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Comparisons Using Methods of Continuum Mechanics and Monte Carlo at Differentially Pumped Chamber

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Abstract:

The article deals with the analysis of gas flows in pumped canals in differential pumped chamber of the Environmental Scanning Electron Microscope (ESEM). The article compares and verifies existing results of differentially pumped chamber flow simulation from ANSYS Fluent system, which uses the mechanics of continuum, with the ones published by D. Danilatos using the Monte Carlo method.

Keywords:

ANSYS Fluent, differentially pumped chamber, EREM, Monte Carlo, SolidWorks

1. Introduction

The article analyses the gas flow within the differentially pumped chamber, which is a part of the Environmental Scanning Electron Microscope (ESEM) [1]. This type of microscope is designed for studying samples which naturally contain water [2]. The differentially pumped chamber's purpose is to separate the high vacuum area (the microscope's tube) 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 while the tube is being drained [3]. The tube of the microscope is pre-drained with a rotatory pump and then the gas pressure is stabilized by a diffusion pump. Another rotatory pump is located in the differentially pumped chamber, stabilizing the gas pressure at a required value with continual pumping.

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The design and the boundary conditions we used are the same as G.D. Danilatos published. He used the Monte Carlo method in order to achieve the best pumping results and the smallest possible losses of the electron beam. The Monte Carlo method is based on running numerous random experiments with the model of the system where their evaluation shows the possibility of specific effect. In this manuscript, there are compared the results obtained by applying the Monte Carlo method with the results obtained by applying the method which uses the mechanics of the continuum used for calculations of the simulations by the ANSYS Fluent program [4]. Mathematical principles of this method are further described in Chapter two. The topic of this work is the comparison of two methods mentioned above and their results for the purpose of deciding which one is more accurate and. It could be used for further simulation calculations for the purpose of additional improvements in design of the ESEM type microscope [5].

1. Mathematical Interpretation

For the modelling of individual apertures, the SolidWorks and ANSYS Fluent were used and thus the flow can be calculated using the finite volumes method. ANSYS Fluent solves a system of three partial differential equations supplemented with a fourth equation of state. It is a type of three-dimensional flow of compressible viscous fluid. Basic equations describing the flow of viscous compressible fluid written in conservative form are the three conservation laws, the Law of Conservation of Mass, Momentum and Energy completed with the Equation of State of the considered fluid [6].

The mathematical-physical model can be found in [8].

1.1. Solver settings

We decided to use the Density-Based Solver because of the compressibility of the flow and the assumption of high gradients associated with the supersonic flow.

The Density-Based Solver solves the governing equations of continuity, momentum, and in this case also energy and species transport simultaneously as a set, or vector, of equations. Governing equations for additional scalars will be solved sequentially (that is, separated from one another and from the coupled set). Two algorithms are available for solving the coupled set of equations, the coupled-explicit formulation and the coupled-implicit formulation.

In this case, we used the Implicit Formulation, where the unknown values are given from the existing ones and also from the unknown values of adjacent cells. Every unknown value appears in more than one equation in the assembly and these equations are solved concurrently.

In this case, we did not use the calculation schema of Roe Flux-Difference Splitting Scheme, but we used the AUSM (Advection Upstream Splitting Method), which is preferable for the supersonic flow solving.

Firstly, the AUSM scheme computes a cell interface Mach number based on the characteristic speeds from the neighbouring cells. The interface Mach number is then used to determine the upwind extrapolation for the convection part of the inviscid fluxes. A separate Mach number splitting is used for the pressure terms.

The AUSM scheme has several desirable properties:

1. It provides an exact resolution of contact and shock discontinuities.
2. It preserves positivity of scalar quantities.

3. It is free from oscillations at stationary and moving shocks.

For discretization we used second Order and Power Law schemas.

The Power Law Scheme interpolates the face value of a variable ϕ using the exact solution to a one-dimensional convection-diffusion equation (1).

