Computer System of Visual Modeling in Design and Research of Processes of Carbon Nanocluster Compounds Synthesis

Dmitriy Petrov, Tamara Chistyakova, and Nikolay Charykov

Abstract The chapter presents a flexible, customizable to the material and technical base of an industrial enterprise, a multi-component man-machine visual simulation system of potentially dangerous, complex in the control of production processes for the synthesis of carbon nanocluster compounds with the prediction of their qualitative characteristics in simulated conditions close to real ones. The task of visual modeling in the design and study of processes of synthesis of carbon nanocluster compounds is formulated. The architecture of the visual modeling system is presented, which includes a database of characteristics of design and control objects, a database of rules and restrictions for the layout of reactor sections and assembly of extraction plants, a database of situational knowledge to support the training of control and production personnel, mathematical support for calculating the qualitative characteristics of the synthesis processes of carbon nanocluster compounds, software including dialog interfaces of the administrator, immersive interfaces of the designer and researcher. The results of functional testing and pilot operation of the visual modeling system in the tasks of decision support in the design and research of technological processes on the example of the model of the reactor section of the industrial enterprise and fullerene C_{60} are presented.

Keywords Visual modeling · Manufacturing process · Design and research · Immersive space · Carbon nanocluster compounds

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1 Introduction

One of the popular trends of the fourth industrial revolution is the development and introduction of digital twins that contribute to the rapid growth of digitalization of production processes in order to optimize their economic and quality indicators, including during the reconfiguration of production lines, as well as increase production safety [1, 2].

The modern market of high-tech interactive tools, graphics libraries, high-performance technical support, and progressive programming languages contributes to the rapid development of the cyber physics system industry [3, 4, 5].

The need for digital transformation and intellectualization of industry is justified by its complexity associated with increased requirements for quality and competitiveness of products. Innovative approaches to the integrated assessment of enterprise activity are being developed [6], as well as methods to support decision-making in industrial cyber-physical systems [7] and flexible product lifecycle control [8]. Construction industry [9], transport sector [10], oil industry [11], high-tech production facilities [12] are characterized by rapid development of intelligent computer simulators [13–16]. One of the most important tasks of computer simulators is ensuring the quality of remote training of personnel, on-the-job [17].

This chapter describes the components of a man-machine visual simulation system as a means to improve quality and reduce the risks of complex, potentially dangerous production through human synergy, as a decision-maker in design and control, with the proposed computer system.

2 Design Object Description

2.1 Historical Information and Market Analysis of Carbon Nano Industry

With the hypothesis of the existence of a stable allotropic carbon modification, physicist E. Osawa (Japan) in 1970 predicted the discovery of closed carbon clusters experimentally obtained in 1985 by scientists Richard Smalley and Robert Kerl (USA) and Harold Croto (UK) with laser irradiation of graphite [18]. Open compounds are called "fullerenes" by the name of the American architect Buckminster Fuller, designing the domes of his buildings with pentagons and hexagons similar in structure to fullerenes molecules.

Currently, the carbon nano industry accounts for 10% of the total nanomaterials market $\approx$ \$100 billion. The main interest in the development of the carbon nano-industry is associated with the high demand for fullerenes and their derivatives both for the purpose of studying their unique structures and for the synthesis of materials with fundamentally new physical and chemical properties. Fullerenes can be used as modifiers to create materials with specified parameters. Regional exporters offer fullerene products of high purity C_{60} at a price of \$86 per gram, C_{70} at a price of \$223 per gram, which is several times more expensive than the gold of a similar mass.

2.2 The Life Cycle of Carbon Nanocluster Compounds

Synthesis of carbon nanocluster compounds belongs to the class of energy-intensive multistage processes, which have special requirements for reactor sites and extraction sites of target components. The life cycle phases of fullerene products covered by the proposed computer visual simulation system are shown in Fig. 1.

The symbols adopted in Fig. 1 are described in detail in item 2.3 Formalized description.

At the stage of the design of production premises, special attention is paid to the presence of a high-voltage network, water main, ventilation system, fire, and explosion safety of the room.

