

# The use of numerical programs in research and academic institutions

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**Abstract.** This paper is conceived on the idea that numerical programs using computer models of physical processes can be used both for scientific research and academic teaching to study different phenomena. Computational Fluid Dynamics (CFD) is used today on a large scale in research and academic institutions. CFD development is not limited to computer simulations of fluid flow phenomena. Analytical solutions for most fluid dynamics problems are already available for ideal or simplified situations for different situations. CFD is based on the Navier-Stokes (N-S) equations characterizing the flow of a single phase of any liquid. For multiphase flows the integrated N-S equations are complemented with equations of the Volume of Fluid Model (VOF) and with energy equations. Different turbulent models were used in the paper, each one of them with practical engineering applications: the flow around aerodynamic surfaces used as unconventional propulsion system, multiphase flows in a settling chamber and pneumatic transport systems, heat transfer in a heat exchanger etc. Some of them numerical results were validated by experimental results. Numerical programs are also used in academic institutions where certain aspects of various phenomena are presented to students (Bachelor, Master and PhD) for a better understanding of the phenomenon itself.

## 1. Introduction

Fluid properties were first researched, studied and deepened since 200 BC (Archimedes principle) and continued by various researchers during ages. In the XX century fluid flow research takes a great extent through the development of numerical calculation using the computer and the appearance of CFD (Computational Fluid Dynamics). CFD is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flow. Computers are used to perform the calculations required to simulate the interaction of liquid and gas with area defined by the boundary conditions. Current research programs help us create more efficient programs by improving the accuracy and the velocity of numerical simulation of complex processes such as transonic or turbulent flow. Validation of these programs is done initially using a wind tunnel, and afterward through a full-scale validation.

CFD development is not limited to computer simulations of fluid flow phenomena. The fact that fluid dynamics research was a problem attractive for researchers/developers does not make the numerical method the first research method. Since 1940 analytical solutions for most fluid dynamics problems, especially those related to aerodynamics, were already available for ideal situations or different simplified situations. However, researchers have realized that a whole range of issues is to be resolved due to the growing demand from the industry. This was a catalyst for the development of asymptotic/semi-analytical methods.



These methods have resulted in solving many problems of flow with viscous fluid flow applications and ideal compressible fluid. In order to use a numerical program it is recommended to understand in detail numerical analytical equations that describe the physical phenomena studied and how these equations are implemented in different numerical calculation methods. A numerical method is an algorithm or the necessary steps to solve a numerical problem. Algorithms have become very important because computers have been used more and more to solve various problems. Modern numerical analysis does not seek exact solutions to problems, because exact solutions are impossible to obtain in practice. Instead, it focuses to obtain approximate solutions while maintaining reasonable errors. Numerical methods are therefore the foundation of a numerical program. Researchers devote their entire attention to two fundamental aspects of a numerical program, namely: physical modeling and numerical values.

The physical modeling has the scope to find a set of equations or mathematical relationships that allow solving the equations that govern a physical process. In addition, the attention to numerical values implies the development of efficient algorithms, robust and reliable to obtain a set of PDE's (Partial Differential Equation). Generally speaking, all physical processes can be described by PDE's. Now the program's goal is to discretize the numeric PDE that govern the physical process. This is done by transforming each differential term in approximate algebraic relationship [1].

From the historical point of view, algorithms were originally developed for solving the linearized equations potential. In the 30's dimensional methods have been developed to solve the flow around a cylinder and the flow around an air-foil [2]. The first application on the computer that has modeled the two-dimensional turbulent fluid flow was conducted at Los Alamos Laboratories in July 1963.

## 2. The structure of a numerical program

Any numerical program consists of three distinct parts: pre-processing, processing (simulation) and post-processing.

Pre-processing is the first stage in building and analyzing the model under study. This stage consists of three main phases: geometrical representation of the model, meshing the model and setting up the border limits. The model can be represented in two-dimensions or in three-dimensions. The model construction can be achieved in a Cartesian coordinate system, a spherical coordinate system or a cylinder coordinate system. The user has at his disposal a multitude of commands common to all CAD (Computer Aided Design) programs [1].

