ABSTRACT

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THE BIOMASS USE TO OBTAIN HIGH-PURITY CARBONACEOUS MATERIALS

The current publication considers the main criteria for biomass utilization instead of combustible fossils for the purpose of obtaining biofuels. The advantages of the biomass in comparison with the traditional non-renewable precursor materials have been shown. The results of the properties of walnut shell studies after conventional pyrolysis at the temperatures from 300 °C to 1000 °C are presented. Additionally, have been highlighted the peculiarities of the oxidative pyrolysis process as the first stage of a two stage technology for the production of high-purity carbonaceous materials from biomass. The possibility of obtaining nanomaterials from the biomass has been established, as instance can serve the hazelnut shell. The obtained results allow implementing the production technology for high-purity carbonaceous materials on an industrial scale.

Key words: biomass, pyrolysis, oxidative pyrolysis, graphitisation, high-purity carbonaceous materials, nanomaterials.

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1.3 METHODS VIRTUALIZATION IN CHEMMOTOLOGY RESEARCHES

Alexandr Moiseev, Alexandr Oreshencov, Nikolay Grishin

The usual purpose of mathematical modelling of technological processes is forecasting course of these processes in various conditions, including not covered by natural experiment. Two basic demands are usually made to similar model – universality and adequacy. Universality allows to use model in a wide range of external conditions, including in structure of models of higher level. Adequacy provides conformity of model to concrete conditions of carrying out of experiment. The specified requirements define typical structure of model. In a basis of last the base model describing process in general is pawned as a skeleton. Adequacy thus is provided during parametrization of model by results of comparison with calibration experiments. It causes the basic requirements to the interface of model – along with the inputs defining conditions of carrying out of numerical experiment, it includes preliminary adjusted calibration parameters. Completeness and consistency of system of these parameters define adequacy of model and are provided during its identification.

Being applied discipline, chemmotology assumes essential domination of experimental methods of the research sold including in the form of qualifying tests of object. At the same time, as it was specified above, construction of base model covering systems or process is carried out within the limits of theoretical, mainly physical and chemical, researches. In turn adequate adjustment of these models is carried out by results of qualifying tests. The main feature of the last is that their basic method is laboratory research of object which basically nothing will differ from maintained [1]. Laboratory installation in these conditions can be considered as physical model of the system covering object. In this sense qualifying tests are a special case of wider concept semi-scale experiment within the limits of which the covering model or its part can be realized as mathematical. In these conditions adequate mathematical model of the system covering object, it is possible to interpret as a certain virtual reality, and numerical experiment in structure of semi-natural – as virtual qualification. Thus the natural experiments spent within the limits of usual qualifying tests, can act as means of identification of created mathematical models [2, 3].

Statement of a question on mathematical modelling any object includes conditionally three stages: *model-algorithm-program* (Fig. 1) [4].

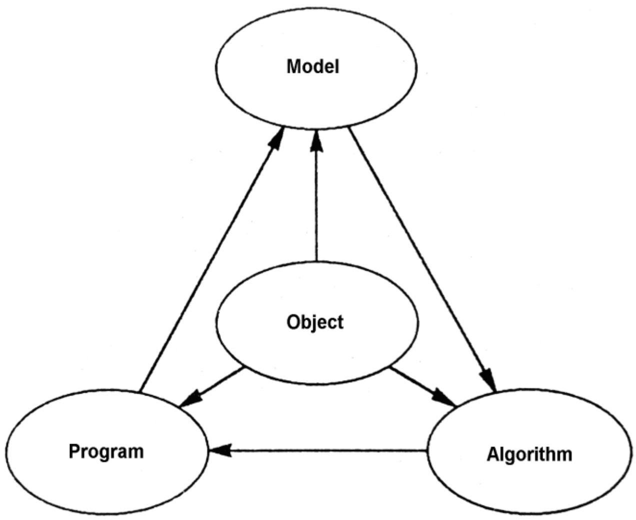

Fig. 1. Scheme of mathematical modeling

At the first stage the «equivalent» of object reflecting in the mathematical form, the major it properties-laws to which it submits, the communications inherent in parts making it, etc. Mathematical model (or its fragments) are researched by theoretical methods that allows to receive the important preliminary knowledge of object is under construction.

