Simulation of Electro-physical Characteristics of the Bulk Material in the Electric Field of Capacitive sensors

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***Abstract*— The present article covers mathematical and computer simulation of behavior of the bulk material with varying particle composition in relation to development of capacitive humidity sensors, which uses wide band of electrical field where a sample of the mentioned bulk material is put during measurements and researches. The developed model of electrical and physical properties of the bulk material is used to receive frequency and humidity characteristics of a matter consisting of particles of two different sizes. There was also a program developed to calculate and visualize frequency and humidity properties, which allows entering different sizes of two particles and changing qualitative characteristics of these materials. Results presented in the article helps to construct multiparameter humidity sensors and improve accuracy of measurements received with their use.**

I. Introduction

Most mathematical bulk material models have such a weak point as that they are not able to obtain frequency and humidity properties of bulk materials with varying particle sizes [1].

In general, a problem of modeling of electrical and physical properties of bulk materials reduces to finding of integral values of the total electrical conductivity of a bulk material sample. A structure consisting of two particles with different geometrical dimensions should be taken from the bulk material sample in order to mathematically describe the whole sample. Such a structure is called the basic or elementary structure of the bulk material. We assume that the whole volume of the bulk material consists of such basic particles. Thus, properties of the whole volume of the bulk material can be inferred when examining characteristics of an individual particle. Since such characteristics are applied to an individual particle they are conventionally called as differential parameters. Specific electrical resistance, specific conductivity, relative permittivity, microhardness, density, heat capacity and other parameters could be investigated. Parameters of the bulk material investigated in the electric field of a capacitive sensor are relative permittivity ε or dielectric loss tangent tgδ. Their volumes depend on bulk material properties such as particle composition, particle nature, moisture content in the bulk material and others [2].

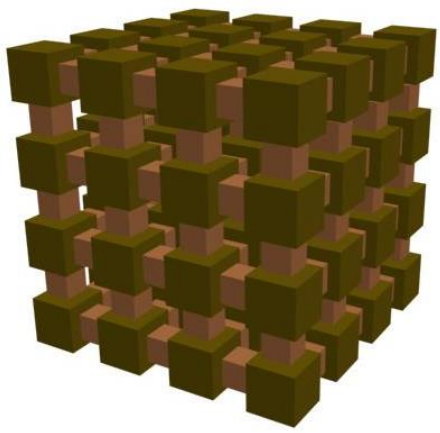

Figure 1. Proposed variant of particle packing of the bulk material consisting of particles with two different sizes (each particle having its own nature)

When developing a mathematical model of bulk material behavior in the frequency spectrum of the electrical field the real chaotic structure is replaced by an adequate ordered structure. Analytical forms are obtained for such simplified structure and used to receive frequency and humidity characteristics of the material under examination in the required frequency range [3].

II. Idealization of the Form and Packing of Bulk Material Particles

We assume that the bulk material under examination consists of two types of cube-shaped particles packed as shown in Figure 1.

Let us consider an idealized structure of the bulk material packed in the manner shown in Figure 2 in one of the orthogonal planes. In order to develop a mathematical model of the bulk material we hypothesize the following facts:

- the bulk material is heterogeneous and two-component;
- Particles 1 and 2 are respectively the first and the second cube-shaped components and have different sizes;
- the particle is evenly moistened;
- packing of particles in relation to each other and the electric field vector E is shown in Figure 2;

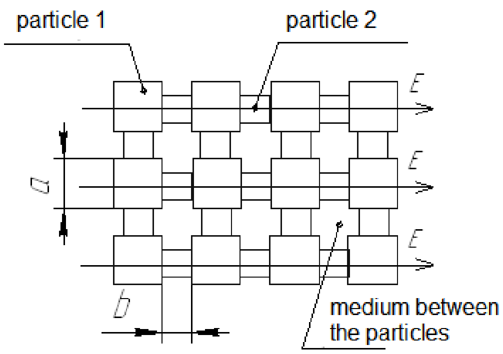

Figure 2. Idealized bulk material structure with cubic packing presented in one of the coordinate planes

- there is some space between particles having the medium with its electrical and physical properties, and porosity of the bulk material structure is determined by a

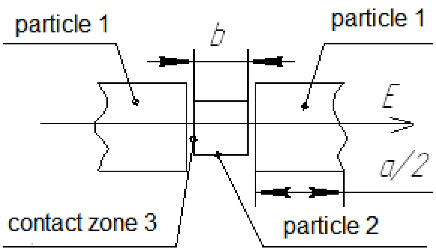

Figure 3. System consisting of two particles

ratio of geometrical dimensions of particles;

- surfaces of particles in the direction of the electric field vector are equipotential;

- current lines in particles are parallel to the electric field vector *E* and are equally distributed in particles.