The most productive method of synthesis of carbon nanocluster compounds is considered an electric arc. Graphite electrodes are burned in a plasma reactor in the medium of inert gas of low pressure. Obtained nano dispersed powder (fullerene carbon soot) by the flow of circulating inert gas is taken from reactor to soot collector [19].

Complexity in process control is due to thermodynamic instability of plasma and increased risk of reactor depressurization. The synthesis of fullerene carbon soot is potentially dangerous to humans because the process takes place at a high temperature in a cooled reactor filled with a harmful inert gas. From the circulation circuit of inert gas during its depressurization, emissions of nano dispersed fullerene carbon soot, which causes damage to respiratory organs, are possible.

Fullerene soot is a carrier of the end product, mainly fullerenes C_{60} and C_{70}. At the next stage, the end product is extracted from fullerene carbon soot, to which production is tuned [20]. When extracting the desired product, rotary vacuum evaporators or Soxhlet extractors are used. Complex combined devices combining extraction, evaporation, and drying can be used.

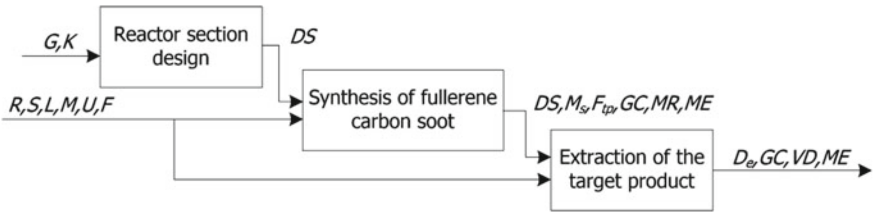

Fig. 1 Fullerene product lifecycle stages

2.3 Formalized Description

We introduce a formalized description of the design and modeling of the process of synthesis of carbon nanocluster structures in the following vector form. Y=f(X, U, F), $X\{G,K,R,S,L,M\}$, $U\{U_A, L_E, G_C, G_G, \upsilon_M, W_H, \tau_1, \tau_2\}$, $F\{\xi_1,\xi_2,\xi_3\}$, Y\{DS,Q\}. X—an initial data vector including components: G—regulatory documents in the field of construction, fire safety, ergonomics and labor protection of personnel and drawings of production facilities (premises and equipment), $K\{H,E\}$—characteristics of production facilities, where H—room characteristics, E—characteristics of the equipment. $H\{Ph_1^s, Ph_2^s, \ldots, Ph_{cps}^s; Ph_1^m, Ph_2^m, \ldots, Ph_{cpm}^m, H_h, W_h, L_h\}$, where Ph_i^s—singlet characteristic (voltage, type of current (direct or alternating), water pressure in the line, etc.), $i \in [1;cps]$, cps—number of singlet characteristics of the room. Ph_j^m – integral characteristic, $j \in [1;cpm]$, cpm—number of integral characteristics of the room. H_h, W_h, L_h—height, width, and length of the room. $E\{E_1,E_2,..,E_{ce}\}$—equipment in the room where $E_p\{PE_1,PE_2,\ldots,PE_{cpe},H_e,W_e,L_e\}$—characteristics of the p-th equipment, $p \in [1;ce]$, ce—number of equipment in the room, cpe—number of characteristics of p-th equipment, H_e, W_e, L_e—height, width, and length of the equipment. $R\{R_1,R_2,R_3,R_4,R_5\}$—system of design and operational rules and requirements. $R_1\{RCM_1,RCM_2,\ldots,RCM_{cpm}\}$, $R_2\{\{\mathrm{D}(E_1,E_2),\mathrm{D}(E_3,E_2),\ldots,\mathrm{D}(E_{ce},E_2),\mathrm{D}(H,E_2)\},\ldots,\{D(E_1,E_{ce}),\mathrm{D}(E_2,E_{ce}),\ldots,\mathrm{D}(E_{ce},E_{ce\text{-}1}),\mathrm{D}(H,E_{ce})\},\{\mathrm{D}(E_1,H),\mathrm{D}(E_2,H),\ldots,\mathrm{D}(E_{ce},H)\}\}$ $R_3\{U_A^{\min}, U_A^{\max}, L_E^{\min}, L_E^{\max}, G_C^{\min}, G_C^{\max}, G_G^{\min}, G_G^{\max}, \upsilon_M^{\min}, \upsilon_M^{\max}\}$. R_1—rules for comparing integral characteristics. RCM_j—the rule of comparison of the integral characteristic of the room Ph_j^m with the equipment of the same name (>, <, ≥, ≤, =). R_2—matrix of spatial constraints. D(E_{p1},E_{p2})—distance requirement between $p1$-th equipment and $p2$-th equipment, maximum—at $p1>p2$ and minimum—at $p1<p2$, at the same time, $p1 \neq p2$, D(H,E_p)—requirement for maximum distance between room walls and p-th equipment, D(E_p,H)—the requirement for minimum distance between room walls and p-th equipment. R_3—requirements to safety and operability of equipment in the form of operating ranges by arc voltage $[U_A^{\min}; U_A^{\max}]$, interelectrode distance $[L_E^{\min}; L_E^{\max}]$, refrigerant volumetric flow rate $[G_C^{\min}, G_C^{\max}]$, volume flow rate of inert gas circulation $[G_G^{\min}, G_G^{\max}]$, anode feed rate to reactor $[\upsilon_M^{\min}, \upsilon_M^{\max}]$. $R_4\{GC_{max},MR_{max},VD_{max},ME_{max}\}$—operational and economic restrictions, where GC_{max}—maximum volumetric flow rate of coolant during the synthesis of fullerene carbon soot and extraction $\tau_1+\tau_2$, MR_{max}—the maximum mass of consumable graphite rods over time τ_1, VD_{max}—the maximum volume of consumable solvent during extraction τ_2, ME_{max}—maximum power consumption for total synthesis time $\tau_1+\tau_2$. $R_5\{m_s^R, F_{tp}^R, D_e^R\}$—requirements for qualitative indicators of the process, where m_s^R—required mass of fullerene carbon soot, F_{tp}^R—required content of synthesized target product in the mass of fullerene carbon soot, D_e^R – required degree of extraction of the end product. $S\{S_1,S_2,\ldots,S_{cs}\}$—material and energy flows of the process, cs—number of flows. $S_f\{S_T,SC_1,SC_2,\ldots,SC_{csc}\}$—characteristics of