The Second stage – development of algorithm for realization of model on a computer. The model is represented in the form of, convenient for application of numerical methods, the sequence of computing and logic operations is defined, which need to be made to find required sizes with the set accuracy. Computing algorithms should not deform the basic properties of model and, hence, initial object to be economic and adapting to features of solved problems and used computers.

At the third stage the programs «translating» model and algorithm on language accessible to a computer are created. Demands of profitability and adaptibility also are made to them. They can be named a «electronic» equivalent of studied object, already suitable for direct test for «experimental installation» – a computer.

Having created a triad «model-algorithm-program», the researcher receives the universal, flexible and inexpensive tool which in the beginning is debugged, tested in «trial» computing experiments in hands. After adequacy of a triad to initial object is certified, with model the various and detailed «experiences», demanded qualitative demanded qualitative and quantitative properties and characteristics of object are spent. Process of modelling is accompanied by improvement and specification, as required, all parts of a triad.

The mathematical model of object is under construction on the basis of its description and can cooperate with the regular software in case of controllability of object. In turn, the mathematical model of covering system is under construction on the basis of its description and can realize the functions which are not sold by physical model. Virtual qualification is carried out during numerical experiment with mathematical models of object and system.

Thus two primary goals are solved: comparative identification of mathematical models in the conditions provided by physical model – laboratory installation; preliminary debugging of the regular software in case of controllability of object.

Example of application of such common approach is modeling internal combustion engine (ICE) displayed in works [5, 6].

First of them is devoted to creation of the simplified mathematical model ICE intended for modelling of influence chemmotology of processes on dynamics of the engine, its efficiency and lubricant ability of used oils. The model allows to spend the numerical experiments reproducing separate stages of bench tests. In the long term, as it is supposed, it will allow to replace carrying out of the same natural experiments by their numerical analogues that will provide economy of time and means.

For identification of model results of qualifying tests on installation IM-1, spent according to GOST 20303 were used. Therefore it is considered, that the virtual engine in structure of model is loaded on the simulator of the asynchronous machine, and losses on friction in the engine are described depending on deterioration cylinder-piston group (CPG) and a degree of its pollution within the limits of Hersey-Stribeck curve. These factors influence factor of friction of pair the piston – the cylinder, and also on size of a backlash between the piston and a wall of the cylinder and, hence, on size of the mixed friction.

The simplified model is based on the ratio of balance and engine load, loaded onto asynchronous machine in generating mode. In the normalized form the equation of balance (1) looks like:

$$T\frac{du}{td} = \pi\sqrt{u} - \pi_{fr}\sqrt{u} - n_0\left(\sqrt{u} - 1\right)\max(1, \sqrt{u}) \qquad (1)$$

where $u = \left(\frac{\omega}{\omega_0}\right)^2$ – normalized a square of frequency; $\pi = \frac{p}{p_0}$ – normalized pressure in the cylinder; $\pi_{fr} = \frac{p_{fr}}{p_0}$ – normalized a pressure of friction; $T = \frac{J\omega_0^2}{2N_0}$ – characteristic time of dispersal, where J – the moment of inertia of a crank; ω_0 – current and nominal cyclic frequency accordingly; p – pressure in the cylinder, Pa; p_{fr} – a pressure of friction, Pa.

The General scheme of the model is shown in Fig. 2. In essence, it is the scheme of realization of the equation solution (1) with an opportunity of a variation of power of the engine and synchronous frequency.

The basic feature of model is that for the description of dynamics of pressure in the cylinder the display diagram of the engine is used. Last represents dependence of pressure in the engine from displacement of the piston on various steps of the engine. To these steps there correspond various ranges of a corner of turn of a crank (a cranked shaft) which is an additional input of the display diagram. In model the display diagram is realized in the form of linear interpolators pressure depending on position of the piston, corresponding various steps of the engine and chosen on size of a corner of turn of a crank. As a rule, the display diagram corresponds to rated power of the engine.

To account for possible nenominalizate used adjustable multiplicative factor g, making sense degrees of opening of a virtual throttle of submission is used. This factor is formed by the simulator of submission which basis is PID a regulator of power.

