COMPARISON OF RESULTS OBTAINED USING MONTE CARLO AND ANSYS FLUENT IN ANALYSIS DIFFERENTIALLY PUMPED CHAMBER

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Abstract: The goal of this thesis is the analysis of a gas flow running through the drain channels within the apertures of differentially pumped chamber of the Environmental Scanning Electron Microscope (ESEM). This thesis contains a verification of current simulation results of gas flow within the differentially pumped chamber published by D. Danilatos using Monte Carlo method in comparison with simulation results achieved by using simulation program ANSYS Fluent, which uses the mechanism of continuum for its calculations.

Keywords: ANYSY Fluent, Environmental Scanning Electron Microscope, ESEM, Monte Carlo

1 INTRODUCTION

This thesis analyses the gas flow within the differentially pumped chamber, which is a part of the Environmental Scanning Electron Microscope (ESEM). This type of microscope is designed for studying samples, which naturally contain water. The purpose of the differentially pumped chamber is to separate the high vacuum area (the microscope's column) from the high pressure area (the sample chamber). This separation is being achieved by two apertures PLA1 and PLA2, preventing the fast equalization of gas pressure throughout the microscope at the time the column is being drained. The microscope column is pre-drained with a rotatory pump and then the gas pressure is stabilized by a diffusion pump. Another rotatory pump is placed into in to the differentially pumped chamber stabilizing the gas pressure at the required figure with continual pumping.

The design and the boundary conditions used for the simulations are the same as G. D. Danilatos [3] published in his calculations, in which he used Monte Carlo method in order to achieve the best pumping results and the minimal loss of the electron beam possible. The Monte Carlo method is based on series of randomly runned expreriments using the model of the system where their evaluation shows the possibility of the specific effect. In this thesis the results obtained using Monte Carlo are compared with the results obtained using the method which deals with the mechanics of the continuum which is also required for calculations of the simulations by the ANSYS Fluent program. The mathematical principles of this method are further described in chapter two. The output of this work is the comparison of the two methods mentioned above and their results for the purpose of deciding, which one is more accurate and could be used for further simulation calculations for the purpose of additional improvements of the construction of the ESEM type microscope.

2 MATHEMATICAL INTERPRETATION OF THE ANSYSFLUENT

The kinetics of the fluids can be described in two ways. The first one is using the Lagrange method which studies the motion of the fluids as individual particles and the second one is using the Euler method which describes the fields of kinetic quantities.

All the calculations were solved with the ANSYS Fluent program. This program solves the system of three partial differential equations, which are extended by an equation of state and the continuity equation. These five equations describe a three dimensional flow of compressible, viscous fluid considering the heat transfer. The Euler method describes the state of the flowing fluid in a specific point. The vector of this point and the time are called the Euler variables. Another term, the "streamline", is connected with the Euler method description of the fluid flow. The streamline is described as a group of points in which the vectors of the fluid flow velocity are tangential at the same moment. This equation can be expressed as (1) :

$$\frac{dx_1}{u_1(x,t)} = \frac{dx_2}{u_2(x,t)} = \frac{dx_3}{u_3(x,t)} \tag{1}$$

where x_i and u_i are components of the position vector which means the velocity in specific point and time, where the time is constant. If the functions are different from zero, they are definite and con-tinuous, so are their first derivations and through every single point of the vector field goes only one single streamline. The streamlines represent the flow in a specific time whereas the trajectories describe the movement of particles in a time interval. [2]

The simulation of a fluid sticks to three basic principles:

- the principle of maintaining the mass (the continuity equation),
- the principle of maintaining the momentum (the Euler equation),
- the principle of maintaining the energy (the Bernoulli equation).

The Continuity equation The continuity equation describes the physical principle of maintaining the mass in the field of mechanics of fluids. The equation states that during the change of velocity, diameter and density the mass of the fluid remains unchanged.

The Euler equation of Hydrodynamics The Euler equation of hydrodynamics describes the equilibrium of forces of mass affecting the fluid from the outside, pressure forces taking effect within the fluid and inertial forces of moving particles of the fluid.

The equation of state The equation of state describes the correction between the pressure, density and temperature of the fluid.

The Bernoulli equation The Bernoulli equation describes the principle of maintaining the mechanical energy of stabilized flow of an ideal fluid.