the f-th flow, where S_T—the type of flow (inert gas, coolant, graphite rod, extractant, etc.), SC_w—characteristic of the f-th flow (density, heat capacity, viscosity, purity, etc.), $w \in [1;csc]$, csc—number of the f-th flow characteristics, $f \in [1;cs]$. $L\{NS,RSN,REC\}$—situational knowledge of the research object in the form of a production-frame model, where $NS\{NS_1,NS_2,\ldots,NS_{nsn}\}$—possible emergency situations, $RSN\{RSN_1^{NS_i}, RSN_2^{NS_i}, \ldots, RSN_{rsnn}^{NS_i}\}$—causes of emergency situations NS_i, where $RSN_k^{NS_i}\{P, [P_{\min}; P_{\max}], \upsilon_{\max}, RM\}$, P—characteristic—initiator of the cause of the emergency situation, $[P_{\min}; P_{\max}]$—its range of identification of an emergency situation, υ_{max}—the limit rate of characteristic change, RM—text of the message to the operator. REC $\{REC_1^{RSN_k^{NS_i}}, REC_2^{RSN_k^{NS_i}}, \ldots, REC_{recn}^{RSN_k^{NS_i}}\}$—recommendations to the researcher to eliminate the cause $RSN_k^{NS_i}$ of emergency situation NS_i. $REC_j^{RSN_k^{NS_i}}\{WR, RCM\}$, where WR—priority of the recommendation, RCM—text of the recommendation to the operator, $j \in [1;recn]$. nsn—number of possible abnormal situations in the simulated process, $i \in [1;nsn]$, $rsnn$—number of causes of emergency situation NS_i, $recn$—number of recommendations to the researcher to eliminate the cause $RSN_k^{NS_i}$ of the emergency situation NS_i, $k \in [1;rsnn]$. M:Q=f(X,U,F)—system of algebraic and differential equations for calculation of qualitative-integral indices Q of the simulated process [21]. U—a variable characteristics vector of a manufacturing process comprising U_A—electric arc voltage, L_E—interelectrode distance, G_C—volumetric flow rate of coolant, G_G—volume flow rate of inert gas circulation, υ_M—anode feed rate to reactor, W_H—extractant heater power, τ_1—fullerene carbon soot synthesis time, τ_2—the time of extraction of the target product. F—a vector of uncontrolled disturbances of the external environment, including ξ_1—errors in the construction of the 3D room and equipment models, ξ_2—heterogeneity of material flow properties, ξ_3—voltage differences in the electrical network. Y—a vector of qualitative-integral indicators, including DS—pre-design specification for manufacturing room sketch, $Q\{M_s$, F_{tp}, D_e, GC, MR, VD, $ME\}$—qualitative and integral indicators of the process, where M_s—the mass of carbon soot synthesized during τ_1, F_{tp}—the content of target product in carbon soot mass, D_e—degree of extraction of the end product, GC—volumetric flow rate of coolant during the synthesis of fullerene carbon soot $\tau_1+\tau_2$, MR—weight of spent graphite rods in time τ_1, VD—the volume of solvent consumed during extraction τ_2, ME—energy consumption during synthesis $\tau_1+\tau_2$.