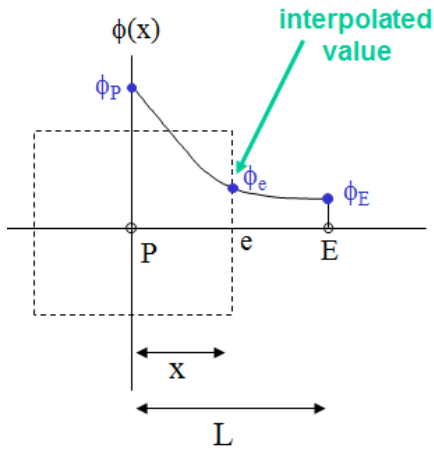

Fig. 1 Power law scheme

$$\phi_e = \phi_P - \frac{(1-0.1\,\mathrm{Pe})^5}{\mathrm{Pe}}(\phi_E - \phi_P), \tag{1}$$

where Pe is the Peclet number given by

$$\mathrm{Pe} = \frac{U\,L}{\alpha}. \tag{2}$$

The Peclet number is defined as the ratio of the rate of convection of a physical quantity by the flow to the rate of diffusion of the same quantity driven by an appropriate gradient [9]. Where U is the freestream velocity, L is the characteristic dimension of the problem, and α is the coefficient of thermal diffusivity.

1.2. Knudsen number

The Knudsen number (Kn) is a dimensionless number defined as the ratio of the molecular mean free path length to a representative physical length scale. The Knudsen number helps determine whether statistical mechanics or the continuum mechanics formulation of fluid dynamics should be used to model a situation (3),

$$\mathrm{Kn} = \frac{I}{L}, \tag{3}$$

where I is the mean free path and L is the characteristic dimension. If the Knudsen number is near or greater than 0.5, the mean free path of a molecule is comparable to a length scale of the problem, and the continuum assumption of fluid mechanics is no longer a good approximation. In such cases, statistical methods should be used.

In practice it is sufficient to approximate the relation for the mean free path in air by

$$\bar{I} = \frac{7 \cdot 10^{-3}}{p}, \tag{4}$$

where p is the air pressure.

2. Results

The comparison of simulation results from the Monte Carlo method with the results obtained using the ANSYS Fluent shows that both methods have had similar results.

Fig. 2 and 3 show a graphical representation of the density number distribution, whereas Fig. 2 shows the results published by D. Danilatos and Fig. 3 shows the results obtained from ANSYS Fluent, respectively. As mentioned above, the comparison of the two figures shows that the results are almost identical, including those for the characteristic gradients caused by a supersonic flow. The comparisons of the values of velocity in Fig. 4 and temperature in Fig. 5 on the trajectory between the two pressure limiting apertures PLA1 and PLA2, which are also almost overlapping, is also worth attention.

The only difference could 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 by D. Danilaos might be caused by a singular point. In this case, the results obtained by the ANSYS Fluent system correspond better to the expected physical processes.

