RESEARCH ARTICLE

Application of computer in Chemical Engineering

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Abstract: In the 21st century, with the rapid development of science and technology, electronic computer applications have penetrated into every field of various disciplines. The further development of various disciplines is increasingly dependent on computers, and the chemical engineering discipline is no exception. . At present, computers have been deeply applied to various levels of chemical engineering disciplines such as chemical simulation, computational chemistry and chemical mapping, which have greatly promoted the development of chemical engineering. Chemists should seize the opportunity to study computer knowledge and master computer tools in the new era, and apply them to chemical design and chemical calculations to enable chemical engineering disciplines to develop faster and higher.

Keywords: Computer; chemistry; chemical industry; application

1. Introduction

Since the advent of electronic computers, various fields of human production activities have been widely infiltrated by computers. Many production fields have achieved unprecedented achievements and remarkable achievements by computer intervention, production efficiency and scientific research results. The field of chemistry and chemical industry has also received its patronage. Especially in recent decades, the application of computers in the field of chemistry and chemical industry has developed by leaps and bounds[1].

With the birth of the first electronic computer, the computer is developing rapidly. Within a few decades, the application of computer has penetrated into various disciplines, such as engineering technology, natural science, military, agriculture, commerce, transportation, health care and daily life and so on. As the development of electronic computers has promoted the development of various departments and disciplines, its far-reaching significance can be compared with the industrial revolution caused by the invention of the steam engine.

As a basic subject, chemical engineering has been developed on the basis of experiment for a long time. It is a subject combining theory with experiment. With the rapid development of computer technology and information technology, computational and computer simulation methods have been added to the research of chemical engineering. It has gradually become the most vigorous research method in chemical engineering. With the wide application of computer in chemical engineering, the traditional chemical engineering discipline has gradually become a comprehensive subject which integrates experiment, calculation and theory.

2. Application of computers in Chemical Engineering

2.1 Chemical simulation

Chemical engineering simulation mainly refers to chemical process simulation.

Chemical engineering is an engineering discipline which studies the common laws of chemical and physical processes in chemical industry and other process industries. The object of chemical engineering is usually very complex,

doi: 10.18063/csa.v1i2.

and analytical methods are often effective in chemical research. Since the 1950s, researchers have been using computers to solve mathematical models of chemical processes, which is an innovation in research methods. After decades of development, chemical process simulation has become a common means, widely used in chemical process research, development, design, control and optimization of production operations, operation training and technical transformation[2].

For chemical simulation, there are different levels of process simulation. A plant's process simulation object is in the range of more than ten meters or even hundreds of meters, and its unit process subsystem is several centimeters to several meters. Further in-depth simulation of the internal transfer process and reaction process of each unit process equipment, the simulation object is as small as millimeters, sub-micron. In the calculation of molecular properties or the development of new drugs, to simulate the performance of the molecule, touch your object even to the nanometer level. Typical chemical simulations are divided into four categories according to the hierarchy: process simulation (102m-100m), unit simulation (100m-10-3m), transfer and reaction kinetics simulation (10-3m-10-7m), molecular simulation (10- 7m - 10-10m).

2.1.1 Process simulation

Chemical process simulation or process simulation is based on data from chemical processes such as material pressure, temperature, flow, composition and associated process operating conditions, process specifications, product specifications, and certain equipment parameters, such as the number of plates in the distillation column. Material position, etc., using appropriate simulation software, a chemical process composed of many unit processes is described by mathematical simulation, the actual production process is simulated by computer, and the required results are obtained by changing various effective conditions on the computer. It includes important data on the most concerned raw material consumption, utility consumption, and production and quality of products and by-products.

Flow simulation is to "reproduce" the actual production process on the computer. Because this "reproducing" process ratio does not involve any changes in pipelines, equipment and energy sources of the actual device, the maximum degree of freedom for chemical industry simulators can be arbitrarily discussed and analyzed on the computer for different schemes and process conditions. Process simulation computer technology is one of the most important applications in chemical industry. Application of process simulation system can not only save time, but also save a lot of money and operating costs, improve product quality and output, reduce consumption. The process simulation system can also comprehensively analyze and accurately evaluate the economic benefits, process optimization and environmental assessment, and can also analyze the planning, research and development of chemical processes and technical reliability, and quickly and accurately analyze and compare various process schemes.

With the development of computer technology and the development of application software technology, process simulation technology has become increasingly mature, and commercial software has appeared widely. The most famous ones are Aspen Plus system and PRO II system[3].

2.1.2 Unit simulation

The process of chemical industry processing is characterized by continuous flow of mass, momentum and energy. The traditional means of dealing with this process is largely dependent on experience and empirical relationships expressed by some macro parameters. In modern process simulation technology, most of the cell processes are still treated as "black box" models. For the design and amplification of cell processes sensitive to flow, mass transfer, heat and reaction, more micro and in-depth information about mass, momentum and energy flow is needed, unit simulation technology is created to solve this problem.