The rated load n_l of the engine is related to the nominal n_0 ratio $n_l = n_0 max(1, \sqrt{u})(\sqrt{u} - 1)$. In turn, the rated load is formed by the simulator of a dynamic brake which basis is the regulator of synchronous frequency. Normalized power of losses is defined normalized by the moment of frictionπ_{fr}.

The further development of the simplified model was carried out in a direction of perfection of imitation of processes in the engine. In work [6] the multipurpose model of an internal combustion engine uniting submodels of the basic subsystems of the engine. These include: model of the internal mixture formation, defining characteristics of a gas mixture; models of a thermal emission and gas exchange in the cylinder, simulating clock processes in the engine; model of crank mechanism model, connecting processes in the engine with external influences.

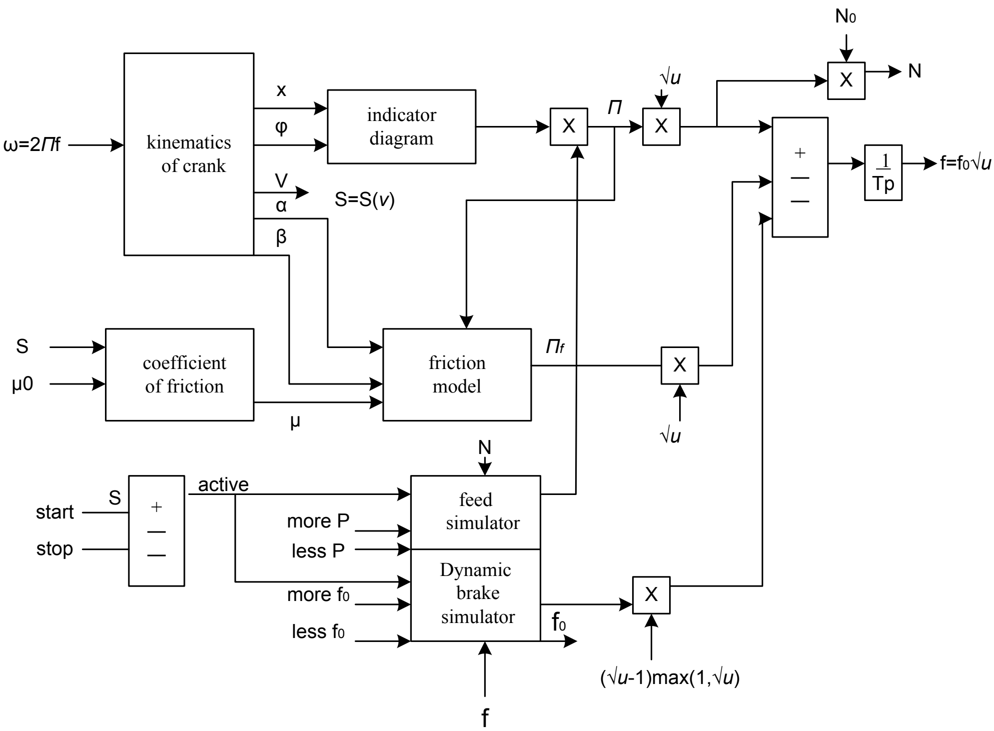

Fig. 2. General control scheme of the engine model

The General scheme of the model is shown on Fig 3. Its inputs are positions of an air throttle, fuel dispenser, and also transfer number of the reducer connecting a running axis with cranked shaft. These inputs naturally interpret controls the engine.

The model also can include the auxiliary submodels intended, in particular, for imitation of structure of an exhaust and cooling of the engine. First of them is based on simplification of system of the kinetic equations of chain process in the quasi-stationary approximation. It allows to simulate dynamics of structure of an exhaust in the form of time dependences of molar fractions its components. The developed technique can be used at forecasting structure of an exhaust for different chain processes with a specified sequence of paired reactions.