In order to solve the equations that characterize the particular flow it is necessary to modify the surfaces or objects, designed in the previous step, into a numerical form to be easily understood by the computer. This technique is called meshing and consists of transforming a surface or a three-dimensional continuous object into distinct parts called cells. The cells can be separated into two categories: flat mesh cells (triangles and quadrilaterals) and spatial mesh cell (tetrahedron, hexahedron, prisms, pyramids and polyhedrons).

Processing (simulation) consists of three distinct phases [1]:

- a) setting conditions: setting boundary conditions (e.g. initial or final pressure, velocity input, input and output flow etc.), defining the flow type (steady or unsteady) and the method of solving (by varying the pressure or by varying the density);
- b) choosing the numerical model: inviscid model (Euler flow), laminar or turbulent model; choosing the method for solving the equations (flow equations, heat equations, equations of vibration, radiation etc.); choosing the tolerance of the residual values;

The most rigorous set of equations which best characterizes the flow of a fluid are the Navier-Stokes equations [1]:

$$\bar{F} - \frac{1}{\rho} \cdot \nabla p + \frac{\eta}{\rho} \Delta \bar{v} + \frac{\nu}{3} \nabla (\nabla \bar{v}) = \frac{d\bar{v}}{dt} \quad (1)$$

or using the scalar form:

$$F_x - \frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \left( \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2} \right) + \frac{\nu}{3} \frac{\partial \theta}{\partial x} = \frac{\partial v_x}{\partial t} + \frac{\partial v_x}{\partial x} v_x + \frac{\partial v_x}{\partial y} v_y + \frac{\partial v_x}{\partial z} v_z \quad (2)$$

$$F_y - \frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \left( \frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2} \right) + \frac{\nu}{3} \frac{\partial \theta}{\partial y} = \frac{\partial v_y}{\partial t} + \frac{\partial v_y}{\partial x} v_x + \frac{\partial v_y}{\partial y} v_y + \frac{\partial v_y}{\partial z} v_z \quad (3)$$

$$F_z - \frac{1}{\rho} \frac{\partial p}{\partial z} + \nu \left( \frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right) + \frac{\nu}{3} \frac{\partial \theta}{\partial z} = \frac{\partial v_z}{\partial t} + \frac{\partial v_z}{\partial x} v_x + \frac{\partial v_z}{\partial y} v_y + \frac{\partial v_z}{\partial z} v_z \quad (4)$$

where:  $\bar{F}$  – unitary mass force;  $\bar{v}$  – velocity;  $p$  – pressure;  $\rho$  – density;  $\eta$  – dynamic viscosity;  $\nu$  – kinematic viscosity,  $\theta$  – velocity divergence.

Navier-Stokes equations are used in many fields of fluid mechanics to model, for example, the movement of currents of air, of ocean currents, the flow of fluids through tubes, the airflow around an airfoil etc. Navier-Stokes equations are also useful in studying the drag force and optimizing the shape of cars and airplanes, when studying the blood flow through the veins, in analyzing the environmental pollutants in air etc. Coupled with Maxwell's equations they can be used to model and study magneto-hydrodynamics.

The unknown quantities are  $\bar{v}$  (velocity field) and  $p$  (pressure field). They are determined by integrating the Navier-Stokes equation knowing the external force per unit mass and knowing the boundary conditions of movement. Once these fields are known, we can get other physical quantities of interest. This is different from what we know from classical mechanics, where solutions regarding the trajectories of particles were found. Determination of velocities instead of positions makes more sense in fluid mechanics; however for a better understanding of the phenomena trajectories are also drawn.

c) organizing all this information and solving all the equations above by finding values for all variables involved in the physical process for each cell of the mesh so that the physical model and boundary conditions are simultaneously satisfied.

Post-processing is the last part of the program dedicated to results analysis. CFD programs give the user a large amount of information collected in different files. The quickest and most effective way to visualize this data is by using a graphical method. Most CFD programs allow the representation of contours of different parameters (pressure, velocity, temperature, flow, density, etc.), power lines, vectors and even combinations of these parameters [3].

