COMPUTER SIMULATION OF TRACK MEMBRANES PORES OVERLAP

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1. INTRODUCTION

One of the main advantages of track membranes (TM) is their great selectivity defined by pores size uniformity and pores forms perfection [1,2]. Different pores should not be overlapped and should not form multiple holes for creating these membranes. It limits membranes porosity and, therefore, their penetrability. Process of track membranes making includes initial matrix exposed to high energy ions beam. It causes stochastic pores distribution and impossibility for regular pores structure creation. Thus overlaps of pores are inevitable and it is necessary to minimize formatting of these overlaps on the way of new type of track membranes development.

For the first time the problem of double and multiple cylindrical pores overlapping was studied in 1977 [3]. In 1979 similar problem for quadratic shape pores was solved [4]. In both works track membranes in which parallel pores system was made by exposing it to the parallel beam of ions was investigated.

Later it was shown in the Laboratory of Nuclear Reaction (JINR, Russia, Dubna) and then in [5], that the divergence of pores orientation allows to decrease pores overlap probability. It is true, because a pore overlapped by another one in one cross-section may be single in another cross-section. This pore do not decrease track membrane selectivity.

The double overlaps is the case when in any membrane cross-section there will be found a pore for a given pore, so as the distances between their axis are less then their diameters. These defects of double overlaps form slit pores which give rise to changes in selectivity for planar rigid particles only (for example disk form).

In the case of triple overlaps for one pore there will be found another two pores so as the conditions of double overlaps are satisfied for each pair. Thus, triple overlaps defects and multiple overlaps defects form pores with larger effective diameters.

Therefore both double overlaps pores probability and multiple (multiplicity equal and more than 3) overlaps pores probability are necessary for track membranes characterization.

2. TRACK MEMBRANE MODEL

For calculation of pores overlaps probability some membrane area with defined pores distribution in co-ordinates and directions is investigated. For each pore placed in this area a checking on double overlaps is made. If this condition is satisfied a checking on triple overlaps is accomplished also. This checking is made for defined number k of membrane cross-section. Apparently it takes the more of computer time the more number of pores n are taken into account. On the other hand decreasing of n makes model of pore system more regular and thus makes the model less correct.

To obtain correct results with acceptable time of calculation initial pores co-ordinates are defined with using Monte-Carlo method on large area. Then some part of this area is considered. This approach allows only the pores belonging to a considered area in some cross-section to be taken into account. Thus the number of pores in considered area is defined by Monte-Carlo method.

Really studied factor is the dependence of pores overlaps probability on the type of pores direction distribution. Tree types of distribution were investigated in present work:

1. All pores are disposed in one plane. Pores are distributed randomly uniformly in the interval ($-\alpha_0<\alpha_x<\alpha_0$) in one plane, and they are oriented normally to membrane surfaces in another plane ($\alpha_y = 0$).

2. Pores are disposed in two planes. Random-uniform distribution in intervals ($-\alpha_0<\alpha_x<\alpha_0$ and $-\alpha_0<\alpha_y<\alpha_0$).

3. Circle distribution: all the pores has the same angle to normal to membrane surface (azimuthal angle $v = \alpha_0$) and they are distributed randomly uniformly in the polar angle ($0<\phi<2\pi$). The advantage of the last case is equivalence of pores length and, consequently, the equivalence of pores hydrodynamics resistance.

3. PARAMETERS OF MODEL

Two dimensionless parameters are introduced: dimensionless diameter of pores χ:

$$\chi = D \cdot \sqrt{N} \qquad (1)$$

Where: N - pores surface density, D - their diameter;
and parameter characterizing pores axis tilt Δ. This parameter is defined as dimensionless projection of pore axis on membrane surface:

$$\Delta = 1 \cdot tg\alpha \cdot \sqrt{N} \qquad (2)$$

Where: l - membrane thickness, α - tilt angle of pore axis to membrane surface normal. Nomogram showing the relationship between parameter Δ, angle α and surface density of pores N for 10 μm thickness TM is given in Fig. 1.

Number of pores on investigated area was 100-1000, the co-ordinates of 10^3-10^4 pores were taken into account. The number of cross-sections, in which pores overlaps were tested, was k = 5 - 20 .

4. RESULTS AND DISCUSSION

Dependencies of double W_2 and triple W_3 overlapping probabilities upon membranes porosity P are shown in Fig. 2 and Fig. 3. The dependencies are presented in co-ordinates of nominal porosity P_n, effective porosity P_{eff}, and dimensionless diameter of pores χ. The nominal porosity is ratio of total pores area to membrane area, in this case pores overlaps are not taken into account. In opposite, real total pores area which are reduced because of their overlappings are used when effective porosity is found.

In the case of parallel pores the results of present investigation correspond well to the results given in [3,4,6].

Dependencies of $W_2(P)$ and $W_3(P)$ for different pores directional distributions are shown in Fig. 3. Even small angle distribution (Δ = 0.01) causes considerable decreasing of pores overlap probabilities. For example, double pores overlap probability equalsto 1% for $\chi \leq$ 0.10 (first method pores directions distribution, in one plane), for $\chi \leq 0.15$ (second variant, distribution in two planes) and for $\chi \leq 0.14$ (third method, circle distribution). It is necessary to note that the same value of probability W_2 for parallel pores system corresponds to $\chi \leq$ 0.05.