In the unit simulation process, the medium inside the unit is basically multi-component or multi-phase, and the mass transfer, heat transfer and reaction processes are coupled to each other. The unit simulation technique solves this coupling system by discrete methods to obtain spatial and temporal velocity distribution, temperature distribution, pressure distribution, concentration distribution, and phase fraction distribution. Unit simulation technology can provide a large amount of information that is difficult to obtain by traditional means, such as spatial distribution and dynamic changes of all parameters in the unit process. Through this information, the internal mechanism of the unit process can be deeply understood, and it is helpful to analyze the cause when an abnormality occurs. Therefore, it is a low-cost tuning method. When the structural form or structural parameters change, the process of changing the process parame-

ters and operating parameters inside the unit process can be easily tested on the computer and directly used for optimization. And the means of transformation, and the calculation of unit simulation is not empirical and reliable. At present, unit simulation is mainly used in engineering amplification, optimization design, diagnosis and expansion transformation, production tuning and control of chemical production.

2.1.3 Reaction kinetics simulation

Chemical reaction kinetics is a science that studies the influence of various factors on reaction rate and reaction mechanism. Based on the experimental results and the study of reaction mechanism, chemical reaction kinetics equations are established. They are essential theoretical basis for the design of reactor and the selection of optimal conditions.

Computer technology has penetrated into the study of chemical reaction kinetics, which is mainly manifested in the following aspects: (1) predicting and establishing a model of chemical reaction. (2) Calculate the parameters of chemical reaction kinetics, such as the number of reaction stages, the number of reaction stages, the rate coefficient, and the activation energy of Arrhenius. (3) Calculate the optimal process conditions for the reaction using the reaction kinetics model.

At present, only a single mathematical method, such as separation of variables or elimination method, is given in the textbooks of physical chemistry for a series of confrontational, parallel and continuous kinetic equations of complex reactions. This method can obtain analytical solutions for very simple and complex reactions, but the reaction mechanism of most chemical reactions is very complicated. Because the differential equations obtained from the reaction mechanism are very inconvenient to be solved, the differential equations obtained from the reaction mechanism can be solved conveniently by means of the numerical method of the computer.

Computer simulation is widely used in the calculation of complex chemical reaction kinetics. The results obtained by computer simulation can predict the change of the concentration of each reaction substance in the process of reaction. By calculating the optimum time of continuous reaction, the reaction time can be controlled to obtain the maximum concentration of the substance needed. By calculating the optimum temperature of parallel reaction and confrontation exothermic reaction, the reaction temperature can be controlled, the reaction conditions can be optimized, and the rate of product can be maximized[4].

2.1.4 Molecular simulation

Molecular modeling is the study of the molecular structure and behavior of molecular scales through molecular models to predict the physical and chemical properties of materials. Molecular simulation can not only study the static structure of the microscopic model, but also simulate the dynamic behavior of the microscopic model. Compared with traditional experimental research methods, molecular simulation not only reduces the research cost, but also improves the research efficiency, and can explain and analyze the molecular scale. At present, molecular simulation methods mainly include quantum mechanical methods, Monte Carlo methods, molecular mechanics methods and molecular dynamics methods.

Chemical engineers urgently need to study the microstructure, macroscopic thermodynamic properties and transfer properties of fluid systems at the molecular level. With the rapid development of computer technology, molecular simulation technology is playing a more and more important role in obtaining the thermodynamic properties and micro-composition properties of chemical products and process development and design. It is undoubtedly an important direction of chemical engineering in the 21st century to study the development and design of chemical processes and products at the molecular level. Computer simulation has become the third important method to understand the natural laws in balance with experimental and theoretical studies. Chemical thermodynamic data plays an important role in the design, operation and optimization of chemical industry processes. Thermodynamic data is generally obtained in three ways: experimental determination, theoretical summary, and computer molecular simulation. Through computer molecular simulation, the macroscopic thermodynamic properties of the fluid can be predicted from the microscopic interaction of the fluid. Especially under some extreme conditions (such as high temperature, high pressure, and highly toxic), it is very difficult to carry out experiments. Computer simulation is easier to implement and economical. By means of computer molecular simulation, the reliable radial distribution function, macroscopic thermodynamic properties and

transport properties of thermodynamic systems can be obtained, which provides a reliable basis for us to establish and improve various theories or models describing actual phenomena.

2.2 Computational chemistry

Chemistry is a basic discipline. It is a combination of theory and experiment developed on the basis of experiment. With the wide application of computer technology in chemistry, it has gradually formed an independent discipline that applies computer research to chemical reactions and material changes. It uses computer as a technical means to perform numerical calculations on chemical reactions. This is computational chemistry.

Computational chemistry is an important branch of theoretical chemistry. It is a methodology that uses electronic computers to solve chemical problems through numerical calculations. Computational chemistry is an emerging, multidisciplinary, edge science that uses mathematical, statistical, and computer programming methods to perform theoretical calculations, experimental design, data and information processing, classification, analysis, and prediction in chemistry. With the increasing demand for automation of chemical instruments, many chemical experiments are difficult to control manually and require reliable control technology systems. Therefore, computer simulation technology has fundamentally changed the chemical experiment technology[5].