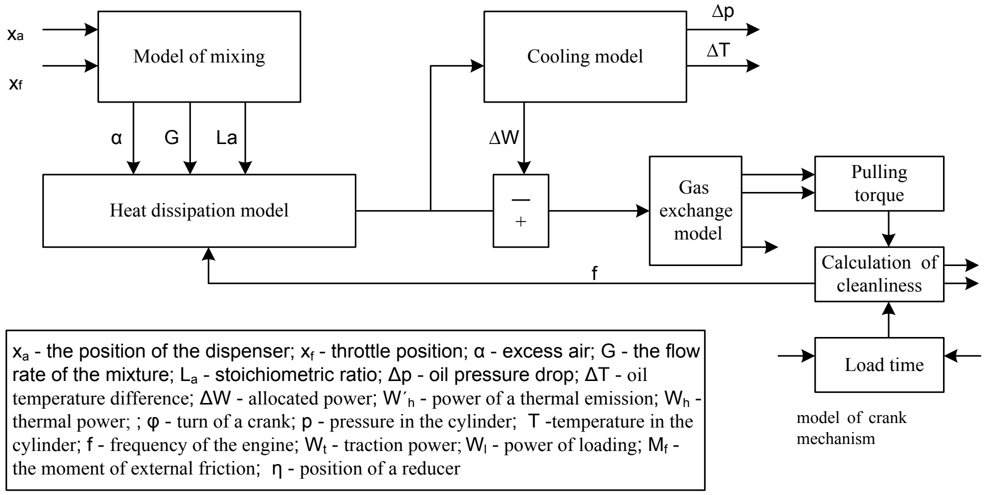

Fig. 3. Scheme of the multi-function models

The model of cooling is based on the developed design procedure of hydraulic circuits. In this calculation linear regulators are used as numerical nonlinear equations Kirchhoff for balance of charges and pressure differences. The given technique is less labour-consuming, than traditionally used, and применима at квазистационарных changes of parameters of a hydraulic circuit. The engine in this model is interpreted as a heat exchanger.

Simulated dynamics of pressure and temperatures of gas in the cylinder according to phases of gas exchange is displayed on Fig. 4.

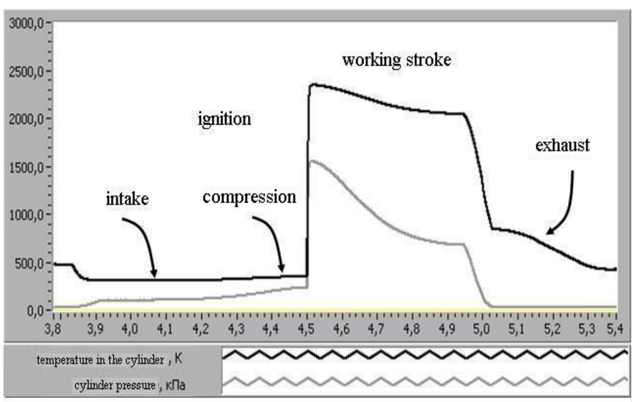

Fig. 4. Cycle without self-ignition

The cycle with spontaneous ignition is presented on Fig. 5. The constructed model was used also for imitation of the basic processes in the engine.

The results of simulation of step loading of the engine are shown in Fig. 6 and 7. Relative loading thus increased with some temporary delay concerning submission.

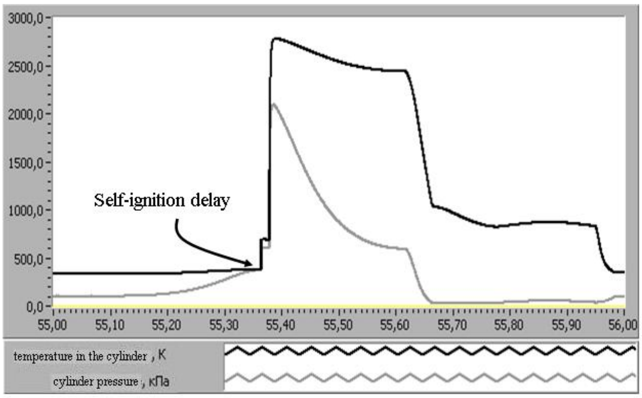

Fig. 5. Self-ignition cycle

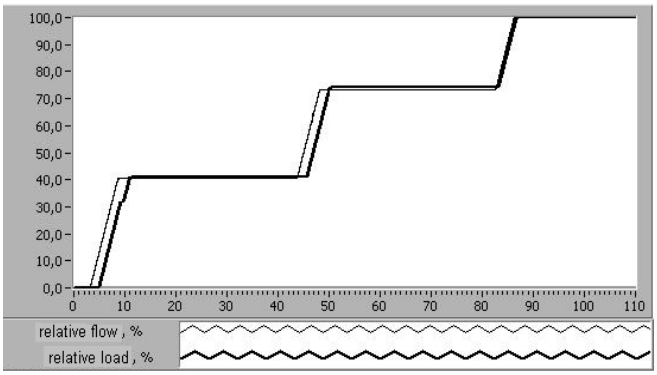

Fig. 6. Stepwise engine loading (feed, load)

