# MODELLING PHYSICAL MATERIAL PROPERTIES USING THE SOFTWARE COMSOL MULTIPHYSIC

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## Abstract

Civil Engineering is a sector that moves within the macroscale. The use of Nanotextile requires an understanding of various phenomena on a basic level, i.e. in the micro and nano-scale. If we move in the macrocosm is the possible influence of some forces to neglect. However, the negligence for nanotextile is not possible. Software, which are used for calculations of diffusion properties of building materials do not provide for modelling the properties of membranes nanotextiles satisfactory results. The probable cause is negligence complex internal structure of these materials. Modelling of physical and chemical properties of nano-membranes is important for their successful use in various technological fields, including construction. As a suitable software seems Comsol MultiPhysic, since it is possible to model multiphysics happening, i.e. that can be added to the modelling include the forces acting on the micro and nano level (for example van der Waals forces). It is also possible to record the program structure and will create a pre e.g. in a text editor or AutoCAD and assign the material parameters.

**Keywords:** COMSOL MultiPhysic, nanotextiles, physical properties, material parameters

## 1. INTRODUCTION

Civil Engineering is a field that so far the use of nanotechnology rather conservatively. In the present nanotechnology is used primarily as nanoparticles, which are scattered in various paint or spray compositions [1]. Nano is used in present are e.g. as filters [2, 3] Protective layer [4], fittings [5]. For use of Nanotextiles in the construction industry, it is essential to know their properties and interactions with the environment. Nanotextiles is a material which has a very high porosity. This property is an obstacle to the use of standard macroscopic models [6]. To create a successful model, it is necessary to establish the structure nanotextile [7, 8, 9]. After determining the structure is another important step in understanding the interactions between environment and nanofibers. Interaction is obviously derived from the problem. The resulting properties of nano should thus be determined as a numerical solution of the corresponding 3D model.

## 2. MODELLING IN COMSOL MULTIPHYSIC

The best program for modelling the properties of nanotextiles seems to be the program Comsol Multiphysic. The program enables the modelling of various physical phenomena. The program serves not only for modelling but also for simulation tasks in many fields of physics (e.g. Engineering, transport of moisture and heat or chemicals). Tasks are described by differential equations of first and second order. For solving individual tasks, the program uses the finite element method. The big advantage is less time-consuming to solve physical problems. Indisputable advantage of this program is the clarity of the model where desktop we have a preview of the model and the process of creating the model. The program uses COMSOL MultiPhysic a clear tree structure.

Before modelling is necessary to accurately specify the problem, i.e. to describe the phenomenon studied using concepts that correspond to the selected computer modelling technique. The model can be defined using particle technique (microscopic level), continuous modelling (macroscopic level), or a combination of the previous two techniques. If the specified problem is to create the model. When creating a model, there are

different simplification, because we do not know all the properties studied phenomenon. In this section it is necessary to pay attention to the possibility of a bad model formulation. The next step is solving the problem itself, which is usually solved system of ordinary and partial differential equations. The final step is to compare modelling results with experimental data. [10]

If the procedure defined in the previous paragraph for modelling in Comsol Multiphysic can be modelling the program to summarise in a few basic steps. The first step is to create a geometry that can be created using CAD Woe For example, in a graphics editor or read formats VRML and STL, 2D files in DXF format and 3D files in NASTRAN. The second step is to enter the property. This step, defines the initial and boundary conditions, i.e. they are assigned to individual areas, surfaces, edges and points variables, expressions or corresponding functions. In this section, we can use the library, where there are predefined materials. The third step is defining the network, which is the basis for the finite element method. The fourth step is solving the model itself. The role is a possible solution COMSOL graphical interface or the command line MATLAB. The last step is processing the results, which can be calculated using different variables to show graphs. The results can be processed graphically or animate formats into AVI or GIF. Solutions can also be exported to text files. [11]

## 2.1. The practical demonstration

The sample is created in 2D space. The model consists of lines formed from polystyrene and the air gaps with a square structure (**Figure 1**). Foam was chosen because it is one of potential materials for the manufacture of nanotextiles usable in construction. Polystyrene is a very good insulator. The demonstration model the linear progression temperatures this structure.