3 Project Objective and Task Setting

At SPbSIT (TU) (St. Petersburg), the Faculty of Chemistry of Substances and Materials laid the foundation for research on innovative multi-stage complex in the control of the synthesis processes of carbon nanocluster compounds. In 2014, the Department of Automated Design and Control Systems, with the support of the Infrastructure and Educational Programs Fund, together with scientists of the Faculty of

Chemistry of Substances and Materials, initiated an interdisciplinary comprehensive project to create a flexible, customizable to technological regulations and the material and technical base of the intelligent simulator complex of the technological process of fullerene synthesis [21]. The software package is implemented and used in the training process. The implementation of the idea of creating a digital twin of the carbon nano-industry to support the life cycle control of fullerene products expanded the functionality of the current software complex by including additional components—the visual designer of the reactor sites for the synthesis of carbon nanocluster compounds and the virtual fullerene extraction site.

The relevance and practical significance of the project are justified by the need to solve the complex problem of designing and studying the processes of synthesis of fullerene compounds, which contributes to:

1. Support decision-making in design activities during the initial design phase of an industrial facility [22];
2. Minimization of risks of equipment breakdown and loss of expensive raw materials in preparation of control and production personnel on the simulation-situational production model [21].
3. Forecasting of quality indicators of the production process at the specified material and technical base and technical regulations of production.

We formulate the goal of creation and implementation of the proposed computer system of visual modeling: ensuring the quality of organization of production of carbon nanocluster compounds with minimization of costs and risks of design and control errors of the chemical-technological process with the prediction of quality characteristics and economic indicators affecting the cost of production.

Setting a complex task of visual design and investigation of the process of synthesis of carbon nanocluster compounds: for a given vector of input parameters X:

- using the dialog mode, visual designer, and 3D models of the room and equipment, in accordance with the system of design and operational rules and requirements R, prepare a 3D model of the reactor area with the specification DS for it;
- varying the characteristics of U in the safety ranges R_3 performing virtual synthesis of the target product taking into account the accepted operational and economic restrictions R_4 and in accordance with the requirements for quality indicators of the process R_5.

Thus, the complex task of designing and researching the processes of synthesis of fullerene compounds covers the product life cycle from the design of a model of a production site to the calculation of qualitative and integral indicators Q, which allows you to correct not only the design solution during the construction of an industrial facility but also the values of varying characteristics in order to obtain the best quality indicators of R_5. Subsequently, targeted products become more accessible to consumers, and the enterprise becomes more competitive.