Although graphical analysis allows the clearest illustration of the results, it is also important to see if the program allows exporting the results in ASCII format, as this is very useful when comparing results with those from other CFD programs [1].

### 3. Illustration of various phenomena in fluids dynamics

In parallel with analytical solutions and equations, we have used ANSYS-Fluent program to investigate the different flows such as: the flow with and without circulation around a cylinder, the development of the boundary layer, the von Karman vortex street etc.

The flow with circulation around a circular cylinder is a plane potential motion that consists of an axial stream (directed along axis Ox), a dipole of moment (with a source at the left of suction) and a whirl (in direct trigonometric sense). The complex potential of motion will be [4]:

$$W(z) = v_0 \left( z + \frac{r_0^2}{z} \right) - \frac{i\Gamma}{2\pi} \ln z \quad (5)$$

If we plot the other streamlines we shall get some asymmetric curves with respect to axis Ox. On the inferior side of the circle, the velocity due to the axial stream is summed up with the velocity due to the whirl (figure 1) [4]. A graphical representation of the velocity distribution will emphasize the non-symmetric distribution of velocity around the profile (figure 2) [1].

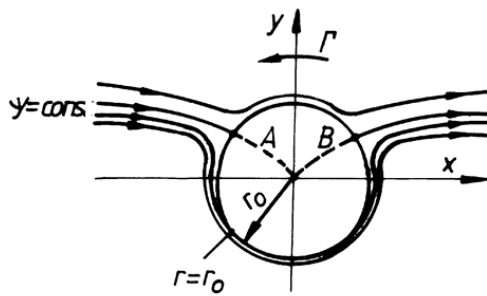


**Figure 1.** Analytical representation of the streamline distribution around a cylinder with circulation.

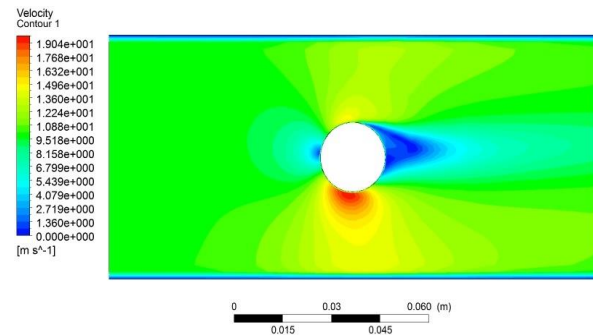


**Figure 2.** Velocity distribution around a cylinder with circulation using numerical programs.

The boundary layer notion is defined as a zone situated near the body surface where the viscosity effect is preponderant at great values of Reynolds number. It is assumed that the entire rotational movement of the fluid is inside the boundary layer, and outside the fluid movement can be considered a potential one. In these conditions, the movement of fluid in the boundary layer can be described by Navier-Stokes equation (the movement equation of real incompressible fluid) for plane movement, in Cartesian coordinate [4]:

$$\begin{aligned} -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \left( \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} \right) &= \frac{\partial v_x}{\partial t} + \frac{\partial v_x}{\partial x} v_x + \frac{\partial v_x}{\partial y} v_y; \\ -\frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \left( \frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} \right) &= \frac{\partial v_y}{\partial t} + \frac{\partial v_y}{\partial x} v_x + \frac{\partial v_y}{\partial y} v_y, \end{aligned} \quad (6)$$

and the equation of continuity:

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} = 0 \quad (7)$$

This analytical model of the flow, near the body, is presented in figure 3 [1], where the velocity of potential movement or the velocity at infinity was denoted by  $V$ . On the other hand, the development of the boundary layer is well pointed out in figure 4 [1] where a gradient of velocity is clearly visible.