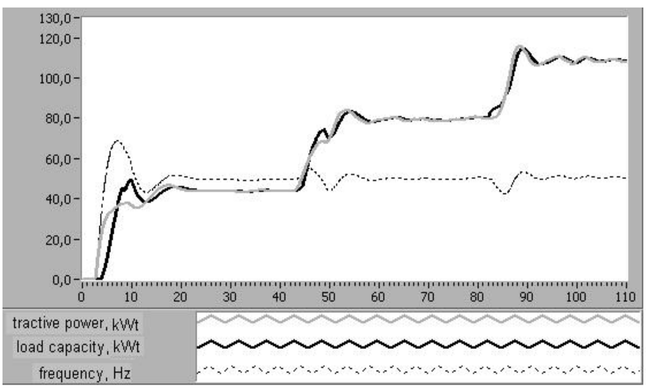

Fig. 7. Stepwise loading of the engine (traction and load power)

During regulation simulated frequency of the engine was stabilized at a nominal level, and traction and loading powers were leveled. Thus, the effect self-regulation of frequency of the engine has been shown at change of loading. Results of compulsory regulation of frequency of the engine are displayed on Fig. 8 and 9.

Installation of regulation was nominal frequency of the engine, and an output – size of relative submission. In an initial condition the size of relative loading was zero. After inclusion of a regulator the size of installation on frequency increased up to nominal frequency. The additional increase in loading led to corresponding increase in submission under action of a regulator. Current frequency thus was stabilized at a nominal level, and traction and loading powers were leveled. The qualitative analysis of simulated dynamics shows, that as a whole the model adequately displays processes in the engine and can be used to study the influence of petroleum products characteristics on the processes in the cylinder.

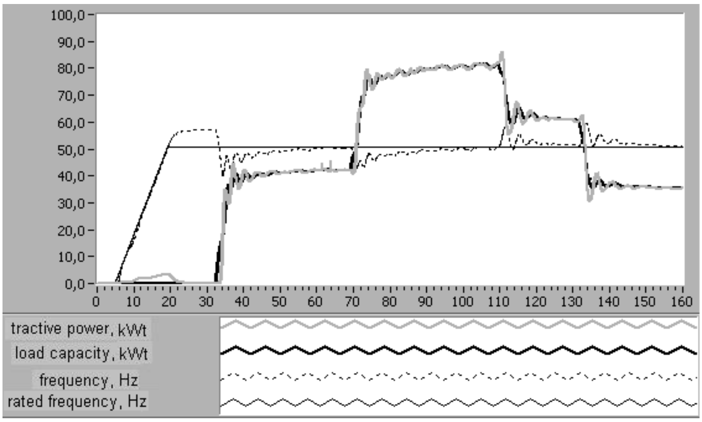

Fig. 8. Frequency control of motor (tractive and load power)

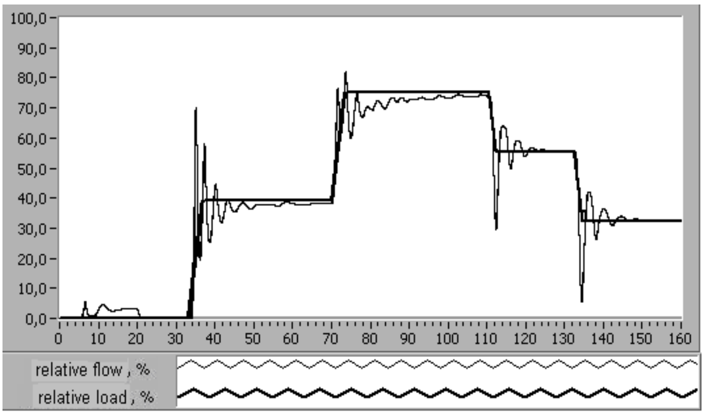

Fig. 9. Engine frequency control (feed, load)

Prominent aspect of application of virtual qualification is extrapolation of laboratory results on regular conditions of operation of researched object. As an example of such extrapolation is the prediction of volumetric wear of the pump plunger head taking into account the anti-wear properties of the lubricating fuel [7–10].