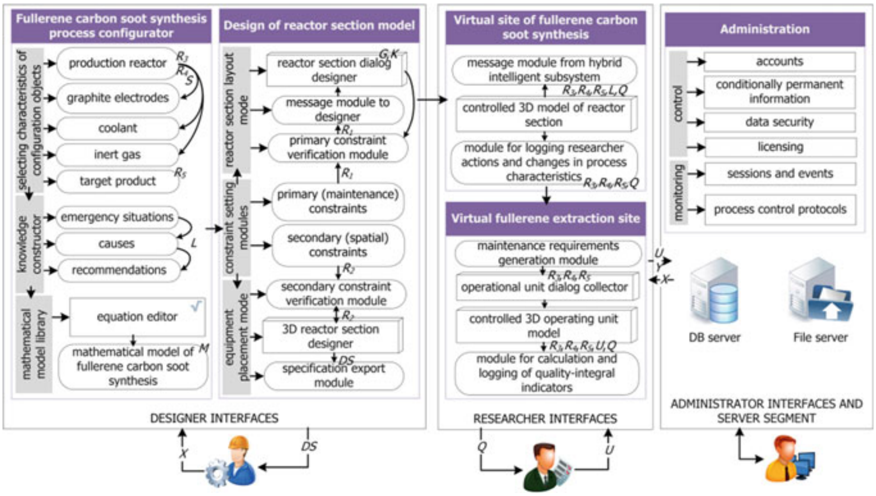

Fig. 2 The architecture of the computer system for processes of carbon nanocluster compounds synthesis visual modeling

4 Visual Simulation Architecture

The architecture of the computer visual modeling system (Fig. 2) includes the dialog and virtual graphical interfaces of the designer, researcher (operator), administrator interface, and server segment. The client-server architecture of the system is two-level.

The main stages of design and research of processes of synthesis of carbon nanocluster compounds are presented in Table 1.

As a result, when the production cycle is successfully completed in simulated production conditions close to the real ones, the resulting qualitative-integral characteristics Q make a decision to adjust the initial data X and the variable characteristics U.

5 Trial Operation

The system is multi-user with a centralized relational database of characteristics and 3D models of premises H and equipment E, material resources S, systems of equations of mathematical model M, situational knowledge L, rules, requirements and limitations R, qualitative-integral indicators of the process Q, as well as users, sessions, events, and protocols.

Pilot operation of the system of visual modeling of the processes of synthesis of carbon nanocluster compounds was carried out on the basis of the Department of

Table 1 Stages of the solution of the problem of visual design and research of processes of synthesis of carbon nanocluster compounds

Stage description	Data sources
1. Entering reference data *E, H, S*	*G*
2. Configuring simulated fullerene carbon soot synthesis process online with restriction entry R_1, R_3, R_4, R_5, situational knowledge *L*, and systems of equations *M*	*E, S*
3. Develop scaled equipment *E* models and space *H* models in the selected 3D graphics editor.	*G, K*
4. In the dialog, select the *K* equipment models to be placed in the *H* room model based on the R_1. Considering *G* enter spatial constraints R_2	*G*, R_1
5. Placement of equipment models *E* in the virtual space of the reactor section *H* in accordance with spatial limitations R_2	R_2
6. Operator, varying U_A, L_E, G_C, G_G, υ_M, τ_1, in the 3D environment of the reactor site model, performs virtual synthesis of fullerene carbon soot with characteristics M_s, F_{tp}, *GC*, *MR*, *ME*, according to regulations R_3, R_4, R_5	*E, H, S*, R_3, R_4, R_5, *U*
7. With the obtained mass of fullerene carbon soot by varying G_C, W_H, τ_2, the process of target product extraction is simulated with the calculation of quality-integral indicators D_e, *GC*, *VD*, *ME*	*E, S*, R_3, R_4, R_5, m_s, F_{tp}, *U*
8. Studying the protocol of virtual synthesis of fullerene, comparing R_4 and R_5 with *Q* with a decision on the techno-cost-effectiveness of the process conducted	

Automated Design and Control Systems in the educational process with the involvement of undergraduates in chemical areas of training—18.04.01 "Chemical Technology" and 18.04.02 "Energy and Resource Saving Processes in Chemical Technology, Petrochemistry and Biotechnology".