The bulk material structure in Figure 2 has two cube-shaped particles, where a and b are edge dimensions of such particles, wherein $a \geq b$ and $a = k \cdot b$. Space between bulk material particles is filled with certain medium. The bulk material under examination is capillary-porous body.

In order to receive differential parameters of the bulk material we choose a section in the volume of the bulk material, which consists of two particles and contact zones. Such a system consisting of two particles is shown in Figure 3.

The Particle 2 is presented in the system as an entire cube with b edge. The Particle 1 is divided into two equal halves with $a/2$ edge in the direction of the electric field vector *E*. Such representation of two particles system allows considering conductivity of particles and contact zones between particles. Change of a and b sizes results in change of the bulk material particle composition.

III. Calculation of Conductivity of the Two-Particle System

We divide the two-particle system into different zones, where active and reactive components of the system conductivity are found using simple methods.

Let us call the zones 1 and 2 in Figure 3 as conduction areas of the Particles 1 and 2, and the zone 3 as the contact area. In this respect we also consider two halves of the zone 1 as the whole zone 1.

We represent the two-particle system as a series connection in the direction of the vector *E*. In order to take into account different polarization states of the bulk material, each part of the connection is represented as active resistance *R* and capacity *C* on zero and infinite frequency. For fast and slow polarization processes we assume parallel and sequential substitutional connections respectively [4]. Equivalent substitutional connection of the two-particle system is shown in Figure 4.

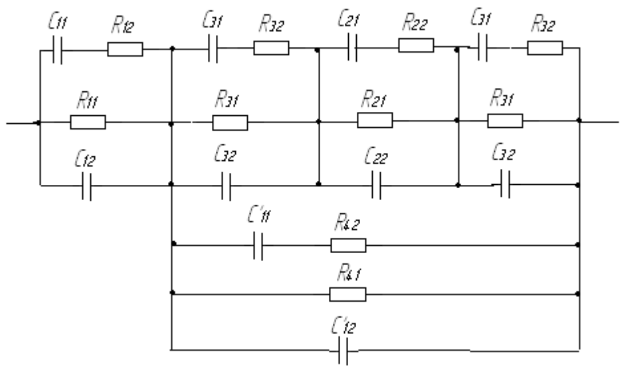

Figure 4. Equivalent substitutional connection of the two-particle system without regard to the effect of inductivities

The following symbols have meanings as follows in Figure 4:

R_{11}, R_{21}, R_{31} and R_{41} respectively mean active resistance of zones 1, 2 Contact Zone 3 and the medium to direct current;

C_{11}, C_{21}, C_{31} and C_{11}' respectively mean additional capacity between proper surfaces of the Zone 1, Zone 2, Contact Zone 3 and between surfaces of different Particles 1 with the deduction of capacity of the Contact Zone 3 under direct current and in the direction of the vector *E*;

R_{12}, R_{22}, R_{32} and R_{42} respectively mean additional active resistance of Zones 1 and 2, Contact Zone and medium on infinite frequency;

$C_{12}, C_{22}, C_{12}', C_{32}$ respectively mean capacity in the direction of the vector E between surfaces of the Particle 1, Particle 2, areas of the different Particles 1 with the deduction of the Contact Zone 3, and the Contact Zone 3 on infinite great frequency of alternate current.

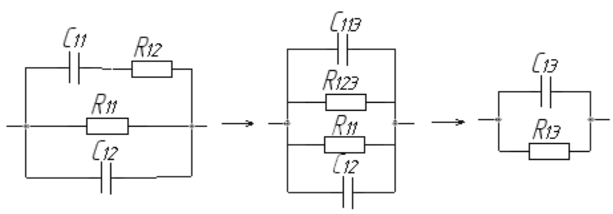

Figure 5. Sequence of conversion of the substituional connection of the Particle 1

The scheme in Figure 4 is simplified with use of formulas of active and reactive resistance when conversing series R and C connection into parallel collection and vice versa [4]. Conversions are carried out sequentially for each part of the substitutional connection (Figures 5, 6 and 7).