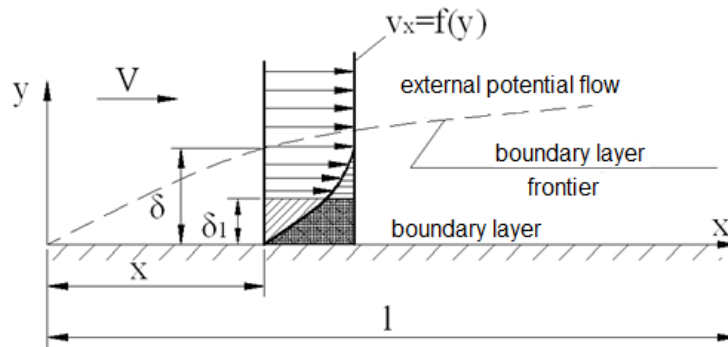


**Figure 3.** Analytical representation for the development of the boundary layer over a plate.

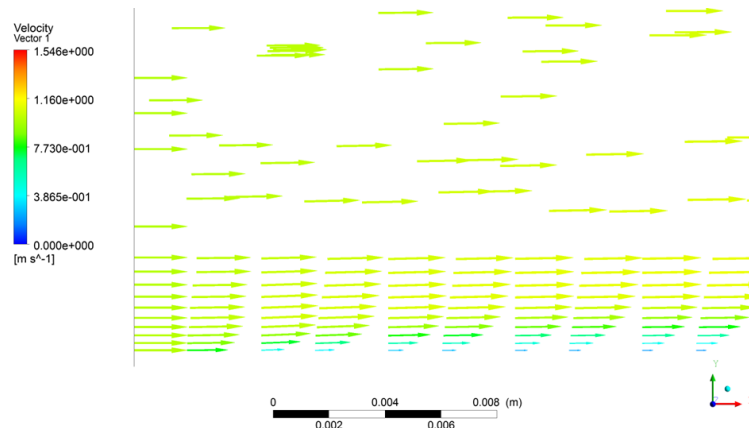


**Figure 4.** Velocity distribution over a plate using numerical programs.

For two or more fluids that move, the analytical relationships are even more complicated, but using numerical programs it makes it easier for a user to understand the phenomenon. The Fluent program offers three possibilities of working with multiple fluids: volume of fluid method (VOF), the mixture model and the Eulerian model. The most common used method is the VOF method. This method relies on the fact that two or more fluids are not interpenetrating. For each additional phase that is added to the model, a variable is introduced: the volume fraction of the phase in the computational cell. In each control volume, the volume fraction of all phases sum to unity. Thus, the variables and properties in any given cell are either purely representative of one of the phases, or representative of a mixture of the phases, depending upon the volume fraction values [5], [6].

$$\frac{1}{\rho_q} \left[ \frac{\partial}{\partial t} (\alpha_q \rho_q) + \nabla \cdot (\alpha_q \rho_q \mathbf{u}) = S_{\alpha_q} + \sum_{p=1}^n (\dot{m}_{qp} - \dot{m}_{pq}) \right] \quad (8)$$

where:  $\dot{m}_{qp}$  is the mass transfer from phase  $q$  to phase  $p$  and  $\dot{m}_{pq}$  is the mass transfer from phase  $p$  to phase  $q$ ;  $\alpha_q$  is the volume fraction of the phase  $q$  and  $S_{\alpha_q}$  is a specific constant.

For turbulent model k-epsilon: the program used the equation for turbulent kinetic energy ( $k$ ), equation (9), and dissipation epsilon ( $\epsilon$ ) (10) [5], [6]:

$$\frac{\partial}{\partial t}(\rho_m k) + \nabla \cdot (\rho_m \bar{v}_m k) = \nabla \cdot \left( \frac{\mu_{t,m}}{\sigma_k} \nabla k \right) + G_{k,m} - \rho_m \varepsilon \quad (9)$$

$$\frac{\partial}{\partial t}(\rho_m \varepsilon) + \nabla \cdot (\rho_m \bar{v}_m \varepsilon) = \nabla \cdot \left( \frac{\mu_{t,m}}{\sigma_\varepsilon} \nabla \varepsilon \right) + \frac{\varepsilon}{k} (C_{1\varepsilon} G_{k,m} - C_{2\varepsilon} \rho_m \varepsilon) \quad (10)$$