As criterion of similarity between laboratory installation and researched plunger the criterion of volumetric deterioration displayed on Fig. 10 has been chosen. Its physical sense – the relation of an impulse износного a material to an impulse of force of friction.

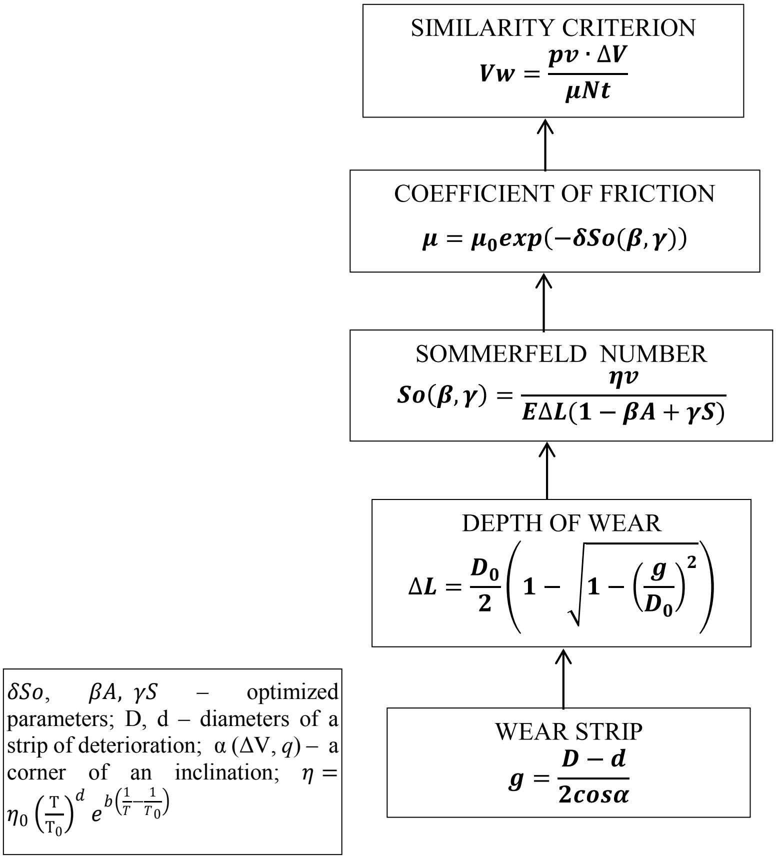

Fig. 10. Criterion of volume of wear

The criterion includes density wear material, speed of sliding and normal pressure in frictional contact, and also the duration of wear. The factor of boundary friction is defined by factor of dry friction and Sommerfeld number. It was assumed that the Sommerfeld number in addition to viscosity, speeds of sliding and hardness depends also from A the greasing environment and percentage of sulfur S in it's.

The size of a backlash in frictional contact was accepted to equal depth of deterioration and was defined by diameter of a spherical measuring element and size of a strip of deterioration. Temperature dependence of viscosity according accordance with the modified Andrade's formula.

The volumetric wear and the wear strip were determined by the maximum and minimum diameters of the wear strip of the measuring element, observable in experiment, and also a corner of an inclination of an axis of this element to a plane of frictional contact. Parameters of model were factor at Sommerfeld number in expression for factor of boundary friction, and also factors at acidity and percentage of sulfur.

The scheme of optimal parameterization of this model is shown on Fig. 11.

