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CONFERENCE OF MSC STUDENTS

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ABSTRACTS

DEVELOPMENT OF COST-EFFECTIVE UPGRADING OF THE NORTH-BUDAPEST WASTEWATER TREATMENT PLANT

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Due the accession to the European Union Hungary has to adopt the new regulations, such as the strict criteria to be applied to the nitrogen concentrations in the treated effluent. The North-Budapest Wastewater Treatment Plant is unable to fulfill these requirements in its current conditions because of the low nitrification rate and insufficient nitrogen removal efficiency. The aim of this work is to examine a technological upgrading process developed in the Department of Agricultural Chemical Technology, Budapest University of Technology and Economics in the most critical winter period operation (12–14 °C). The comparative model experiments were carried out on site with the usage of the incoming wastewater. Implementation of this technological process would require about just half of the costs of those of other solutions.

One of the pilot-scale systems was run as a reference without any chemical used for primary sedimentation, however, the sludge concentration was set at a high value according to the proposed clarifier capacity expansion: *Reference* $x = 3.0$–4.0 g/l. In the two other model systems Fe(III)-chlorid was fed continuously to the raw wastewater in order to increase the efficiency of primary clarification. The concentration of the biomass was different in these two systems: *Chemical* $x = 2.0$–3.0 g/l and *Chemical* $x = 3.0$–4.0 g/l. The total bioreactor volume was 13.3 l per system; with the anoxic reactor (1.3 l), the 1st aerated reactor (4 l), and the 2nd aerated reactor (8 l). The flow rate of the raw wastewater was set to the average hydraulic retention time of the full-scale system. The results confirmed that the wastewater temperature could be maintained in the range of 12 to 14 °C during 21 days of the experiment, accomplished by a cooling system. The necessary biomass concentrations were assured by the excess sludge removal strategy. It was verified that the chemically enhanced primary sedimentation has a considerable reducing effect on the load of the bioreactors, whereby the sludge retention time increases at a given sludge concentration. During the experiment the effluent total nitrogen concentration limit of 30 mg/l could be fulfilled in all of the three model systems. However, in the case of the *Reference* system the effluent NH_4-N concentration exceeded the 5 mg/l limit value when the load increased. There was no considerable inhibition detected on the biodegradation processes, since the results calculated by the ASM1 simulation model adequately approached the measured data, if using the kinetic parameters applied for describing the domestic wastewater treatment.

The results of the experiment verified that the required upgrading can be cost-effectively achieved by the capacity expansion of the secondary clarifier and feeding chemicals in winter time into the primary clarifier. Experimental studies combined with simulation modelling proved to be a useful tool in finding a cost-effective procedure for enhanced performance.

COMPARISON OF THE MATHEMATICAL PROGRAMMING MODEL TYPES OF CHEMICAL PROCESS SYNTHESIS

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Investment in chemical industry is so large that determining optimality is an important aspect at both levels design and operation. Process synthesis is a series of decisions aimed to select optimal structure and operation from a given set of units and their possible connections. Mathematical programming (optimization) is used to define the optimal system via solving exact mathematical models.

The object of my study is a comparison of known strategies used for creating mathematical programming models, from the viewpoint of process synthesis. I studied and compared the known strategies on small-scale test problems.

Our research group often faced problems with several local optima. That is why our aim is to apply global optimization tools for process synthesis. My particular research task was a conceptual examination and comparison of the known model-creating strategies, and extracting conceptual information about them, from the perspective of their combination with the interval optimization methodology which is able to find global optima. My final aim was to choose the strategy that seems to be the best candidate to handle the interval optimization software.

Our final target is elaborating a mathematical model which is optimal for applying the global optimizing software to solve MINLP representation of process synthesis problems occurring in chemical industry.