$$R_{12Э} = R_{12}\left[1+\frac{1}{(\omega C_{11}R_{12})^2}\right]$$

$$C_{11Э} = \frac{C_{11}}{1+(\omega C_{11}R_{12})^2}$$

$$R_{1Э} = \frac{R_{12Э}R_{11}}{R_{12Э}+R_{11}} = \frac{R_{11}R_{12}\left[1+\frac{1}{(\omega C_{11}R_{12})^2}\right]}{R_{11}R_{12}\left[1+\frac{1}{(\omega C_{11}R_{12})^2}\right]}$$

$$C_{1Э} = C_{11Э}+C_{12} = \frac{C_{11}}{1+(\omega C_{11}R_{12})^2}+C_{12}$$

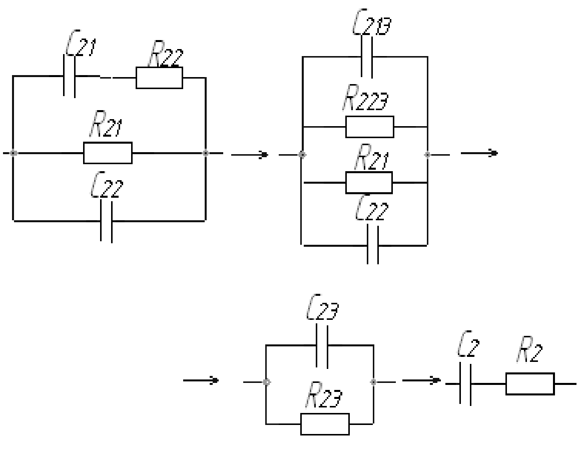

Figure 6. Sequence of conversion of the substitutional connection of the Particle 2 and substitutional connection of the Contact Zone 3

$$R_{22Э} = R_{22}\left[1+\frac{1}{(\omega C_{21}R_{22})^2}\right]$$

$$C_{21Э} = \frac{C_{21}}{1+(\omega C_{21}R_{22})^2}$$

$$R_{2Э} = \frac{R_{22Э}R_{21}}{R_{22Э}+R_{21}} = \frac{R_{21}R_{22}\left[1+\frac{1}{(\omega C_{21}R_{22})^2}\right]}{R_{21}R_{22}\left[1+\frac{1}{(\omega C_{21}R_{22})^2}\right]}$$

$$C_{2Э} = C_{21Э}+C_{22} = \frac{C_{21}}{1+(\omega C_{21}R_{22})^2}+C_{22}$$

$$R_2 = R_{2Э}\frac{1}{1+(\omega C_{2Э}R_{2Э})^2} = \frac{R_{21}R_{22}\left[1+\frac{1}{(\omega C_{21}R_{22})^2}\right]}{R_{21}R_{22}\left[1+\frac{1}{(\omega C_{21}R_{22})^2}\right]}\times$$

$$\times\frac{1}{1+\left[\omega\left(\frac{C_{21}}{1+(\omega C_{21}R_{22})^2}+C_{22}\right)\frac{R_{21}R_{22}\left[1+\frac{1}{(\omega C_{21}R_{22})^2}\right]}{R_{21}R_{22}\left[1+\frac{1}{(\omega C_{21}R_{12})^2}\right]}\right]^2}$$

$$C_2 = C_{2Э}\left(1+\frac{1}{(\omega C_{21Э}R_{21Э})^2}\right) = \left[\frac{C_{21}}{1+(\omega C_{21}R_{22})^2}+C_{22}\right]\times$$

$$\times\left(1+\frac{1}{\left(\omega\left(\frac{C_{21}}{1+(\omega C_{21}R_{22})^2}+C_{22}\right)\cdot\frac{R_{21}R_{22}\left[1+\frac{1}{(\omega C_{21}R_{22})^2}\right]}{R_{21}R_{22}\left[1+\frac{1}{(\omega C_{21}R_{22})^2}\right]}\right)^2}\right)$$

For the Contact Zone:

$$R_{32Э} = R_{32}\left[1+\frac{1}{(\omega C_{31}R_{32})^2}\right]$$

$$C_{31Э} = \frac{C_{31}}{1+(\omega C_{31}R_{32})^2}$$

$$R_{3Э} = \frac{R_{32Э}R_{31}}{R_{32Э}+R_{31}} = \frac{R_{31}R_{32}\left[1+\frac{1}{(\omega C_{31}R_{32})^2}\right]}{R_{31}R_{32}\left[1+\frac{1}{(\omega C_{31}R_{32})^2}\right]}$$

