Contemporary Engineering Sciences, Vol. 8, 2015, no. 9, 393 - 399
HIKARI Ltd, www.m-hikari.com
http://dx.doi.org/10.12988/ces.2015.5227

Model Research of Bitumen Composition with Nanoscale Structural Units

Evgeny Valeryevich Korolev

«Nanomaterials and Nanotechnology» Scientific and Educational Center
Moscow State University of Civil Engineering, Moscow, Russia

Roman Viktorovich Tarasov

Department of Quality management and technology of building production
«Penza State University of Architecture and Construction», Penza, Russia

Ludmila Viktorovna Makarova

Department of Quality management and technology of building production
«Penza State University of Architecture and Construction», Penza, Russia

Vladimir Alekseevich Smirnov

«Nanomaterials and Nanotechnology» Scientific and Educational Center
Moscow State University of Civil Engineering, Moscow, Russia

Abstract

On the basis of simulation principles the assessment of a scale range of structural units of the developed organic-mineral nano-dimensional modifier for asphalt concrete is carried out.

Keywords: model research, nano-dimensional modifier, dimensional effect, bitumen compositions

1 Introduction

The condition of a road network is an indicator of welfare and development of

national economy. Use of road-building materials with the raised indicators of operational properties is one of elements.

Traditional asphalt concrete at modern loads of an axis of vehicles and intensity of the movement on roads of the highest categories cannot provide durability of the top layers of pavings. Researches on search of the new materials allowing to raise significantly service life of asphalt concrete coverings are actual now.

Bitumens and compositions of bitumens and minerals are one of the most widespread materials that are used in road construction. Development of ways of improving quality and durability of bitumens and materials on their basis is the actual task allowing to solve a problem of reliability and durability of pavings' work. This task can be solved by modifying asphalt concrete mixes with various additives [1-6].

The researches conducted by the authors have showed that the best effect can be reached due to using an organic-mineral additive that based on slime and a poly-dimensional leaving (Butonal NS 198) which disperse phase contains particles of nanometer range.

Methods and simulars are used along with theoretical researches for justification and a choice of parameters of a product.

The description of the modeled system – bitumen composition – can represent itself as a set of the differential, algebraic, logical and difference equations that describe physical processes in structural elements (mutual movements, transfer of warmth and radiation).

Within the system analysis the general stages of mathematical modeling have been established. The iterative "triune" essence of process of modeling is expressed by the scheme "model – algorithm – program" [7].

Theoretical prerequisites have been formulated and practical questions of creation of composite materials [8] have been developed in the polystructural theory. The paradigm of modern science of construction materials – system and structural approach – has to become a methodological basis of modeling structural levels of asphalt concrete (fig. 1).

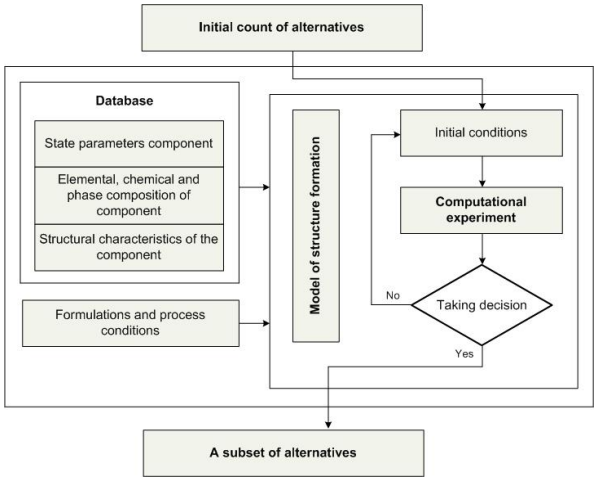

Figure 1:Basic data and algorithm of modeling

Cyclic three-stage process of modeling – from a model in terms of science of construction materials through calculating experiment to subject interpretation – at each structural level has to be added with necessary basic data (density and laws of distribution of disperse phases, parameters of technological modes of the consolidation, temporary dependences of dynamic viscosity of a binder) and settlement procedures (algorithms of numerical integration of systems of ordinary differential equations and equations in partial derivatives, algorithms of generation of selections of the pseudorandom numbers that subordinate to given one- and multidimensional distributions).

2 Experimental study

Let's use the principles of modeling for forming judgments about the dimensional range of structural units of the developed organic-mineral nano-dimensional modifier.

Let's go to dimensional features of disperse system. Dimensional effects have impact on rheological properties and characteristic values of superficial energy of the system. Importance of analysing dimensional effects is defined by that fact that known regularities of macroscopic properties' change are often failed for the systems that have been formed by small-sized structural units (the number of atoms of structural unit is comparable with the number of atoms on its surface). In practice the abnormal change of physical properties of finely dispersed materials is observed because of this reason.