As initial data, the characteristics of the reactor section of the industrial enterprise "Closed Joint-Stock Company" Innovations of Leningrad Institutes and Enterprises", St. Petersburg and the reactor section with an industrial reactor of the Kretschmer design [19] were used. Material resources: technical water as a refrigerant, inert gas—helium, graphite rods of a high degree of purification. Fullerene C_{60} is used as a target product.

Three-dimensional graphics editor selected to develop 3D equipment models "Autodesk 3ds Max". Scaled equipment and space models are obtained. In the configurator dialog, you have entered reference data for designing the manufacturing process model.

The knowledge designer introduces situational knowledge frames. Frame example of situational knowledge: NS_1: Electric arc break. $RSN_1^{NS_1}$ {Ta, [0;300], 100, "Electrode fracture, massive protuberance"}, $REC_1^{RSN_1^{NS_1}}$ {1, "Turn off electrode voltage, shut off inert gas and coolant"}, $REC_2^{RSN_1^{NS_1}}$ {2, "Replace electrode"}. $RSN_2^{NS_1}$

$\{L_E, [0.1;10], 0.3,$ “Failure of inter-electrode distance ACS”$\}$, $REC_1^{RSN_2^{NS_1}}$ $\{1,$ “Turn off electrode voltage, shut off inert gas and coolant”$\}$, $REC_2^{RSN_2^{NS_1}}$ $\{2,$ “Eliminate malfunction of inter-electrode distance ACS”$\}$.

Among the process parameters for tracking their values by the researcher are direct ones corresponding to the vector of varying characteristics U and indirect ones calculated by model (for example, arc temperature T_a, coolant temperature, inert gas pressure).

A semi-empirical system of equations is introduced as a mathematical model, reflecting the dependence of safety and operability characteristics and qualitative-integral parameters of the simulated process on technical, operational, and variable characteristics of the process [21].

When generating the characteristics of the room, rules for comparing the integral characteristics of the R_1 are introduced. The integral characteristics are: the power of the power grid, volume airflow rate of plenum-exhaust ventilation, light flux power of lighting devices. The singlet characteristics of the room are: electrical voltage, water pressure in the main, temperature, and humidity of the environment.

Taking into account G, R_2 spatial constraints are formulated and introduced into the matrix. The requirements of safety standards, ergonomics, and speed of personnel, requirements of safety and operability of equipment and tools of instrumentation were taken into account.

The design of the reactor section with regard to spatial limitations is carried out using the 3D designer (Fig. 3). The designer, using visual positioning tools with regard to the matrix of spatial constraints R_2 places equipment models in the model space of the reactor section.

The 3D designer tracks collisions and collisions, which imposes additional spatial constraints. It is not excluded that the equipment cannot be placed according to the spatial constraint matrix R_2. In this case, the R_2 is corrected, the designer continues the placement until the equipment in the parcel model assumes the position according to R_2.

In the designed reactor area, the process of synthesis of fullerene carbon soot is simulated (Fig. 4).

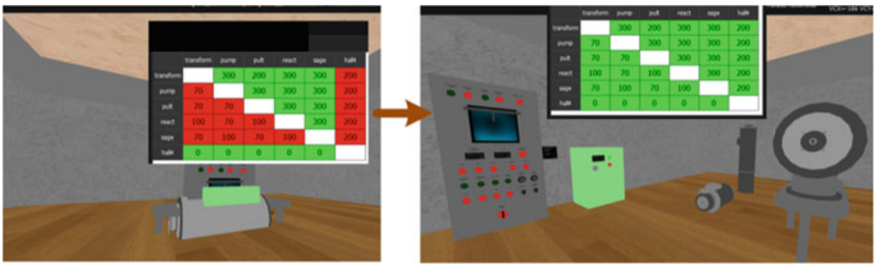

Fig. 3 Space and equipment models in the 3D designer before placement (left) and after placement according to spatial constraints R_2 (right). If the distance is R_2, the matrix element changes color from red to green

Fig. 4 Fragments of virtual reactor site operator interface for fullerene carbon soot synthesis

With the observance of the accepted ranges of safety and operability of the equipment R_3 and operational and economic restrictions of R_4 the operator, varying characteristics of U makes the synthesis of fullerene soot of the required weight m_s^R with the required weight of the target product F_{tp}^R. Incorrect or untimely action of the operator, as well as setting a variable characteristic outside its safety range increases the risk of an emergency, as well as reduces the main qualitative indicator of the process—the content of fullerene C_{60} in the soot.