During my research I studied (1) a Generalized Disjunctive Programming (GDP) strategy which handles the logical variables in a direct way. I also studied (2) a strategy which eliminates the binary variables of the Mixed-Integer Nonlinear Programming (MINLP) formulation and formulates an NLP problem, instead. The third strategy I tested is (3) a method which applies a binary minimal MINLP representation (BMMR) via coding the feasible structures by using the least possible number of binary variables. The logical conditions of the synthesis problem are formulated in this case in a disjunctive normal form (DNF). A test problem featuring many local optima was applied for testing the interval optimization method.

According to my results, the best candidate for global optimization methods is a combination of the BMMR and the NLP representations. The GDP algorithm behaves well for optimizing chemical industrial problems; however, applying it to interval methods is useless because the sequential solution of sub-problems leads to difficulty in maintaining the mathematical certainty of the results. This certainty is an essential component of interval methodologies.

CATALYTIC REDUCTION OF ARYL-PIRIDYL METHANOLS

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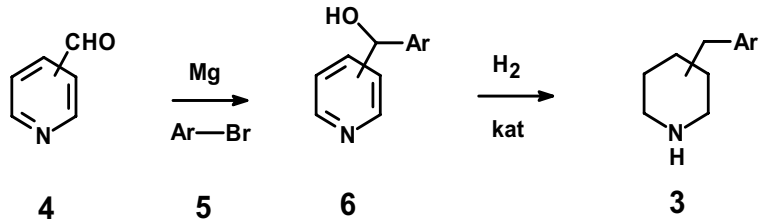
The interest in NMDA receptor antagonists has grown in the recent years. The abnormal functioning of these receptors causes many neurodegenerative diseases (e.g.: Parkinsonism, Huntington disease, Alzheimer disease). Extremely important members of NMDA receptor antagonists are benzylpiperidines.

The preparations known from literature, proceed from piperidinecarboxilic acids, providing the target compound in 5 to 6 steps and with 15 to 19% yield. A whale of harmful waste is prepared, however, the main problem is due to the Friedel Crafts acylation, which is not convenient to prepare all derivatives because of the directing rules.

The synthesis worked out in our department a few years ago provides benzylpiperidines in only two steps and by a 60 to 85% yield.



4 pyridinealdehydes react with **5** arylbromides (Grignard reaction). The **6** arylpyridilmethanol is then catalytically hydrogenated and gives **3** benzylpiperidine.

The expensive catalyst is an essential factor by industrial realization. Thus, we tried a new, more active catalyst, the Hereaus K 0218. By the optimal conditions the reaction resulted in byproducts, the most significant was the N-ethyl derivative. In our opinion this alkylation was induced by the in situ generated acetaldehyde on the surface of the Hereaus catalyst.

By size enlarging it is necessary to eliminate all byproducts from the procedure.

A solution may be the change of the solvent. Acetic acid is a good alternative, but technologically not the best choice, because it must be evaporated and regenerated.

The reduction carried out in water containing mineral acid, at the optimal temperature needed more time, but resulted in a unitary end product without any byproduct.

The reduction carried out in ethanol or acetic acid caused the catalyst to be damaged, and it was not possible to use it more than two times, because the activity decreased dramatically. By the defecation of the Grignard product with boneblack removed the catalyst banes. So the catalyst could be used more times without activity decrease. By the size enlarged experiments we used the same catalyst eight times with constant activity. Further advantage of the water is the lack of flammability. We obtained a good reproducible 80 to 86% yield for the isolated, distilled product by the enlarged experiments.

I proved that the repeated use of the catalyst can be carried out without cross-contamination. I changed the solvent of the processing. The ethers used earlier were very flammable and dangerous so I substituted them with methylcyclohexane. This solvent is favourable for environmental and safety causes.