By consideration of aggregate stability in disperse systems an expression has been offered [9]

$$\sigma_m = \gamma \frac{kT}{a^2} \tag{1}$$

where $\gamma \sim 10$ (is a dimensionless coefficient), k is a Boltzmann's constant, T is an absolute temperature, a is a size of a structural unit.

Expression (1) has dimension of a superficial tension and actually represents the characteristic energy of the thermal movement that have been referred to a surface of structural unit. It is noted [9] that spontaneous dispergating becomes possible (the heterogeneous system thermodynamic is steady) if (1) exceeds the superficial energy ($\sigma_{12} \sim 0{,}01...0{,}1$ J/m^2) in system (the power profit of a particle's participation in the thermal movement exceeds energy expenses at increase in the area of interphase border).

Existence in a numerator of expression (1) of the constant of Boltzmann predetermines an assessment for the size of structural unit – $a \sim 10^{-9}$ m. This quantity can be accepted as the lower bound defining the nano-dimensional modifier: dimensional effects are essential to the material that has been formed by such particles.

There is [10] dependence of viscosity of the system formed by monodisperse particles on the enclosed tension:

$$\eta = \eta_0 \frac{1}{3} \frac{z^3}{z \operatorname{ch} z - \operatorname{sh} z} = \frac{\kappa \tau k T}{\lambda a^2} \frac{z^3}{z \operatorname{ch} z - \operatorname{sh} z} \tag{2}$$

where $z = \dfrac{\lambda a^2 P}{kT}$, λ is an average distance between equilibrium provisions of structural (kinetic) unit, a is a size of structural unit, P is a mechanical tension, $\kappa \sim 1$, τ is an average time of being structural unit in balance position ($\tau \neq \tau(a)$).

The authors [10] have had interest in the dependence $\eta = \eta(P)$ of viscosity on mechanical tension. That is why the detailed analysis of behavior of the second multiplier is provided in the work [10]

$$\varphi(z) = \frac{z^3}{3(z \operatorname{ch} z - \operatorname{sh} z)} \tag{3}$$

in the right part (2). In range of definition the function (3) monotonously decreases, asymptotically coming nearer to zero. Thus the maximum value $\lim\limits_{z \to +0} \varphi(z) = 1$ – corresponding to the greatest viscosity of disperse system – is reached in a stationary point (3):

$$\lim_{z \to +0} \frac{d\varphi}{dz} = \frac{1}{3} \lim_{z \to +0} \frac{z^2 \left(3z \operatorname{ch} z - 3\operatorname{sh} z - z^2 \operatorname{sh} z\right)}{\left(z \operatorname{ch} z - \operatorname{sh} z\right)^2} = 0 \tag{4}$$

The multiplier $\eta_0 = \dfrac{3\kappa \tau k T}{\lambda a^2}$ besides the multiplier (3) has impact on dependence $\eta = \eta(a)$ of viscosity on the size of structural unit. Like the dependence (3), the dependence

$$\eta(a) = \frac{\tau \lambda^2 a^4 P^3}{(kT)^2} \left(\frac{\lambda a^2 P}{kT} \operatorname{ch} \frac{\lambda a^2 P}{kT} - \operatorname{sh} \frac{\lambda a^2 P}{kT} \right)^{-1} \tag{5}$$

monotonously decreases, but at $a \to +0$ it suffers a rupture of the II sort:

$$\lim_{a \to +0} \eta(a) = +\infty \tag{6}$$

$$\lim_{a \to +0} \frac{\partial \eta}{\partial a} = \lim_{a \to +0} \frac{2\tau \lambda^2 a^3 P^3 \left(2kT\lambda a^2 P \operatorname{ch} \dfrac{\lambda a^2 P}{kT} - \left(2k^2 T^2 + \lambda^2 a^4 P^2\right) \operatorname{sh} \dfrac{\lambda a^2 P}{kT} \right)}{k^2 T^2 \left(\lambda a^2 P \operatorname{ch} \dfrac{\lambda a^2 P}{kT} - kT \operatorname{sh} \dfrac{\lambda a^2 P}{kT} \right)} = -\infty \tag{7}$$

Correlations (6) and (7) testifies that dependence (2) can be a model of rheological properties of disperse system, only since some characteristic size of particles of a disperse phase; at $a \to +\infty$ a small deviation Δa of the size of particles complies with an essential change of viscosity of system.