The operator assembles the extraction plant before the extraction. The criterion constraints when assembling an extraction plant are D_e^R, VD_{max}, ME_{max}. In addition, the geometric characteristics of the parts of the extraction plant (a type of the bottom of the flask, slips) are taken into account, as well as calculated by the solubility of the extracted target product, the selected extractant, and the requirement D_e^R bulb working volume. After assembly of the extraction plant, the operator, including the heater and the coolant supply, initiates the fullerene C_{60} extraction process (Fig. 5).

After the completion of the simulation of the production cycle, the following results were obtained: the mass of the synthesized carbon soot $Ms = 0.9$ kg, fullerene content in it C_{60} $F_{tp} = 14.8\%$, mass of fullerene in the soot $m_{tp} = M_s \cdot F_{tp}/100 =$

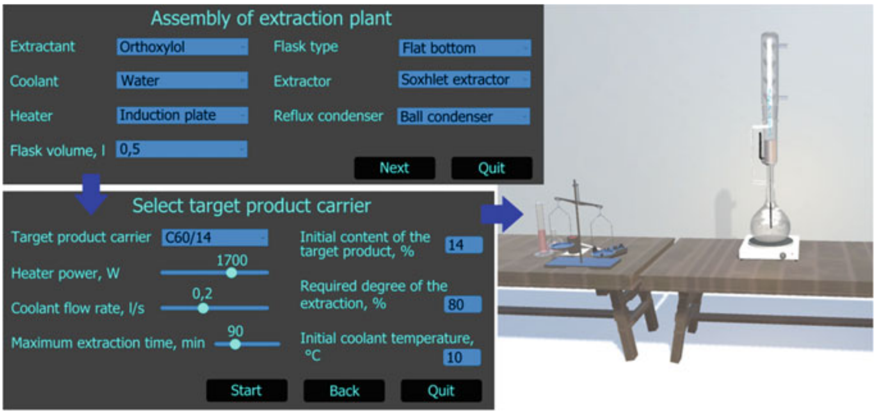

Fig. 5 Operator interface fragments for assembly of extraction plant model and virtual extraction of fullerene

0.133 kg, that is more than the required mass C_{60} $m_{tp}^{R1} = 0.126$ kg than 0.007 kg. The resulting difference is not critical for the first synthesis step. For the second stage of synthesis—extraction, with the required degree of extraction of fullerene C_{60} $D_e^R = 90\%$ and actual $D_e = 87\%$ the weight of fullerene in the extractant was 0.116 kg, which is higher than the required weight C_{60} $m_{tp}^{R2} = m_{tp}^{R1} \cdot D_e^R = 0.126 \cdot 0.9 = 0.113$ kg for 0.003 kg.

The obtained results of the pilot operation make it possible to conclude the applicability of the visual modeling system for design tasks, research of the process of synthesis of carbon nanocluster compounds, as well as the tasks of training control and production personnel in process control in both working and abnormal conditions.

6 Conclusions

It is known that the cost of unadjusted design errors of production facilities at subsequent stages of the product life cycle increases many times. Deviation from the process regulations in the process management not only leads to a decrease in the profitability of the enterprise, but also increases the intensity of wear and tear and the risk of equipment breakdown, and can also pose a potential danger to the health and life of control and production personnel.

The proposed system of visual modeling allows not only to reduce time and errors of design of the production area but also to increase qualitative and integral indicators of the process of synthesis of carbon nanocluster compounds. The obtained computer visual simulation system can be recommended both to enterprises in the field of synthesis of carbon nanocluster structures and scientific and educational centers and to educational institutions that carry out training in educational programs of automated design and control.

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