SYNTHESIS OF NEW CROWN ETHERS CONTAINING 9-CARBOXY-ACRIDINO UNIT

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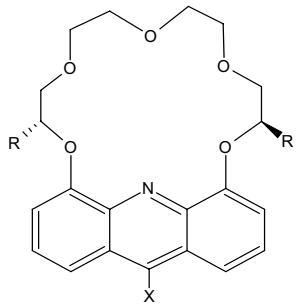
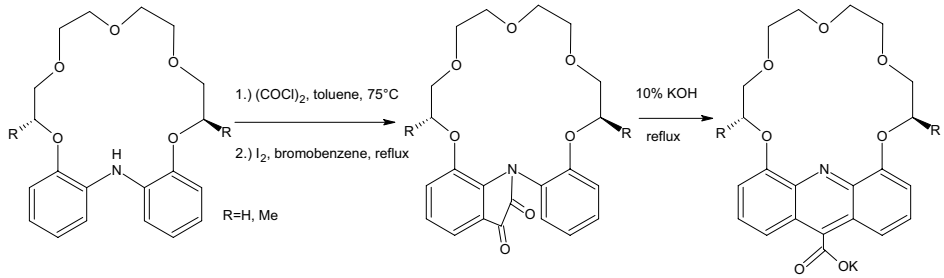
The importance of chiral crown ethers is expected firstly in the field of resolution of racemates. Earlier, a couple of crown ethers containing an acridino unit (**1**) were synthesized. These macrocycles showed advantageous complexing abilities. Our goal was to prepare such functionalized acridino crown ethers (**2**, **3**) which can be attached covalently to silica gel.



1 X=H
2 X=COOK (**2A**), COOH, CONH-CH_2-CH=CH_2
3 X=C_6H_4COOK, C_6H_4COOH, C_6H_4CONH-CH_2-CH=CH_2

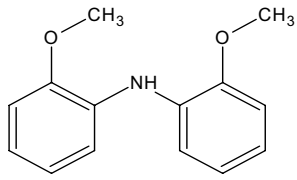
During our work it turned out that compounds of type **3** cannot be synthetized in the planned way. However, we worked out a new way to obtain novel crown ethers type **2** from compounds of type **4**.



4 **5** **2A**

The greatest difficulties were caused by the side reactions during the formation of isatin derivates (**5**). These side reactions were rationalized by doing model experi-

ments using compound **6**. Based on the latter model experiments we worked out a procedure to significantly decrease the undesired side reactions. Compound type **2**



6

containing terminal double bond is being studied for enantioselective complexation and it is also being bonded covalently to silica gel to obtain a chiral stationary phase for the enantioseparation of racemic protonated organic primary amines. The latter studies are carried out by Péter Huszthy and his co-workers.

NEW KINETIC MODEL OF THE REGULATION OF CYCLIN DEGRADATION

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Eukaryotic cell division is regulated by a highly complex network of proteins. The elements of the network are characterized separately and it is still to explain how the typical behaviour of cells emerges from the interactions of these proteins. The elements are involved in complex feedback loops that make verbal reasoning insufficient.

We constructed a new mathematical model describing early embryonic cell cycles of *Xenopus laevis* (african clawed frog) (CILIBERTO et al., [1]). We created a new wiring diagram, detailing the source of delay in the mitotic exit on the basis of new experimental results published since the appearance of the original model (NOVAK and TYSON [2]). Cyclin is essential in mitosis and Cdc20 is needed to carry out the degradation of cyclin at the end of mitosis. We studied the system to clear the role of Cdc20 phosphorylation. In the new approach Cdc20 is inactivated by phosphorylation. We translated the interactions of the network as ordinary differential equations by the help of the biochemical reaction kinetics and analysed the system with numerical simulations and with the tools of dynamical systems. Simulations show cycle oscillations in the case of normal and two types of mutant cells. We concluded that our system is able to perform periodic activation of MPF (dimer of Cdk1 and cyclin B), typical of embryonic cells, if MPF activates and inactivates its own degradation machinery at the same time. By this model we can get a better understanding how mutual inactivation of MPF and Cdc20 corresponds to the delay in the exit from mitosis.

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DESIGN OF BATCH REACTIVE DISTILLATION WITH EQUILIBRIUM LIMITED CONSECUTIVE REACTIONS

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Reactive distillation (RD) is a hybrid procedure to integrate separation and reaction in the same operation unit. The main advantages of reactive distillation over sequential processes include reduced initial investment and operating costs, reduced heat usage, higher reaction conversions and selectivity. Although reactive distillation has received increasing attention in recent years, there is no current and overall design method of RD.