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\bar{v}(\rho E + p)) = \nabla \cdot \left( k_{eff} \nabla T - \sum_j h_j \bar{J}_j + (\bar{\tau}_{eff} \bar{v}) \right) + S_h \quad (11)$$

where:

$$\rho_m = \sum_{i=1}^N \alpha_i \rho_i \quad (12)$$

$$\bar{v}_m = \frac{\sum_{i=1}^N \alpha_i \rho_i \bar{v}_i}{\sum_{i=1}^N \alpha_i \rho_i} \quad (13)$$

$$\mu_{t,m} = \rho_m C_\mu \frac{k^2}{\varepsilon} \quad (14)$$

$$G_{k,m} = \mu_{t,m} \left( \nabla \bar{v}_m + (\nabla \bar{v}_m)^T \right) : \nabla \bar{v}_m \quad (15)$$

Good results have been reported when performing a multiphase flows in a settling chamber [7], a separation of fluids in a separation tank [8] and pneumatic transport systems for cereals [9], by using VOF model. According to [7], figure 5 a, b and c, shows how two immiscible fluids (diesel oil which has the density of 730 kg/m<sup>3</sup> and water which has the density of 1000 kg/m<sup>3</sup>) are separating in a short period of time.

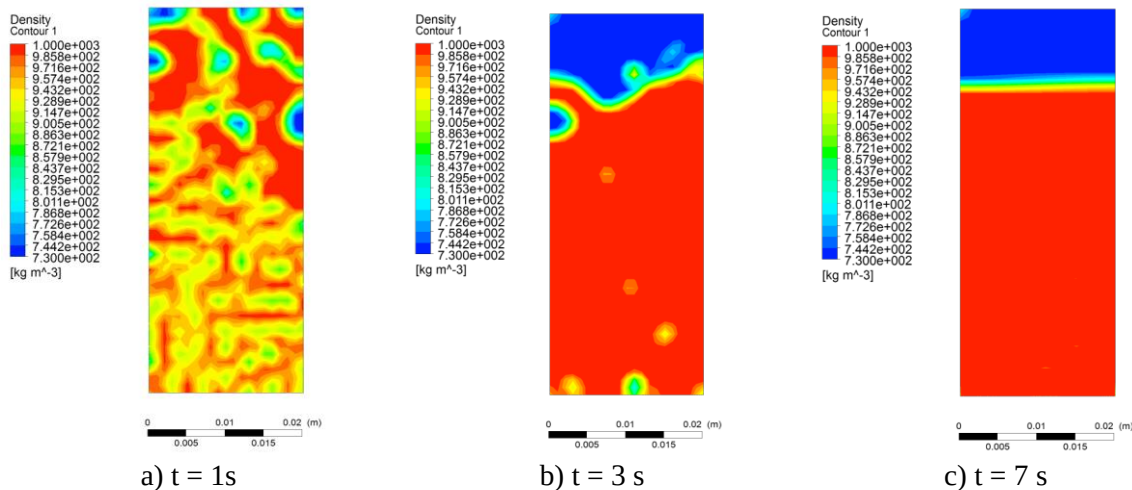


**Figure 5.** Diesel oil - water density separation.

Usually the VOF model is usually complemented by energy equations (11) provided by ANSYS program [5], [6].

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\bar{v}(\rho E + p)) = \nabla \cdot \left( k_{eff} \nabla T - \sum_j h_j \bar{J}_j + \left( \bar{\tau}_{eff} \bar{v} \right) \right) + S_h \quad (11)$$

where  $k_{eff}$  is effective conductivity;  $\bar{J}_j$  fluid diffusion flux  $j$ ;  $S_h$  heat due to chemical reaction. In the equation (11) we have:

$$E = h - \frac{p}{\rho} + \frac{v^2}{2} \quad (12)$$

where  $h$  – enthalpy; for ideal fluids (13) and for real fluid (14):