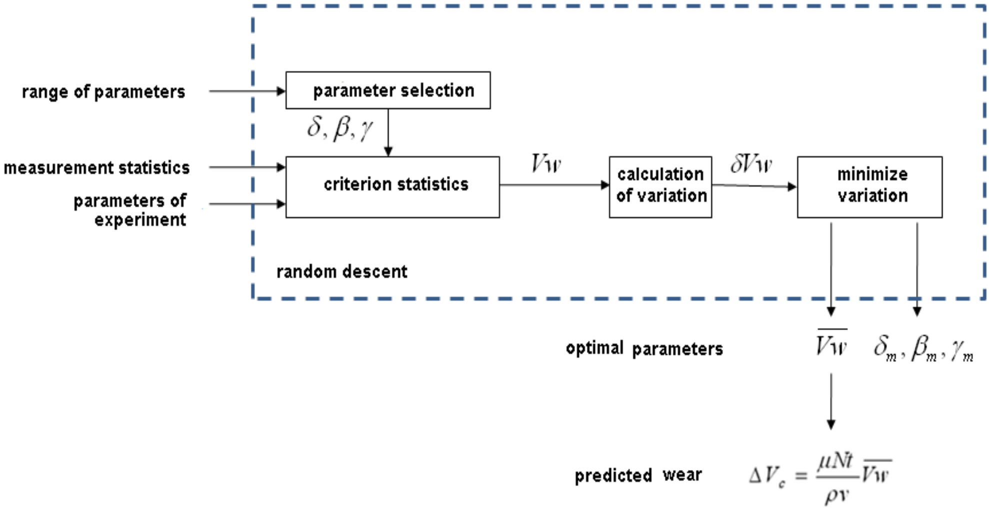

Fig. 11. Optimal parameterization

The first stage of parametrization included formation of statistics of criterion of similarity according to measurements and to the chosen values of parameters. On measurements and the chosen parameters the criterion of volumetric deterioration paid off. Thus the received statistics was used for calculation of a variation of criterion δVw for the chosen values of parameters. Optimum parameters got out a method of casual descent of a condition of a minimality of the specified variation. The size of the average criterion of similarity $\overline{Vw}$ on which predicted wear.

By parameterized model forecasting deterioration on the basis of equality of predicted and settlement deterioration was carried out. This equality was interpreted as the equation concerning depth and strips of deterioration. It was solved by minimization of the module of a mismatch between settlement and predicted deterioration for various duration according to Fig. 12.

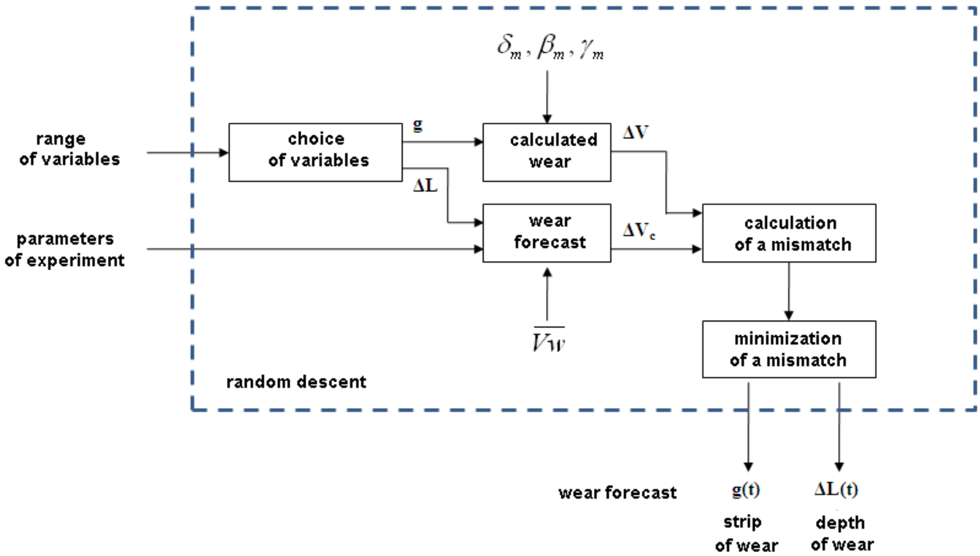

Fig. 12. Wear prediction

Result of this minimization which are carried out by a method of casual descent, temporary dependences of depth and the strips of deterioration interpreted as forecasts of deterioration are. Thus, the developed model of deterioration can be used for formation of qualifying norms on the basis of operational restrictions on the depth wear, corresponding specified duration of last.

Carrying out of tests is preceded with a preliminary choice of their extreme conditions. Parametrization criteria model models by results of qualifying tests in the given conditions allows to lead forecasting of frictional deterioration which results can be interpreted as the guaranteed norms of deterioration.