The objective of my research work was the creation of a general design method of batch reactive distillation (BRD), including all the steps of the design, like conceptual design, detailed design, and experiments.

A feasibility study has been developed to treat two or more equilibrium limited reactions with three or more components and complex column configurations including reactive and non-reactive sections in rectifier, stripper, and middle-vessel column configurations.

I have performed a feasibility study of the transesterification of dimethylcarbonate in two cascade reversible reactions with an intermediate methylethylcarbonate in BRD procedure, in order to verify and demonstrate the method. Only complex configurations have been found feasible.

An adequate model has also been established, for the detailed design. The detailed design is usually performed with commercial software in order to have precise and realistic results. Commercial software is not yet available to handle the complex batch configurations, and it is hard to implement equilibrium limited reactions in dynamic models. Moreover, the start-up of distillation processes is usually not implemented in commercial software, however, the start-up procedure can significantly affect the efficiency of the whole process. Therefore, an adequate model has been created for the detailed design of batch reactive rectifier in gPROMS environment. The model has been validated successfully with batch extractive distillation separating acetone and methanol with water as an entrainer.

COMPARATIVE STUDY OF β-NUCLEATING AGENTS

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The simplest procedure for β-modification of iPP in industrial conditions is using β-nucleating agents. The aim of my work is to compare the efficiency and selectivity of β-nucleating agents used in industrial and laboratorial practice, and study their behaviour. The crystallization and melting characteristics of β-nucleated and non-nucleated iPP were studied by calorimetric methods (DSC, TMDSC), and the supermolecular structures were investigated by polarization optical microscope (POM).

The calcium salt of two dicarboxylic acids (suberic acid and pimelic acid) developed at the department proved to be β-nucleating agents with extremely high efficiency and selectivity. Only these agents were able to exceed pure β-iPP and the efficiency of the wide-range advertised NJ-Star NU-100 commercial β-nucleating agent was more or less the same. The nucleating agents having qualification (CG, IRG) had relatively small β-nucleating ability. The linear trans γ qinacridon was the first applied β-nucleating agent, but its efficiency and selectivity is lower than the recently developed nucleating agents.

Investigating the NJ-Star NU-100 we realized that the nucleating agent's efficiency and selectivity in low concentration range strongly depend on the end temperature of the heating run. We examined this effect in details. In the light of our results we can say that at a given temperature this compound partially dissolves in the iPP till it reaches the saturation concentration. Our researches raise additional questions. The most important is whether the partial dissolution can be exhibited on every β-nucleating agents, or this occurrence is single and is typical for only NJ-Star NU-100. Answering these questions needs further investigations.

NEW TARGET PROTEIN AGAINST TUBERCULOSIS; THE CLONING AND CHARACTERIZATION OF *MYCOBACTERIUM TUBERCULOSIS* dUTPase

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Within the EU FP6 program, my studies were involved in a targeted project against *Mycobacterium tuberculosis*. The project funds cover two years of research and my goal was to characterize the dUTPase enzyme of *Mycobacterium tuberculosis* and to design screening methods with medium or high throughput capacity to be used for screening for potential antagonists. Within the full project, potential antagonist molecules are identified by computer scientists and mathematicians by the help of computer-assisted docking. The database of potential drug-like compounds used in the docking includes all those active substances that are used in therapeutics nowadays. Biological participants in the full project analyze and screen potential antagonists by biochemical methods. The aims of my work were the followings:

1. Cloning and expression of the *Mycobacterium tuberculosis* dUTPase enzyme.
2. Enzymological and structural characterization of the *M. tub.* dUTPase enzyme.
3. Development of fast screening methods with medium throughput to be used in screening of potential antagonists.
4. Crystallization of *M. tub.* dUTPase with the aim to determine the three dimensional structure of the protein.