In the processing example first selects the physical environment. In the menu is set space in which will be modelled (in our case 2D) and the application mode, which is in this case the transport of heat. It is also necessary to set up whether the case is stationary or non-stationary. In this case will be used stationary calculation. Further parameters are set, i.e. the dimensions of individual segments (**Figure 1**), and at the same time, the value of individual constants. In this case it is necessary to define the dependence of the equivalent thermal conductivity on the thickness, which will allow any change in the dimensions of the air cavities is automatically changed and thermal conductivity of the air cavity temperature (**Table 1**). Since there is only a table of specific values, this is a function of the interpolation. It is also necessary to choose how the function will behave if it comes out of the defined values. In this case will have a linear approximation.
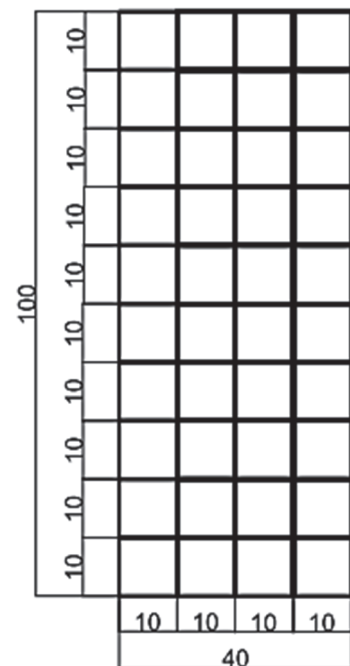


**Figure 1** The schema of the problem

**Table 1** The equivalent thermal conductivity depending on the thickness of the air gap [12]

| Air layer thickness [mm] | 5 | 10 | 50 | 300 |
|---|---|---|---|---|
| The equivalent thermal conductivity [W/mK] | 0.045 | 0.067 | 0.313 | 1.88 |

The next step is to define the geometry according to the specified example and choice of materials. COMSOL MultiPhysic program includes a library of materials. It is therefore possible to select the material from the library or define a new one. For this example was chosen polystyrene, which was in the library of materials. After entering the geometry and materials is defined way to spread heat. It spreads when heat is only one way (in this sample leadership) you should not need to modify the default settings. Characteristics required to calculate
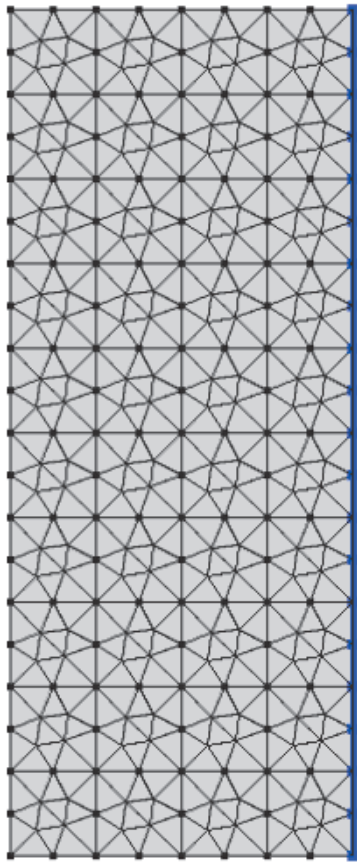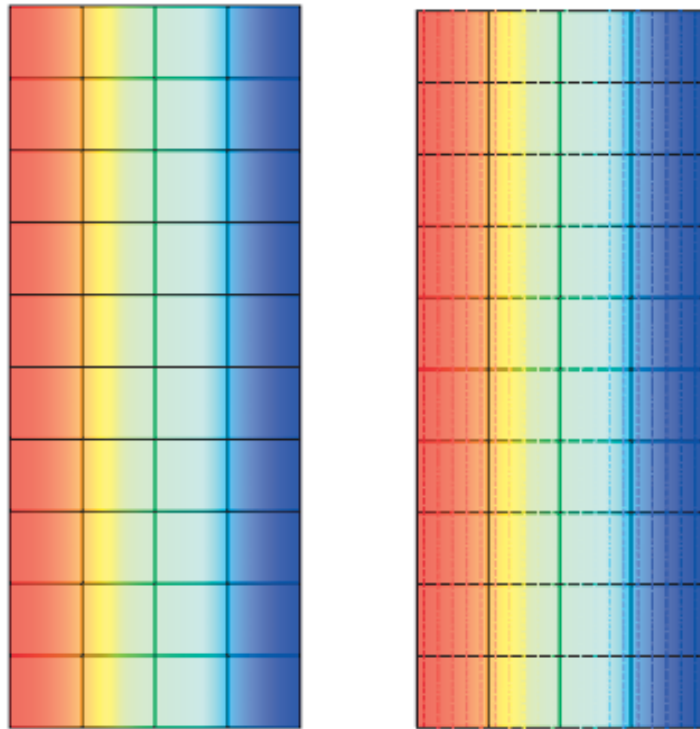
Figure 2 The finite element mesh