The Navier – Stokes equations The equilibrium of forces affecting the flow of a real fluid is described by Navier - Stokes equations.

$$\underbrace{\frac{\delta(\rho v_i)}{\delta t} + v_j \frac{\delta(\rho v_i)}{\delta x_j}}_{1} = \underbrace{-\frac{\delta p}{\delta x_i}}_{2} + \underbrace{\eta \frac{\delta^2 v_i}{\delta x_j^2} + \eta \frac{1}{3} \frac{\delta}{\delta x_i} \left(\frac{\delta v_j}{\delta x_j} \right)}_{3} + \underbrace{\rho a_i}_{4} + \underbrace{F_i}_{5} \tag{2}$$

The forces affecting the elementary volume in real fluid flow are:

1. Inertial forces; 2. Pressure forces; 3. Viscous forces; 4. Gravitational forces; 5. Centrifugal forces, electromagnetic forces and others

Where:
ρ – is fluid density $[kgm^{-3}]$; t – is time $[s]$; v – is velocity $[ms^{-1}]$; p – is pressure $[Pa]$; x – is trajectory $[m]$; η – is dynamical viscosity $[Nsm^{-2}]$; a – is acceleration $[ms^{-2}]$; F – is force $[N]$; indexes $_i$ and $_j$ are parts of individual directions of axes (x,y,z) [1]

Atomic Number Density The number of atoms or molecules(n) in a mass (m) of a pure material having atomic or molecular weight (M) is easily computed from the following equation using Avogadro's number ($N_A = 6.022 * 10^{23}$ atoms or molecules per gram-mole):

$$n = \frac{mN_A}{M} \tag{3}$$

In some situations, the atomic number density (N), which is the concentration of atoms or molecules per unit volume (V), is an easier quantity to find when the material density (ρ) is given[4].

$$N = \frac{n}{V} = \frac{\rho N_A}{M} \tag{4}$$

3 CALCULATION SETTINGS

3.1 Boundary conditions settings

In the figure 1 is shown the part of the differentially pumped chamber in which is plotted the dimensions of the apertures PLA1 and PLA2. There are also described boundary conditions as the pressure in the specimen chamber, the pressure in the differentially pumped chamber or the pressure in the microscope column.

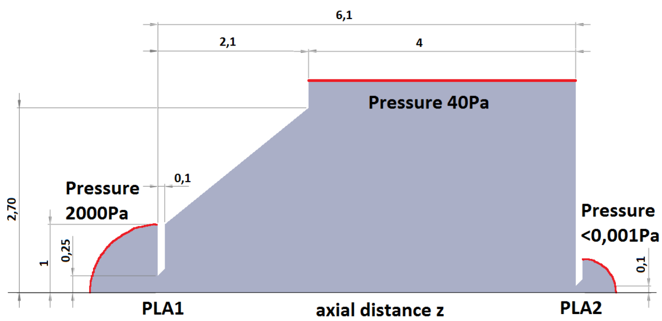

Figure 1: Boundary conditions settings

3.2 Solver settings

It was used Density based settings, which carried out by a coupled calculation pressure, speed, energy and so on. Additionally were used the settings Flux type AUSM, which is better suited for supersonic flow than type Reo-FDS. AUSM stands for Advection Upstream Splitting Method. It is developed as a numerical inviscid flux function for solving a general system of conservation equations. The AUSM first recognizes that the inviscid flux consist in two physically distinct parts, i.e. convective and pressure fluxes. The former is associated with the flow (advection) speed, while the latter with the acoustic speed; or respectively classified as the linear and nonlinear fields. Currently, the convective and pressure fluxes are formulated using the eigenvalues of the flux Jacobian matrices. Discretization was done in a second order with respect to the complexity of calculation in the area of low pressure and supersonic flow. This required careful preparation of the mash and calculation had to be steering at low values Curant the number of decreased relaxation factors.

4 RESULTS

The comparison of simulation results from Monte Carlo method with the results obtained using the ANSYS Fluent shows both methods having similar results. Comparing the graphical expression of the distribution of Number density shown on figure 2 in the left part, where the results published by D. Danilatos are shown, with the distribution shown on figure 2 in the right part, which were obtained using the system ANSYS Fluent, shows almost identical results including characteristics gradients caused by supersonic flow. The comparisons of values of velocity (on the graph 3 in the left part) and temperature (on the graph 3 in the right part) on the trajectory between the two pressure limiting apertures PLA1 and PLA2, which are also almost overlapping, is also worth attention. The only small difference can be found at the temperature curve showing the area near the aperture PLA2, where the value obtained by the ANSYS Fluent system changes slower. The sharp transition between the values published D. Danilaos may be caused by a singular point. In this case the resulting curve obtained by the ANSYS Fluent system is from its nature physically more.