In the same situation triple pores overlap probability equals to 1% for χ 0.35 (method 1), for $\chi \leq 0.40$ (method 2), for $\chi \leq 0.39$ (method 3)and for $\chi \leq 0.29$

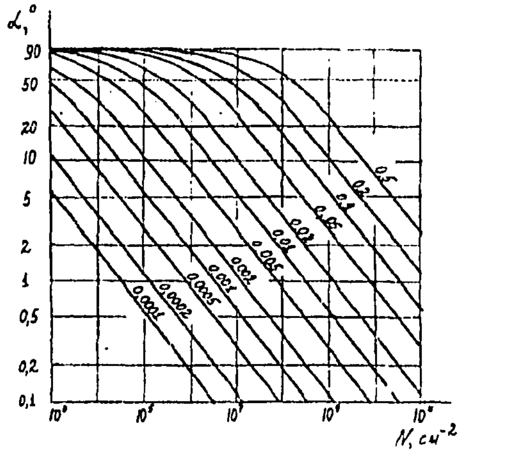

Fig. 1. Nomogram connecting α — angle of pores tilt with the normal, N — surface density of pores, and parameter Δ

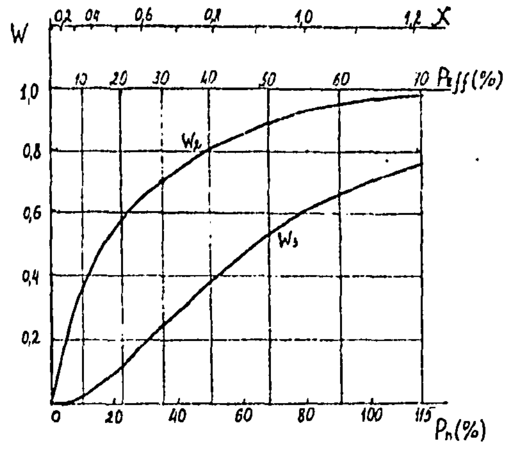

Fig. 2. Dependencies of double W2 and triple W3 overlapping probabilities upon nominal porosity Pn, effective porosity Peff, and dimensionless diameter of pores χ for track membrane with parallel pores

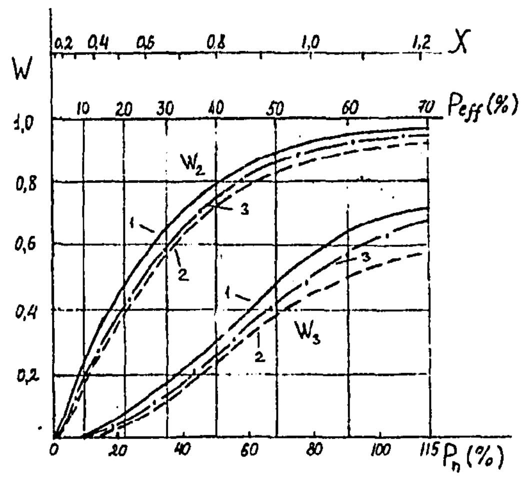

Fig. 3. Dependencies of double W_2 and triple W_3 overlapping probabilities upon nominal porosity P_3, effective porosity Peff, and dimensionless diameter of pores χ for track membrane with non-parallel pores. Parameter of pores axis tilt is D = 0.01

1 — random-uniform in one plane;

2 — random-uniform in two planes;

3 — random-uniform in a circle

(parallel pores).

For small porosity, pores overlap probabilities for the second and the third variants of pores angle distributions (in two planes) are approximately equivalent. The pores overlap probability for the first variant (distribution in one plane) is larger. In the case of large value of porosity the difference between the second and the third variants distributions appears.

For all considered variants the smaller values of pores overlap probabilities |are realised when random distribution of pores direction in two planes is used.

When large value of parameter characterizing pores axis tilt $\Delta = 0.1$ is used the probabilities are $W2 < 1\%$ for $\chi \leq 0.34$ (effective porosity $P_{eff.} = 9\%$) and $W3 < 1\%$ for $\chi \leq 0.65$ ($P_{eff.} = 28\%$).

5. CONCLUSION

Numerical model for estimation of the double pores overlaps (slit pores) probability and the triple pores overlaps probability was developed for the case of track membranes with non-parallel pores system.

Three methods of pores directions distribution were investigated:

1) random-uniform in one plane;
2) random-uniform in two planes;
3) random-uniform in a circle.

The last two methods are approximatly

equivalent, but give less values of pores overlaps probabilities in comparison with the first method.

Using large angles of pores axis with the normal gave the possibility to decrease pores overlaps probabilities. In particular, when $\Delta = 0.1$ is used the probabilities are $W_2 < 1\%$ for $\chi \leq 0.34$ (effective porosity $P_{eff} = 9\%$) and $W_3 < 1\%$ for $\chi \leq 0.65$ ($P_{eff.} = 28\%$).

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