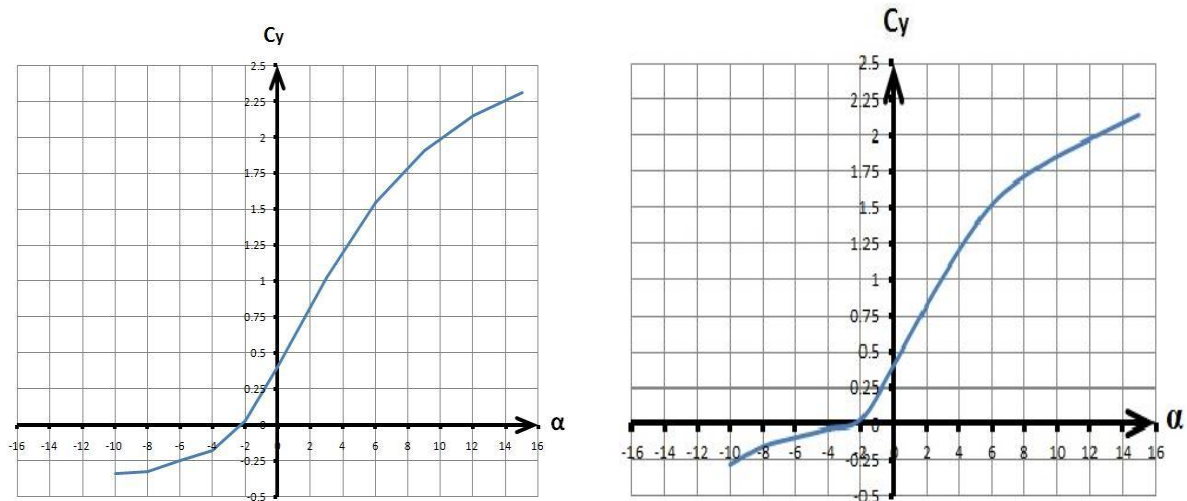
$$h = \sum_j Y_j h_j \quad (13)$$

$$h = \sum_j Y_j h_j + \frac{p}{\rho} \quad (14)$$

$$h_j = \int_{T_{ref}}^T c_{p,j} dT \quad (15)$$

Reasonable results have been reported when simulating a heat transfer system used to heat up the LNG after is transferred on shore in specialized plants [10], or when simulating a heat exchanger used in a complex installation that uses heat transfer pumps [11].

Also, similar results have been obtained when comparing experimental results with numerical ones, e.g. when calculating the lift and the drag force over a hydrodynamic wing [12]. In Figure 6 a), b) are presented the lift force graphics obtained from the two methods mentioned above and in Figure 7 a), b) the compared drag force graphics [12].