Results

1. Cloning of the native protein was successful and the expression is of high yield.
2. Catalytic activity of the protein was very low, however magnesium (II) ions showed a co-factor effect in increasing activity.
3. Substrate ligand induced a protein conformational change that could be detected by CD spectroscopy.
4. With the help of limited trypsinolysis and mass spectrometry, the peptide bond preferentially cleaved in the absence of substrate but protected against cleavage by the substrate could be identified.
5. The measurement of enzyme activity and the limited trypsinolysis are adaptable for screening numerous antagonists. Both methods allow screening of approximately 10 antagonists per day.
6. Protein crystals suitable for X-ray analysis were obtained in nine different precipitation solutions. It is expected that these conditions may prove to be useful in the case of the protein co-crystallized with the antagonists.

SYNTHESIS OF HEPARIN OLIGOSACCHARIDES: AN EFFICIENT SYNTHESIS USING L-IDURONIC ACID THIOGLYCOSIDES

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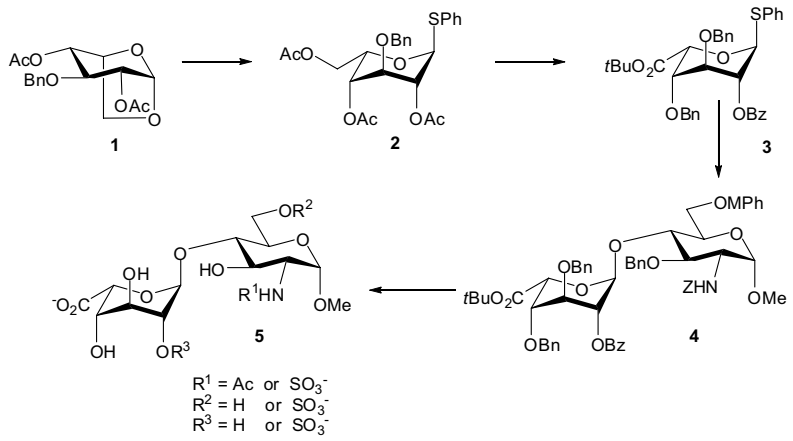
Heparin and heparan sulphate are heterogeneous polysaccharides that bind to a large number of biologically important proteins. Specific oligosaccharide sequences within the polysaccharide chain are responsible for the interactions with individual proteins and for the diverse biological effects. Chemical synthesis of homogeneous fragments of heparin is a valuable tool for studying heparin-protein interactions. These syntheses present a series of difficulties compared to common oligosaccharide syntheses, one of them is due to the presence of uronic acids, which are well-known to be poor glycosyl donors in glycosylation reactions.

Various types of glycosyl donors have been studied in the literature to find a useful glycosyl donor of L-iduronic acid. We have developed a stereospecific synthesis method for the preparation of an L-iduronic acid thioglycoside (**3**) starting from the readily available 1,6-anhydro derivative (**1**). We have studied the glycosyl donor capability of **3** and found that in contrast to literature reports, L-iduronic acid thioglycosides are highly efficient donors in oligosaccharide syntheses.



With the aid of the thioglycoside donor a new synthesis strategy was developed for the synthesis of heparin oligosaccharides, this approach allows for the synthesis of multiple sulphated products from a single protected precursor. This synthesis strategy is based on orthogonal protection of the positions which are optionally sulphated in the target compounds. Thus, using **3** as glycosyl donor, the orthogonally protected disaccharide **4** was synthesized, from which all eight basic disaccharide units (**5**) of heparin and heparan sulphate were prepared.

APPLIED INFORMATICS IN SENSORY PROFILE ANALYSIS

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Applying descriptive sensory test methods by means of profile analysis has lately gained significantly growing importance in supporting the pursuit of holding a competitive position in the market. An adequate informatic background gives a high–level promotion in designing and carrying out professional sensory analyses, essential in the determination of food quality.