$$C_{3Э} = C_{31Э}+C_{32} = \frac{C_{31}}{1+(\omega C_{31}R_{32})^2}+C_{32}$$

$$R_3 = R_{3Э}\frac{1}{1+(\omega C_{3Э}R_{3Э})^2} = \frac{R_{31}R_{32}\left[1+\frac{1}{(\omega C_{31}R_{32})^2}\right]}{R_{31}R_{32}\left[1+\frac{1}{(\omega C_{31}R_{32})^2}\right]}\times$$

$$\times \frac{1}{1+\left[\omega\left(\frac{C_{31}}{1+(\omega C_{31}R_{32})^2}+C_{32}\right)\frac{R_{31}R_{32}\left[1+\frac{1}{(\omega C_{31}R_{32})^2}\right]}{R_{31}R_{32}\left[1+\frac{1}{(\omega C_{31}R_{32})^2}\right]}\right]^2}$$

$$C_3 = C_{3\text{Э}}\left(1+\frac{1}{(\omega C_{3\text{Э}}R_{3\text{Э}})^2}\right) = \left[\frac{C_{31}}{1+(\omega C_{31}R_{32})^2}+C_{32}\right]\times$$

$$\times\left[1+\frac{1}{\left(\omega\left(\frac{C_{31}}{1+(\omega C_{31}R_{32})^2}+C_{32}\right)\cdot\frac{R_{31}R_{32}\left[1+\frac{1}{(\omega C_{31}R_{32})^2}\right]}{R_{31}R_{32}\left[1+\frac{1}{(\omega C_{31}R_{32})^2}\right]}\right)^2}\right].$$

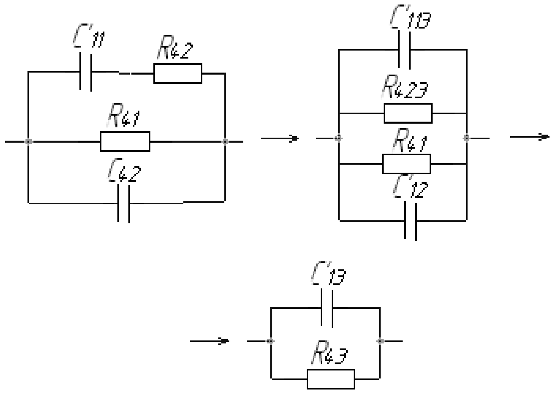

Figure 7. Sequence of the conversion of the substitutional connection of themedium

$$R_{42\text{Э}} = R_{42}\left[1+\frac{1}{(\omega C'_{11}R_{42})^2}\right]$$

$$C'_{11\text{Э}} = \frac{C'_{11}}{1+(\omega C'_{11}R_{42})^2}$$

$$R_{4\text{Э}} = \frac{R_{42\text{Э}}R_{41}}{R_{42\text{Э}}+R_{41}} = \frac{R_{41}R_{42}\left[1+\frac{1}{(\omega C'_{11}R_{42})^2}\right]}{R_{41}R_{42}\left[1+\frac{1}{(\omega C'_{11}R_{42})^2}\right]}$$

$$C'_{1\text{Э}} = C'_{11\text{Э}} + C'_{12} = \frac{C'_{11}}{1+(\omega C'_{11}R_{42})^2} + C'_{12}$$

Taking into account all conversions, scheme shown in Figure 4 takes the form shown in Figure 8.

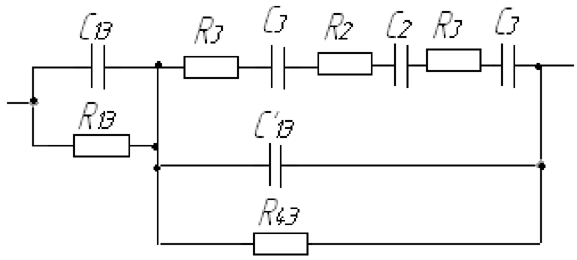

Figure 8. Substitutional connection of the two-particle system with the consideration of intermediate conversions

Further conversion of the substitutional connection is shown in Figure 9. Parameters of the scheme are calculated according to the formulas given below.