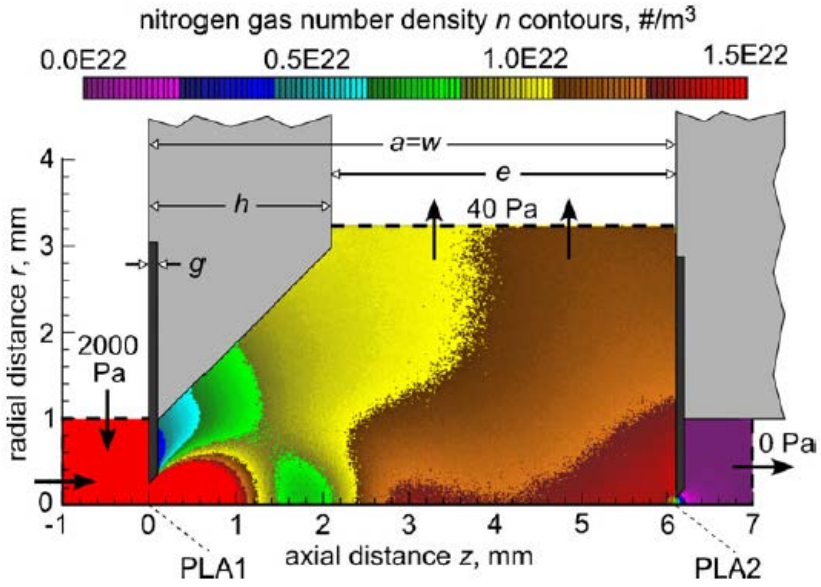

Fig. 2 Inter-aperture flow field with plane geometry PLA2 calculated using the Monte Carlo method [7]

In the second case of the differentially pumped chamber with deflector shape given in Fig. 6, the results of the density number decomposition values are similar.

The results in Fig. 6 show lower pressure values in the area of supersonic flow and also higher values in the area of interfering gas, where velocity of the gas declines from the supersonic velocity area to subsonic area.

The results in Fig. 7 show the ability of the deflector to deflect the pumped gas stream to the required direction and to prevent the density number values fluctuations in the area of primary beam between the apertures.

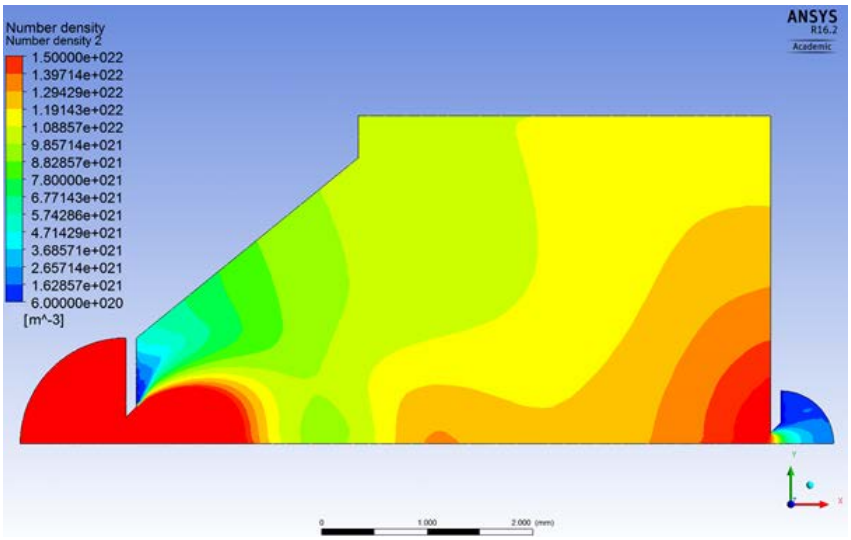

Fig. 3 Inter-aperture flow field with plane geometry PLA2 - calculated using the ANSYS Fluent