As the characteristic size it is natural to accept the value corresponding to a point of the greatest curvature (2):

$$k = \zeta \left| \frac{\partial^2 \eta}{\partial a^2} \right| \left(1 + \left(\zeta \frac{\partial \eta}{\partial a} \right)^2 \right)^{-\frac{3}{2}} \tag{8}$$

where ζ is a normalizing multiplier (after multiplication on which, in particular, the second item in brackets becomes dimensionless) that is equal

$$\zeta = \left| \left\langle \frac{\partial \eta}{\partial a} \right\rangle \right|^{-1} = \left| \frac{1}{L} \int_{a_0}^{a_0+L} \frac{\partial \eta}{\partial a} da \right|^{-1} = \left| \frac{L}{\eta(a_0 + L) - \eta(a_0)} \right| \tag{9}$$

3 Results and discussion

The sign of the normalizing multiplier is arbitrary and has no impact on value (8). For the chosen parameters of system the normalizing multiplier is equal

$$\zeta \approx 2{,}8 \cdot 10^{-5} \tag{10}$$

The dependence (8) constructed with (10) is represented in the figure 2.

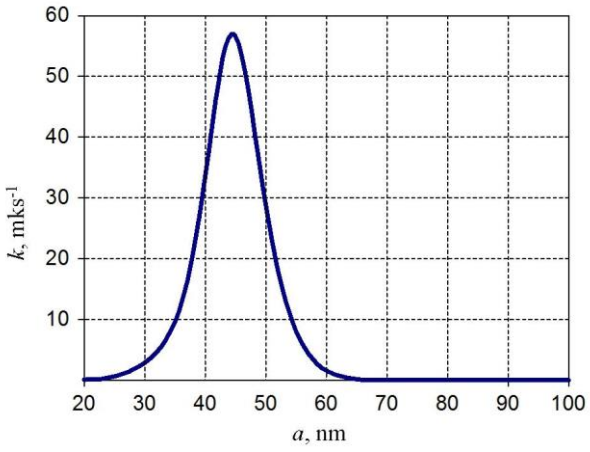

Figure 2: Curvature's coefficient of dependence of system's viscosity on the size of particles

The abscissa of a point of an extremum (8) can be found numerically:

$$a_{k,\max} \sim 50 \text{ nm} \tag{11}$$

4 Conclusion

Consequently, the range of sizes of structural units that complies with manifestation of dimensional effects in disperse system appears in equal $1 \sim a \sim 50$ nm. This range corresponds to using nanodispersed materials that has to provide an increase of known effects' quantity.

It should be noted that achievement of characteristic parameters can be reached not only with dispergating of a phase of the modifier (this is connected not only with considerable expenses of energy, but also with accompanying toxicological and technological problems of technology), but also organizing on a surface of a mineral phase of the microscopic sizes a layer of the modifier with given sizes.

References

[1] S. K. Illiopolov, Organic binders for road construction, Rostov-on-Don.: South. 2003. 428 p.

[2] A. B. Solomentsev, Classification and nomenclature of modifying additives for bitumen, Science and technology road, 2008, no. 1, pp. 14-16.

[3] V.V. Leonenko, G.A. Safonov, Some aspects of bitumen modification polymeric materials, Chemistry and technology of fuels and oils, 2001, no. 5, pp. 43-45.

[4] L.M. Hochman, O. Babak, T. Starks, The use of polymer-bitumen binders in road construction, Building machinery and technology, 2001, no. 5, pp. 72-76.

[5] S.V. Cats, G.V. Timofeev, S.V. Livanov and others, Road bitumen with modifying additives, Chemistry and technology of fuels and oils, 2003, no. 3, pp. 52-53.

[6] D.A. Ayupov, A.V. Murafa, Y.N. Khakimullin, V.G. Khozin, Nanomodified bituminous binders for asphalt concrete, Building materials, 2010, no. 10, pp. 34-35.

[7] A.A. Samarsky, A.P. Mikhailov, Mathematical modeling: the ideas, Methods, Examples, Fizmatlit, 2001, 320 p.

[8] V.I. Solomatov, Development polystructural theory of composite building materials, Proceedings of the jubilee conference, Engineering, 2001, pp. 56-66.

[9] P. A. Rebinder, Physical and chemical mechanics of dispersed structures, Physico-chemical mechanics of dispersed structures, Collection of articles colloid journal, 1966, pp. 3-16.

[10] G.M. Bartenev and others, The theory of the rheological properties of disperse systems, Physico-chemical mechanics of dispersed structures, Collection of articles colloid journal, 1966, pp 371-377.

Received: February 17, 2015; Published: March 24, 2015