$$R'_{\text{Э}} = 2R_3 + R_2$$

$$C'_{\text{Э}} = \frac{2C_2\cdot C_3}{2C_2 + C_3}$$

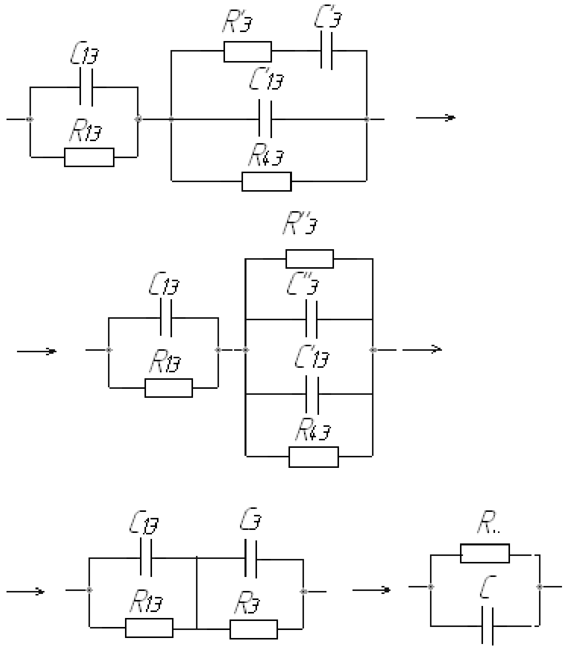

Figure 9. Subsitutional connection of the two-particle system with the consideration of intermediate conversions

$$R''_{\text{Э}} = R'_{\text{Э}}\left[1+\frac{1}{(\omega C'_{\text{Э}}R'_{\text{Э}})^2}\right]$$

$$C''_{\text{Э}} = \frac{C'_{\text{Э}}}{1+(\omega C'_{\text{Э}}R'_{\text{Э}})^2}$$

$$C_Э = \frac{C'_Э}{1+(\omega C'_Э R'_Э)^2} + C'_{1Э} \quad (1)$$

$$R_Э = \frac{R_{4Э} \cdot R'_Э \left[1+\frac{1}{(\omega C'_Э R'_Э)^2}\right]}{R_{4Э} + R'_Э \left[1+\frac{1}{(\omega C'_Э R'_Э)^2}\right]} \quad (2)$$

For cubic packing of the bulk material shown in Figure 1, conductivity along any of the x, y, z axes equals to a sum of conductivities of individual chains parallel to a respective axis; and resistance of each of the chains is equal to a sum of resistance of individual particles [3]. If the electric field vector *E* is collinear to any of the reference axes, components of total conductivity of the cubic volume of the bulk material with number of particles on each side equaling *n* is equal to components of conductivity along the corresponding axis:

$$C_M = nC \ ; \qquad \gamma_M = \frac{n}{R},$$

where *C* means capacity of the two-particle system (1), *R* means resistance of the two-particle system (2).

Substituting *C* and *R* we obtain the following formulas:

$$C_M = \frac{n \cdot \left(R_{1Э}^2 C_{1Э} + C_Э R_Э{}^2 + (\omega R_{1Э} R_Э)^2 \cdot C_{1Э} C_Э (C_{1Э} + C_Э)\right)}{(R_{1Э} + R_Э)^2 + [\omega R_{1Э} R_Э (C_{1Э} + C_Э)]^2}$$

$$\gamma_M = \frac{n \cdot \left(R_{1Э} + R_Э + \omega^2 R_{1Э} R_Э \left(R_{1Э} C^2{}_{1Э} + R_Э C_Э{}^2\right)\right)}{(R_{1Э} + R_Э)^2 + [\omega R_{1Э} R_Э (C_{1Э} + C_Э)]^2}$$

If particles are cubic packed, value of the total conductivity of the bulk material does not depend on the direction of the electric field. Based on the mathematical model of the bulk material behavior, we could find dependence of the dielectric loss tangent of the finite volume of the bulk material on frequency change of the applied electric field, where this volume of the material is put.

$$tg\delta_M = \frac{1}{\omega \cdot n^2 \cdot R_M C_M},$$

where resistance of the cubic volume of the bulk material on the relevant axis is calculated according to the following formula:

$$R_M = \frac{1}{\gamma_M}$$

The present mathematical model has distinctive features as follows: firstly, it analytically describes behavior of the two-component bulk material in the electric field; and secondly, it takes into account particle size composition of the bulk material. Abovementioned features make it possible to improve applicability of the mathematical model to analysis of bulk materials with different component and particle size compositions.

Analytical frequency and humidity characteristics of the bulk material found with the use of the present mathematical model could be considered as basis for selection of the optimal frequency of humidity sensors, and for mathematical description of behavior of capacity sensors in the electric field of measuring circuit of a signal converter to a signal convenient for further processing.