Our research group has been performing the IT support of profile analysis since 2001 by the development of a Visual Basic for Excel based software: ProfiSens, featuring

- ✓ support for group design of the qualification system and the scoresheets,
- ✓ the choice of using either just right scales or unstructured scales,
- ✓ a database storing the former qualification aspects, thus speeding up the design phase of the assessment and opening the possibility of industrial applications,
- ✓ automatic generation of scoresheets, including sample codes, pads and kitchen lists,
- ✓ the electronic distribution, fill–in and recollection of scoresheets through LAN (local area network),
- ✓ an independent evaluation module for statistical analysis and displaying the results,
- ✓ bilingual (and extensible) communication for every step of the above process,
- ✓ a new extension for the qualification of the assessment panel (reliability).

Experimental background and development guidelines have been provided by the experiences gathered during the continuous design, implementation and evaluation of assessments at the Sensory Laboratory of Budapest Corvinus University. The ProfiSens software has been regularly used in the Sensory Laboratory of BCU since the very first version (2002), primarily in research and education, but also for industrial purposes. The application of the software is part of the special engineering courses at BME Dept. of Biochemistry and Food Technology since 2004. The number of assessments carried out in a fully electronical way with the support of ProfiSens is over 1500.

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DNA-BASED IDENTIFICATION OF GENETICALLY MODIFIED MAIZE

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The introduction of genetically modified food on the market has risen worldwide concern. According to the EC1829/2003 directive of the European Union, products containing more than 0.9% GMOs must be labelled. This regulation requires the development of validated analytical methods for detection of GMOs.

Traditional and real-time PCR methods have been developed for GMO analysis in our laboratory. Both raw material (maize) and processed products (maize germ, starch, gluten) were investigated. One part of the samples were from Hungary (GMO free territory), and the other part of them were from Romania and from the USA (biotech mega-countries). DNA was isolated by Promega's Wizard Kit and modified CTAB methods.

Two different DNA parts of the maize genome were amplified: the CaMV 35S sequence, which proves the genetic modification, and a sequence of zein (housekeeping) gene. To detect each of these sequences two sets of primers were designed that give two different size amplification products. A 79bp and a 195bp long fragment of the CaMV sequence and a 69bp and a 419bp long fragment of the zein gene were amplified. In the real-time PCR experiments fluorogenic hybridization probes were also used. The probes were labelled with FAM (35S) and Texas Red (zein) fluorescent dyes.

Using traditional PCR technique the appropriate DNA isolation method was chosen and adapted for the further real-time PCR experiments. The detection of 419bp-sized fragment was successful for most samples, but in case of gluten and starch samples amplification products could not be detected. However, the use of primers resulting 69bp-sized products led to amplification products in all samples. In order to detect 35S promoter three different mixtures of maize seed were created (containing 1%, 10%, 100% GMO). The use of primers providing 195 bp long PCR product indicated the presence of GMO in gel electrophoresis even in samples containing 1% GM material. The multiplex PCR examinations proved that the protocol was suitable for real-time PCR measurements.

The real-time PCR experiments have been tested by known GM rate samples (1%, 10%, 100%). The fact and the exact rate of modification could be determined. Based on our results we established that maize gluten sample from the USA and maize germ sample from Romania were both genetically modified.

Eventually, we have managed to develop a real-time PCR method for quantitative detection of GMOs in maize and processed products. The prevalidation steps required for validation have shown that our method is specific, limit of detection is 0,5%, working range is 0,5 to 100%. The newly developed GMO detection method can be applied in the Hungarian food industry after its extensive validation.

COMPUTER SIMULATION OF THE SMALL ANGLE X-RAY SCATTERING OF GRANULAR SYSTEMS

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Researches on nanostructures have great importance these days. One special and often forthcoming class of them is usually named as 'granular systems'. These aggregates, e.g. macromolecules and polymers, can be approximated with systems constructed from small, spherical structural units, with fixed electron density, which is homogeneous in each unit. The resulting structures could have many conformations and shapes. The goal of nanotechnology is to follow the change of their conformation, when they go through some kind of treatment, e.g. heating or adding different molecules.