a) Lift force graphic experimentally obtained

b) Lift force graphic obtained by using numerical programs

**Figure 6.** Lift force graphics.

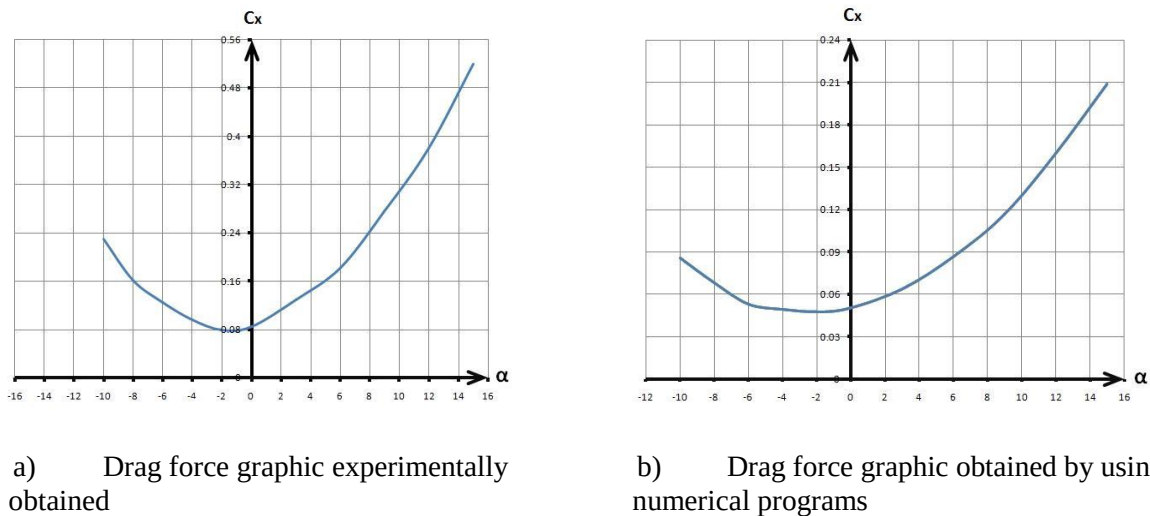


**Figure 7.** Drag force graphics.

Very good results were also obtained when calculating the drag force over a bluff body used as an auxiliary propulsion system [13]. The bluff body was attacked by an incompressible fluid under various angles of incidence. In this case study it was used a different turbulent model named Large Eddy Simulation with Wall-Adapting Local Eddy-Viscosity (LES) as a sub-grid modeling scale. In figures 8 and 9 are presented the lift force graphics obtained from the two methods mentioned above for different angle of incidence.

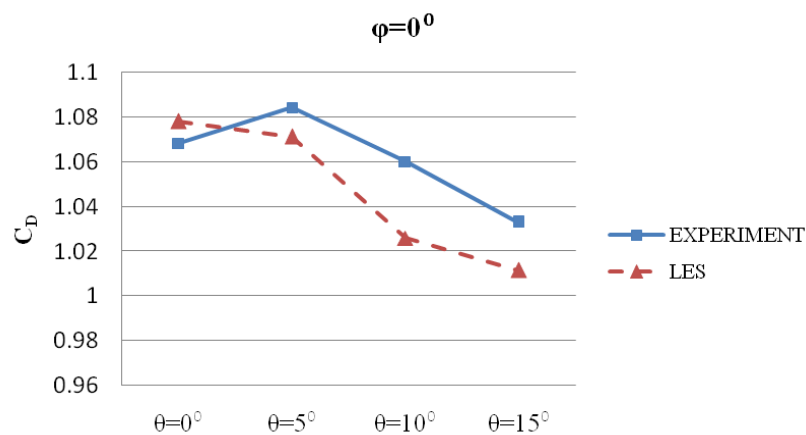


**Figure 8.** Drag coefficient variation with the pitch angle  $\theta$  that is plotted for the yaw angle  $\phi = 0^\circ$ .

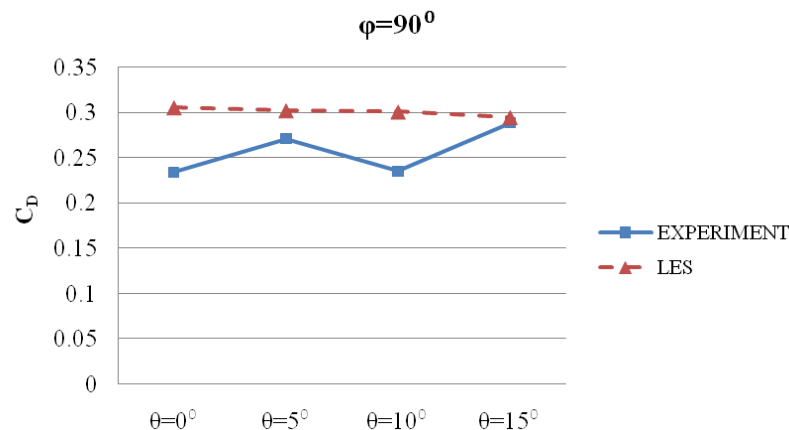


**Figure 9.** Drag coefficient variation with the pitch angle  $\theta$  that is plotted for the yaw angle  $\varphi = 90^\circ$ .

#### 4. Conclusions

Numerical methods begin to be used increasingly often compared to the experimental methods due to their numerous advantages (inexpensive, reliable, give lots of details, etc.). But to harness fully this new method of research we must well understand the physical processes that take place, how the software operates, how to set the correct data and we need to be able to correctly interpret the output data of the computer based model.

As shown in the paper we have a good correlation between the theoretical results (analytical and numerical) and those from experimental ones. We should emphasize that numerical programs can be used in academics institutions for a better explanation and understanding of the phenomenon which in many cases has only an analytical form. Also, they are extensively used in industrial companies for optimizing of different working elements, items, parameters.

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