IV. Program of Visualization of Frequency Characteristics of the Bulk Material

Need in development of a program for calculation and visualization of calculation results originates from the fact that MathCad 8 computer-aided design system has no option for enlargement of the frequency range of the applied voltage over 1 MHz. Whilst the required variation frequency range is determined by need in stressing of a volume of the bulk material in a capacity cell of the sensor by changing of the voltage frequency over 1 MHz.

There was a software tool developed in the Microsoft Visual Studio [5] environment with options as presented below.

1) Updatability of input data, such as:

a) particle size:

a – edge length of the cube-shaped Particle 1, m;

k – ratio of dimensions of the cube-shaped Particle 1 and cube-shaped Particle 2.

Frequency change range in increments of subintervals equaling to W:=(w1,w2,w3):

w1 – voltage frequency variation range increment;

w2 – lower limit of the voltage frequency range;

w3 – upper limit of the voltage frequency range.

The following constant is used:

e – electric constant, $8{,}85\ 10^{-12}$, Fm^{-1}.

b) electrical and physical properties of the particles, such as:

b – dielectric permittivity of the Particles 1 and 2 under direct current;

c – dielectric permittivity of the Particles 1 and 2 on infinite frequency;

d – specific resistance of the Particles 1 and 2 under direct current;

f – specific resistance of the Particle 1 and 2 material on infinite frequency;

p – specific resistance of the Contact Zone under direct current;

q – specific resistance of the Contact Zone on infinite frequency;

g – dielectric permittivity of the medium under direct current;

h – dielectric permittivity of the medium on infinite frequency.

Electrical and physical parameters of the medium, such as:

l – specific conductivity of the medium under direct current;

m – specific conductivity of the medium on infinite frequency.

Other data such as:

n – number of Contact Zones of the Particle 1 and 2;

j – radius of the Contact Zone, m..

2) Wide variation range of the voltage frequency.

3) Ability to improve the software tool in connection with changes in requirements to the process of calculation and visualization of results.

Data for experimental calculations were taken from [1] taking into account the varying particle loose medium (Figure 1).

Work with the application (Figure 10) is carried out sequentially as described below:

1) data are input or default data are loaded ("Default" («Умолчание») button);

2) any change of data requires acceptance of such changes ("Accept" («Принять») button);

3) activity and calculation results in real time could be reviewed at the "Terminal" («Терминал») tab;

4) having results of calculations different tabs could be used. "FW Results Array" («Массив результатов FW») represents a list of results of the "Calculation 1" («Расчет-1») function, shows calculations of all the variables for the present FW, pointwise calculations. "W Results Array" («Массив результатов W») represents array of calculations in accordance with the given frequency W(w1,w2,w3), execution of a group of 33 functions, which are located on the tools menu for each W value. Calculation results are presented on the tab called "W Results Array" («Массив результатов W»). The "W Results Array" («Массив результатов W») tab shows first 500 lines of the array with 33 values of variables in order to optimize the process time needed for data output. It supports viewing of any number of lines in the capacity of the array part.

5) calculating panel allows calculating separate functions or running one of the two automatic functions called "Calculation-1" and "Calculation-2" («Расчет-1» and «Расчет-2») for FW and W respectively.

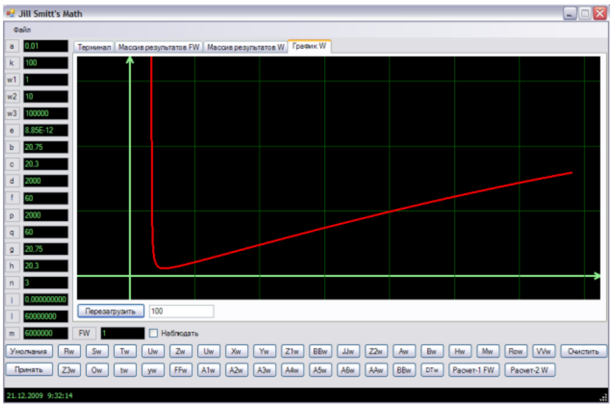

Figure 10. Visualization window of the program of calculation of the dielectric loss tangent of the finite volume of the bulk material on the sensor voltage frequency

THE RESULTS OF THE RESEARCH

We developed a mathematical model of behavior of finite volume of the two-component bulk material with varying particle size composition in the alternate electric field of the capacity sensor [6], which allows calculating dependence of the dielectric loss tangent on frequency of alternate field of the capacity sensor.

There was a program developed to calculate and visualize calculation results and dielectric loss tangent dependence on frequency of alternate field of the capacity sensor in the Microsoft Visual Studio environment, which has an ability to change source data.

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