For such examinations, small angle X-ray scattering (SAXS) could be a powerful method. However, due to the diverse effects occurring in the resulting curves, it is often difficult to interpret the measured data. Therefore one would need an instrument, for example a computer simulation, which can create these effects to be separated from each other, so their results could be examined more precisely.

In this study, I have created a special PC-program. It consists of three functional parts: one to generate the structure (to construct the form of the spherical units); the second one to calculate its simulated SAXS-curve and the third part to visualize the generated aggregate (i.e. to draw it on the screen or write the image to a file).

One could examine the results of different effects by controlling the development of the system. This can be made by restricting the constructing algorithm. The main parameters, which can be set are the radius and the electron density of the spherical units and the quasi-dimension of the generated granular system (cluster). The latter determines the conformation of the structure, there are three building methods: one unrestricted (3D); one quasi-planar (2D, one of the dimensions of the generated unit is much smaller than the other ones); and one quasi-linear (1D, we restrict the cluster formation in a line). There is a second step building algorithm too, when one uses these small clusters to generate greater aggregates. This latter step could be easily repeated: the program is able to construct huge structures by using these greater aggregates and so on.

Moreover, the program makes possible to build other structures too: e.g. crystal-like and gas-like systems.

My software seems to be useful if attached to real measurements: by using the program the expected changes in the SAXS-curve can be predicted by assuming a hypothesis for the change in the conformation. For example, the measured curve in *Fig. 1* represents a cubic structure, and one could see, that the peaks coincide with the peaks of the simulated curve of a $10 \times 10 \times 10$ cubic structure in *Fig. 2*.

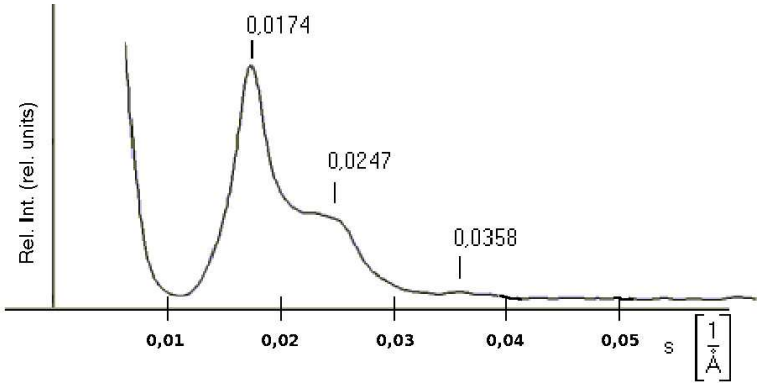

Fig. 1. Measured SAXS-curve of a cubic system

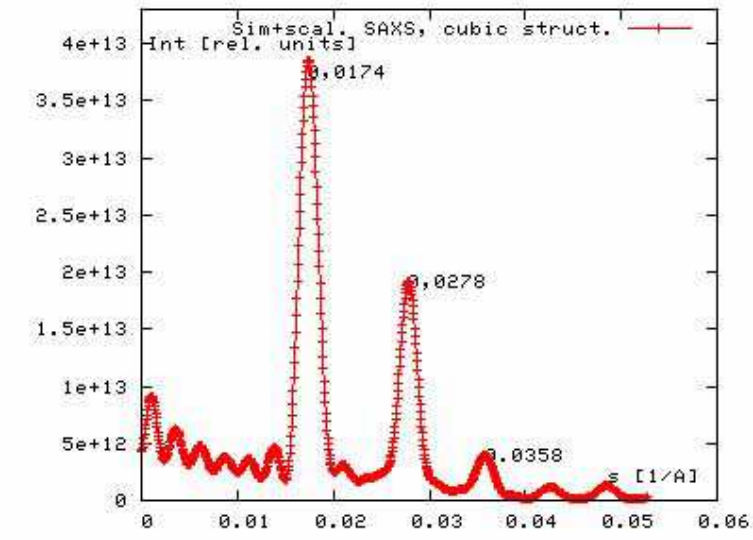

Fig. 2. Simulated SAXS-curve of a cubic system