetrated the academic world and is often used in the professional world, especially by large engineering companies.

The capacities of these methods go beyond their present use, especially in the professional world. It is also the case of procedures that are already common in research, but have not yet been transferred into practice, either by regulatory rigidity, by distrust of novelty or lack of knowledge by the end users.

In all cases, there should be greater dissemination of academia developments among professionals and companies. Congresses and conferences are a good showcase for the exchange of ideas, sometimes work better or can complement scientific publications, often too restricted to academic and research world.

There are fields in agricultural/biosystems engineering that could take advantage of these methods in the near future and are waiting to young professionals eager to learn and innovate. Imagination and analytical skills of our young researchers and professionals will help them to develop these applications, but this requires that due attention to the teaching of these tools and procedures will be paid at University.

Today we can simulate engineering problems with solids, engineering problems with fluids and engineering problems with particles, but very few have been made so far.

This paper has highlighted the current applications in one of the many aspects covered by biosystems engineering, buildings and infrastructures, and even within these particular areas, there are many things to improve. For example in a building for animal housing, warehouses, factories or greenhouses, the structure can be simulated by FEM considering the interaction between structural elements and all other construction elements (walls, roof, etc.). No matter if the structure is made of wood, steel or reinforced concrete, it is now possible to simulate the whole building considering all its elements. But besides the global analysis of structures, multitude of problems dealing with construction details can be studied, such as the behaviour of the connections between structural elements of the same material or different materials, or the interaction between structure and ground, this time using FEM or FEM-DEM combinations. Also environmental conditions inside the building can be fully simulated, using CFD and FEM. Effects of livestock manure over building materials, interactions of animals and machines with the building elements, vibration or noise propagation could also be studied using numerical simulation.

In the field of granular materials, handling of forage or energy products (biomass) is still to be studied and also its conveying and storage. All topics related to earthworks: excavation, transport, compaction etc., are subject to further analysis using FEM and DEM.

Other rural infrastructures such as pipelines, reservoirs, canals and ditches etc., need also improvements in the knowledge of their structural behaviour, some of which could be solved or at least could be better understood with the most intense use of numerical methods, yet underused.

Finally, all problems derived from interaction of different materials (granular solids and continuum solids, fluids and solids, etc.) show complex behavioural problems that can only be adequately addressed by numerical methods and probably by their combination.

The generation of all these models, the detection of the physical parameters required for the numerical simulation of problems, and experimental validation of the outcome, consideration of scale effects and calibration models are tasks awaiting engineers and researchers who want to venture into this exciting world of numerical simulation of engineering problems.

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