**Figure 3** The resulting temperature curve (on the right with the isotherms)

the heat conduction to take on the assignment of materials. Now it is necessary to set the boundary conditions. At the beginning, all boundaries assume adiabatic conditions. These conditions need to be changed at borders that are exposed to known conditions. In this example, is defined inner (20 °C) and outdoor (10 °C), which is governed by Newton boundary condition. The last step is necessary to create a finite element mesh, which will be used for this demonstration predefined styles (**Figure 2**). Now we can proceed to the actual calculation. The calculation results can be displayed using different graphs (**Figure 3**) or generate the calculated values to the table.

## 3.    CONCLUSION

COMSOL MultiPhysic program can be a very good tool in solving various physical phenomena that take place in nanotextiles. First, it is necessary to analyze the problem, determine the basic physical interactions studied phenomena and then choose the appropriate mathematical model for the phenomenon. The results also depend on the selected geometry of the material structure. Effect of structure on the properties of the nanotextiles can be performed using various simulations using numerical methods. Examples of such structures include computations involving chaotic network of lines and multi-layer systems.

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## REFERENCES

[1] HOCHMANOVÁ L., VYTŘASOVÁ J. Vliv nanočástic TiO$_2$ a ZnO na fotokatalytické a antimikrobiální účinky silikátových nátěrů. Chemické Listy, Vol. 104, 2010, pp. 940-944.

[2] DETVANOVA L., PRICHYSTALOVA J., DOSEK M., KALHOTKA L. Using of the nanotextiles for removing of microbial pollution. MendelNet 2014, pp. 534-536.

[3] LEV J., KALHOTKA L., ČERNÝ M. Water filtration by nanotextiles. Nanocon 2010.

[4] SOUČEK J., TICHÁ P. Modelling Interior Environment of Historical Building and Determination of Critical Places for Application of Nanotextiles Protection", Advanced Materials Research, Vol. 1025-1026, 2014, pp. 1141-1144.

[5] WEI B., XU F., AZHAR S. W., LI W., LOU L., LIU W., QUI Y. Fabrication and property of discarded denim fabric/polypropylene composites. Journal of Industrial Textiles, Vol. 44, No. 5, 2015, pp. 798-812.

[6] MADĚRA J. Transmat-S. 2009. At: http://tpm.fsv.cvut.cz/vz/software10.php

[7] SAMBAER W., ZATLOUKAL M., KIMMER D. 3D air filtration modelling for nanofiber based filters in the ultrafine particle size range. Chemical Engineering Science, Vol. 82, 2012, pp. 299-311.

[8] GHASEMI-MOBARAKEH L., SEMNAMI D., MORSHED M. A novel method for porosity measurement of various surface layers of nanofibers mat using image analysis for tissue engineering applications. Journal of Applied Polymer Science, Vol. 106, No. 4, 2007, pp. 2536-2542.

[9] KLICMANOVÁ I. Diploma thesis: Analýza mikroskopické struktury polymerních nanotextilií. Praha, 2015.

[10] HRACH R. Počítačová fyzika I. University J. E Purkyně, Ústí nad Labem. 2003. ISBN 80-7044-521-1.

[11] HUMUSOFT. Software: COMSOL MultiPhysic. 2016. Homepage: https://www.comsol.com/comsol-multiphysics

[12] ČESKÝ NORMALIZAČNÍ INSTITUT. Tepelná ochrana budov - Část 3: Návrhové hodnoty veličin. Prague. 2005. ČSN 730540-3.