Computational chemistry is based on numerical calculations. It uses high-level language and its programming techniques to solve numerical calculation problems in chemistry. It applies mathematical calculation methods to chemical processes through computer programs. It is usually used to study some commonly used chemistry. Common, more common calculation methods are the core of chemical calculations. Interpolation of experimental data, function fitting, solving linear equations, solving higher-order equations, solving differential equations, finding eigenvalues and eigenvectors, etc., all of which are related to quantum chemistry, analytical chemistry, chemical equilibrium, Chemical kinetics are closely related to experimental data processing. The development of modern computational chemistry technology has been able to quantitatively link the relationship between various chemical properties and molecular structure. Chemistry is therefore moving from experimental science to a comprehensive discipline combining experiment, calculation and theory. The experiment is less computational, and the evolution is the first experiment and then the calculation, and it will gradually evolve into the first calculation and then the experiment.

Computational chemistry has developed greatly in the 1970s and 1980s because it was born to meet the needs of the times. By the 1990s, it had become an independent discipline and was accepted by the international chemical community. Wide attention. It is a new growth point that is highly interwoven and interpenetrated with mathematics, computer science, physics, pharmacology, materials science and other disciplines. It is the basis of many practical technologies and is deeply influenced by the rapid development of computer and network communication technologies today. It is in rapid development and constant evolution. This characteristic of computational chemistry determines its position in chemistry and is intended to help chemists, promote research methods in the chemical industry and continuously innovate production methods in the industry. At the same time, it is closely related to the rapid rise of high-tech, is the foundation of green chemistry and green chemistry, and is a bridge linking chemistry and chemical industry to the sustainable development of the national economy. Therefore, the role of computational chemistry in promoting the development of chemistry can not be underestimated. Without its development, there would be no modern chemistry[3].

At present, computational chemistry is widely used in inorganic chemistry, analytical chemistry, organic chemistry, physical chemistry, and structural chemistry. Specifically, computational chemistry is mainly accomplished by quantum structure calculation, molecular ab initio calculation, semi-empirical calculation and numerator. Quantum chemistry and structural chemistry, such as mechanical calculations, and calculation of physicochemical parameters, including reaction enthalpy, dipole moment, vibration frequency, spectral entropy, reaction free energy, reaction rate, etc., which are chemical thermodynamics, chemical kinetics, and statistics. Thermodynamic category. In computational chemistry, numerical calculation is the most fundamental task. Its purpose is to obtain a expected result from appropriate mathematical calculations. This result can be compared with experimental results or compared with previous research results. Finally, conclusions are drawn to guide the implementation of chemical experiments.

2.3 Computer graphics

Computer Aided Design (CAD) is a general term for engineers and technicians who use computers as tools to design, draw, model, analyze and write technical documents for products and projects. There are many software for computer-aided design. Among them, Auto CAD (Auto Computer Aided Design) software has the highest versatility and the most widely used. Because of its high-speed computing, data processing, large-capacity storage, and powerful drawing editing capabilities, Auto CAD has been widely used in chemical engineering. It takes advantage of the convenience, speed, accuracy, reuse, and artificial intelligence of computing to help people solve all the problems encountered in the design process.

Auto CAD is a general-purpose computer-aided design software package for computer graphics design work. It is a modern drawing tool widely used in various design fields today, and is no exception in the chemical industry. The software has powerful chemical drawing capabilities, which can be used not only to draw general 2D drawings, but also to perform 3D solid modeling to generate three realistic graphics.[6] In addition, secondary development can be carried out on this basis to form a broader professional application field.

Drawing chemical drawings with Auto CAD can be done in a human-machine dialogue or in a way that becomes. Because Auto CAD is widely used and easy to learn medical, it is one of the favorite CAD software for chemical designers. It is widely used in the chemical industry at home and abroad.

The specific tasks of chemical design involve material balance calculation, energy balance calculation, plant layout drawing, workshop layout drawing, equipment and equipment drawing, pipeline layout drawing, process flow chart with control point, equipment selection and strength check calculation. Waiting for a lot of work, so many jobs, such as the introduction of computer aid, will greatly reduce the intensity of chemical design work. In the past, the use of ordinary paper and pen to draw chemical drawings, the use of rulers and calculators will be replaced by a variety of computer software applications. Comparing with ordinary drawing, CAD drawing not only has the advantages of drawing accurately and neatly, but also has the characteristics that ordinary manual drawing can not have, such as arbitrary modification, reuse, on-demand printing and so on.

3. Conclusion

With the rapid development of modern science and technology, computer application has penetrated into every field of various disciplines, and society has entered the post-computer era. The further development and promotion of the subject depend on computer more and more, chemistry and chemical engineering are no exception.

At present, electronic computers have been widely used in chemical engineering, such as chemical simulation, computational chemistry, computer graphics and other fields, which has played a great role in promoting the construction and development of chemical engineering discipline. Chemical engineers, technicians and scientific researchers should seize the opportunity to grasp the knowledge of computer technology and strengthen the skills of computer application while learning this professional knowledge so as to combine computer, a new subject, with traditional subjects such as chemistry and chemical engineering. The application of computer in the scientific research of chemical engineering can make the subject of chemical engineering develop better with the help of advanced scientific research means such as computer.

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