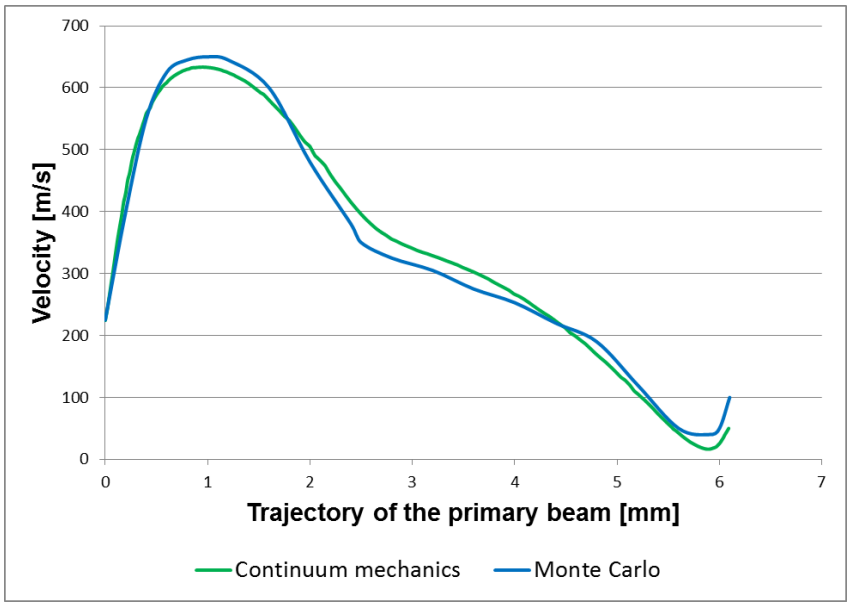

Fig 4. Velocity on the trajectory of the primary beam in comparison of both methods

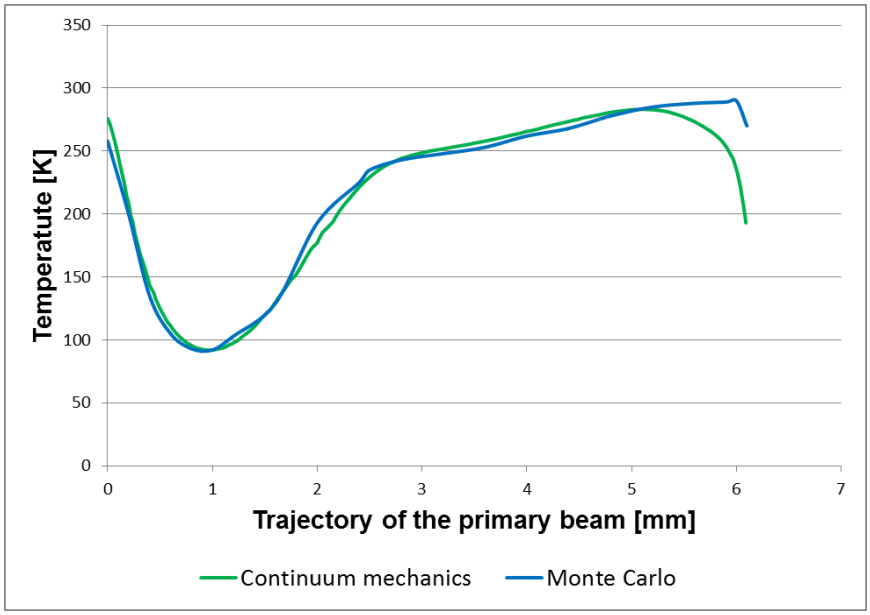

Fig. 5 Temperature on the trajectory of the primary beam in comparison of both methods

