NEW APPLICATIONS OF ARTIFICIAL INTELLIGENCE TOOLS IN MODELING AND DETERMINING CERTAIN PHYSICAL-CHEMICAL CHARACTERISTICS

Idei Programe PNCDI-II, Project ID _600 (Contract no. 64/1.10.2007)

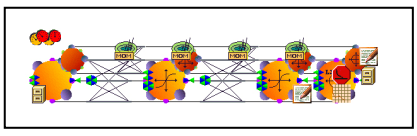
Significant efforts have been noticed at international level these latest years, to reduce the number of experimental determinations, which has also become a more frequent requirement in the study of physical, chemical and biological processes. This trend is particularly supported by the economic advantages that may result from it, like, for instance, less time-consuming and less expensive experimental research. The use of artificial intelligence tools in modelling and determining certain physical-chemical characteristics helps the achievement of this desideratum.

To support the above considerations, the overall objective of the grant proposition is the assessment of the applicability of various artificial intelligence tools like: neuronal networks and genetic algorithms in modeling and determining certain physical-chemical characteristics, while one of the specific objectives of the project would be aimed at discovering new applications for artificial intelligence tools in the study of the characteristics of real systems by means of proper models. Also, it tries to contribute to the establishment of new mathematical models, by means of modern and topical methods, namely – neuronal networks and genetic algorithms. The new calculus concept – neuronal calculus – that led to concrete achievements also known as artificial neuronal networks (in short neuronal networks) distinguishes itself through its applicability to very different fields.

The calculus based on neuronal networks is one of the artificial intelligence areas with the fastest development due to the ability of neuronal networks to memorize different types of relations. Neuronal networks proved able to estimate any continuous non-linear function, which means that they may be applied to non-linear system modelling.

The project theme has a multi-disciplinary nature, as it combines experimental abilities with high performance computational methods, thus providing useful tools to chemical engineering and also observing the preoccupations of the researchers at international level.

The project theme is an applicative and fundamental research area based on the synergy of pluri-disciplinary approach in physics, chemistry and mathematics.



It has a multi-disciplinary nature and it is compliant with the national society computerization policy, by the transfer and implementation of the most recent information technologies in chemical engineering, aimed at obtaining high performance solutions for new technologies and products.

The scientific importance of the theme replies on the two directions of application of the artificial intelligence tools we approached: 1. – modeling and especially determination of certain physical-chemical characteristics like: excess refraction index, excess molar volume and excess superficial stress of binary fluid systems and 2. – prediction of the thermal stability of certain organic compounds based on their molecular structure.

The design of materials having certain compulsory biological, chemical and physical characteristics requires the modeling of significant interactions between the basic structural units for characteristic prediction, as well as the efficient localization of viable structures that could help achieve the wanted synthesis performance. This area of molecular design is a way to combine neuronal networks and genetic algorithms. Neuronal networks model the non-linear structure-characteristics correlations more accurately and more easily as compared to other conventional approaches and that is why they are used to solve the direct problem. The opposite problem concerning molecular design is also solved by means of neuronal networks optimized with genetic algorithms, based on the fact that, wishing to obtain certain macroscopic characteristics, molecular structures are built that could provide such characteristics. Both research directions shall contribute to the achievement of the project desideratum, namely the reduction of the number of experimental determinations required for the establishment of certain physical-chemical characteristics with implications on time and money saving.

For more information on the PN-II-ID _600 project please visit the project site at: *http://www.ch.tuiasi.ro/cercetare/PNCDI/glisa/en/index.html*

Project Director
Dr.ing. Gabriela Lisa
Department of Chemical Engineering
"Gh. Asachi" Technical University of Iasi, Romania,
gapreot@ch.tuiasi.ro