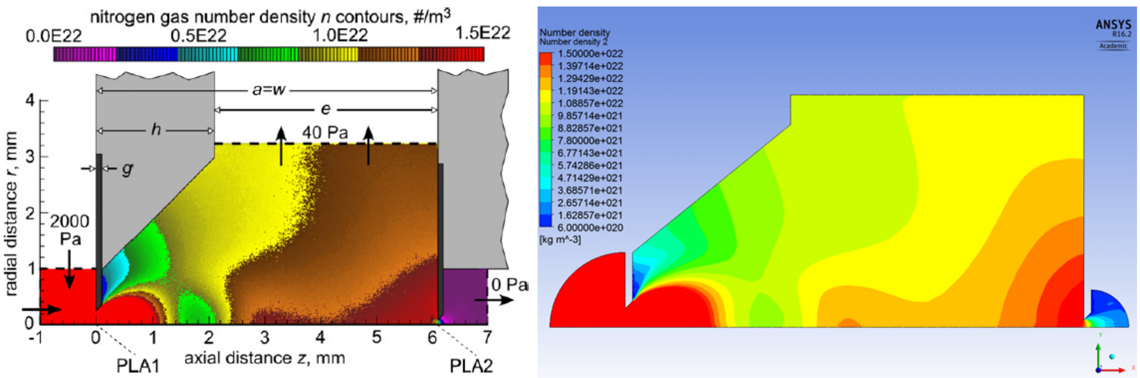

Figure 2: In the left part of inter-aperture flow field with plane geometry PLA2 calculated using the Monte Carlo [3] in the right part calculated using the AnsysFluent

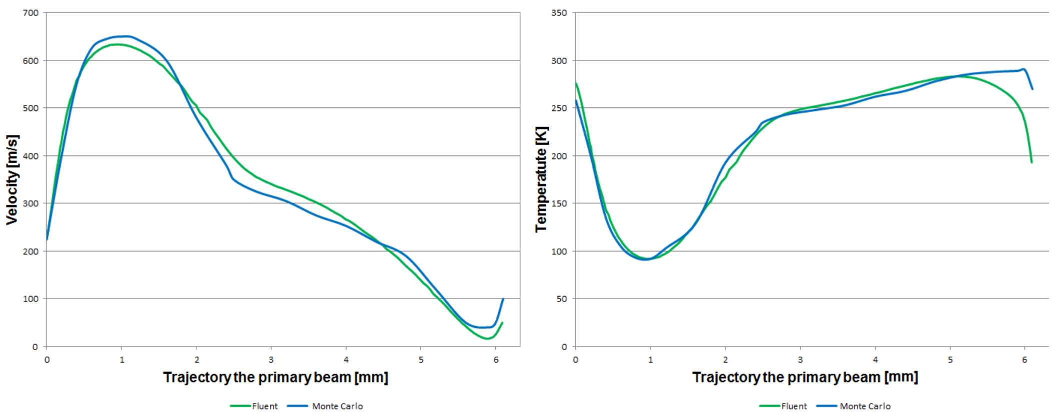

Figure 3: In the left part velocity on the trajectory of the primary beam in the right part temperature on the trajectory of the primary beam

5 CONCLUSIONS

The results published by D. Danilatos, who used for his calculations the Monte Carlo method, are practically identical with the results obtained using the ASYS Fluent system, which uses the method of finite volumes meaning the mechanics of continuum.

Method Monte Carlo does not require the connections between individual subdomains and thus it can describe the effects that are impossible to describe with continuous function, but on the other hand it can also give us wrong results, because it is not conditioned by the continuity condition. The Monte Carlo method is suitable only for the cases, where it is about solving the movement the lone molecules, also called the particulate movement, which has a stochastic character. So it is there, where Navier-Stokes equations are no longer valid. At the opposite, in the cases of a continuous environment is the usage of Navier-Stokes equations definitely an advantage because of its exact description of continuity, because the Navier-Stokes equations are derived from the forces affecting the individual parts of the fluid: gravitation, pressure, friction between adjacent parts of the fluid, formation of the turbulence. The liquids state is described by its velocity and pressures at all points forming the liquid.

Each element of the fluid in a continuum is affected by two forces: the volume one (simple) and the surface one (complicated) which is caused by neighboring elements. What's more the surface force consists of two parts: the first one is related to the pressure and the second one which is more complicated to describe, is describes the shear of the surfaces of individual elements of fluid between each other, which is the viscosity (the internal friction). This complex process of continuum can be precisely evaluated by the Navier-Stokes equations, which compared to the Monte Carlo method do not solve the problem stochastically, but with accurate description of the complex behavior of the fluids. The Navier-Stokes equation is an emblematic example of very complex partial differential equation.

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