Traditional qualifying tests are interpreted as a special case semi-scale experiment in which laboratory installation plays a role of physical model of the system including researched object. Virtualization represents transition from physical to mathematical models of system and object and supposes virtual qualification, that is realization of qualifying tests in the form of numerical experiment. Obvious advantage of virtual qualification is restriction of quantity of the natural experiments used only for calibration of mathematical models, and, hence, reduction in expenses for their carrying out.

Virtualization allows to carry out extrapolation of results of qualifying tests for regular conditions of operation. Efficiency virtualization is shown on examples of optimization of mathematical models, perfection of qualifying experiments and forecasting of their results.

Simplified model internal combustion engine is intended for modelling influence chemmotology and tribological factors on dynamics of the engine and its efficiency. It was based on a ratio for balance of power of the engine and its loading created by asynchronous machine in a generating mode. Its feature is that for imitation of dynamics of pressure in the cylinder the display diagram of the engine was used. The account of friction within the limits of model was based on approximation of Hersey-Stribeck curve and its use for calculation of factor of the mixed friction depending on Sommerfeld number. Input in structure of this number of the factors considering deterioration and pollution of pair the piston – the cylinder, has allowed to carry out modelling of these processes and qualitatively to estimate their influence on dynamics of lubricant ability and efficiency of the engine.

On the basis of the analysis anti-wear properties of greasing fuel the model of the volumetric deterioration intended for forecasting of size of last under set conditions. Optimum parametrization criterion model was based on interpretation of criterion of wear as an invariant with the minimal variation. Thus the ratio, connecting criterion of volumetric wear with its average value, was interpreted as the equation of communication between size of wear and factors influencing it. It has allowed to use the given equation for forecasting size of deterioration in the set conditions and for various terms of operation. Synthesized thus criterion model was offered for using for forecasting wear in extreme conditions and formations of corresponding qualifying specifications.

РЕФЕРАТ

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МЕТОДИ ВІРТУАЛІЗАЦІЇ У ХІММОТОЛОГІЧНИХ ДОСЛІДЖЕННЯХ

Віртуалізація в хіммотології дозволяє здійснити екстраполяцію лабораторних результатів на штатні умови експлуатації, а також зворотний перерахунок цих умов в адекватні параметри кваліфікаційного експерименту. Ефективність віртуалізації продемонстрована на прикладах оптимізації математичних моделей, вдосконалення кваліфікаційних експериментів і прогнозування їх результатів.

Ключові слова: кваліфікаційні випробування, напівнатурний експеримент, чисельний експеримент, фізична модель, віртуалізація, віртуальна кваліфікація, критеріальна модель, крива Герсі-Штрібека, число Зоммерфельда, протизносні властивості, ідентифікація.

РЕФЕРАТ

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МЕТОДЫ ВИРТУАЛИЗАЦИИ В ХИММОТОЛОГИЧЕСКИХ ИССЛЕДОВАНИЯХ

Виртуализация в химмотологи позволяет осуществить экстраполяцию лабораторных результатов на штатные условия эксплуатации, а также обратный пересчет этих условий в адекватные параметры квалификационного эксперимента. Эффективность виртуализации продемонстрирована на примерах оптимизации математических моделей, совершенствования квалификационных экспериментов и прогнозирования их результатов.

Ключевые слова: квалификационные испытания, полунатурный эксперимент, численный эксперимент, физическая модель, виртуализация, виртуальная квалификация, критериальная модель, кривая Герси–Штрибека, число Зоммерфельда, противоизносные свойства, идентификация.

ABSTRACT

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METHODS VIRTUALIZATION IN CHEMMOTOLOGY RESEARCHES

Virtualization in chemmotology allows to carry out extrapolation of laboratory results on regular conditions of operation, and also return recalculation of these conditions in adequate parameters of qualifying experiment. Efficiency virtualization is shown on examples of optimization of mathematical models, perfection of qualifying experiments and forecasting of their results.

Key words: qualifying tests, semi-scale experiment, numerical experiment, physical model, virtualization, virtual qualification, criterion model, Hersey-Stribeck curve, Sommerfeld number, anti-wear properties, identification.

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