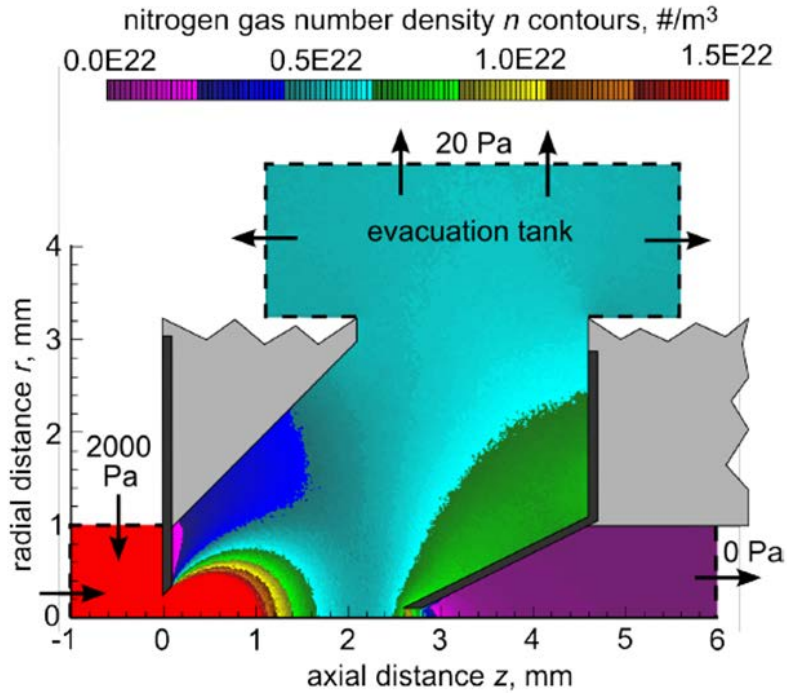

Fig. 6 Inter-aperture flow field with conical PLA2 geometry calculated using the Monte Carlo method [7]

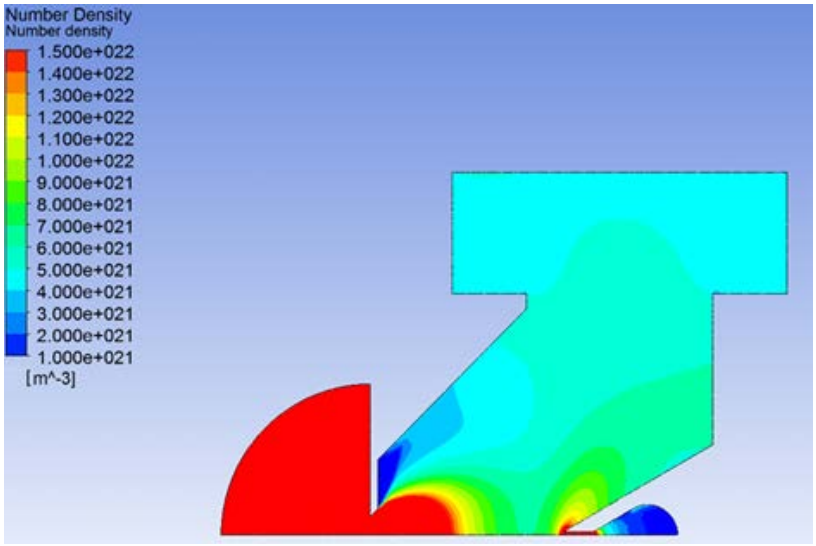

Fig. 7 Inter-aperture flow field with conical PLA2 geometry - calculated using the ANSYS Fluent

3. Conclusions

The results published by D. Danilatos, who used the Monte Carlo method, are practically identical to the results obtained by ANSYS Fluent, which uses the finite volume method and the continuum mechanics assumption.

The Monte Carlo method does not impose the basic requirement of individual connections between subdomains and thus it can afford to describe the one-side effect, which is not possible to describe with a continuous function. On the other hand, however, this method can lead to a wrong result, because it is not constrained by the continuity assumption. The Monte Carlo method is applicable only when one needs to solve the movement of individual molecules when it comes to a particulate movement, which has a stochastic character. Under these conditions, the Navier-Stokes equations become no longer valid. In contrast, when the continuity assumption is appropriately justified, it is always better to use the Navier-Stokes equations, which are mathematically better able to describe the physical connections in the fluid. This is because the Navier-Stokes equations are derived from the forces which affect individual parts of the fluid: gravitation, pressure, friction between neighbouring particles of the fluid, and the onset of turbulence. The state of the fluid is described by its speed and pressures at all points, in which this fluid is present. In a continuum, two forces are acting on each element of fluid: the volume (simpler) and surface (more complicated), which are conducted by adjacent fluid elements. Moreover, the surface force is composed of two parts: the first is related to the pressure and the second, which is more difficult to describe, is attributed to the shear on the surfaces of individual fluid elements, known as viscosity (the internal friction). This complex process under the continuum assumption can be precisely balanced in the Navier-Stokes equations, which, compared to the Monte Carlo method, do not allow for solving the problem stochastically, but are able to provide an accurate description of the behaviour of complex fluids.

The Navier-Stokes equations are an emblematic example of a set of equations that appear simple, but are very complex partial differential equations internally.

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