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Modeling of Chemical and Technological Processes: A New Scientific Specialty

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Abstract The article analyses the scientific essence, object, subject and research directions of the new specialty 02.00.20 — "Modelling of Chemical and Technological Processes", introduced into the list of specialties of scientific and scientific-pedagogical personnel of the Republic of Uzbekistan by Decision No. 386/6 of the Higher Attestation Commission (HAC) dated 10 June 2026. Based on the specialty passport proposed by the authors, the scientific and socio-economic significance of the field is revealed. It is shown that, although extensive research in mathematical modelling of chemical-technological processes, computational fluid dynamics (CFD), process systems engineering (PSE), artificial intelligence and digital-twin technologies is being carried out worldwide, in most countries this direction has not been institutionalised as an independent specialty. Uzbekistan is among the first states to officially register this field as a separate scientific specialty.

Keywords Chemical technology, Mathematical modelling, Computational fluid dynamics

1. Introduction

The development of modern chemical industry and technology is increasingly dependent on computational methods, mathematical modeling, and digital technologies. At the stages of design, optimization, control, and scale-up of chemical and technological processes, the high cost of experimental investigations and stringent safety requirements have made modeling techniques an indispensable tool. As emphasized in the journal *Processes*, published by MDPI, the modeling and simulation of chemical and technological processes have become a central pillar of contemporary industrial practice, encompassing activities ranging from process design to operational control and maintenance management [1,2].

Chemical and technological process modeling emerged at the intersection of several independent scientific disciplines, including the school of Neal R. Amundson and Rutherford Aris, which introduced mathematical analysis into chemical reaction engineering; the research direction established by Roger W. H. Sargent, widely recognized as the founder of Process Systems Engineering (PSE); as well as the fields of Computational Fluid Dynamics (CFD) and computational chemistry [3]. The common scientific foundation of these disciplines lies in representing the parameters of physicochemical systems through systems of mathematical equations based on the conservation laws of mass, momentum, and energy, followed by their solution using computational methods and numerical tools [4]. In countries such as France, Japan, China, and India, this field is incorporated into the official descriptors of existing academic specialties as a recognized research area. Nevertheless, despite its broad spectrum of fundamental and applied research directions and its extensive range of research objects, the field of chemical and technological process modeling has not yet been formally recognized worldwide as an independent scientific specialty.

This article provides brief information about the scientific and methodological foundations of the specialty 02.00.20 - "Modeling of Chemical and Technological Processes", proposed by us and officially registered by the Higher Attestation Commission (HAC) of the Republic of Uzbekistan, its place in the world scientific arena, and the significance of this direction being officially registered as a separate specialty for the first time in Uzbekistan.

To address the aforementioned issue, the specialty passport for **02.00.20 – "Modeling of Chemical and Technological Processes"**, developed by the authors, was prepared in accordance with Clause 7 of the Regulation on the Higher Attestation Commission. Following positive evaluations by the Expert Council on Chemical Sciences of the Higher Attestation Commission of the Republic of Uzbekistan, as well as by leading research and educational institutions and prominent scholars in the field, the specialty was officially included in the national nomenclature of

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scientific and scientific-pedagogical specialties by Resolution No. 386/6 of the Higher Attestation Commission dated June 10, 2026, as a new specialty designated **02.00.20 – "Modeling of Chemical and Technological Processes"** [5].

The scientific object of the specialization is chemical, petrochemical, biotechnological and other technological processes and the devices and technological systems that implement them. The subject of the specialization is the creation of mathematical, physical and computational models of mass, heat and momentum transfer, chemical kinetics, hydrodynamics and thermodynamic phenomena occurring in these processes, their identification, verification and optimization [5,6].

The principal research areas of the specialty include:

- the development and theoretical substantiation of mathematical models of chemical and technological processes, including deterministic, statistical, and hybrid modeling approaches;
- modeling and numerical analysis of mass, heat, and momentum transfer processes, as well as chemical reactors;
- investigation of flow structures and mixing phenomena in process equipment using Computational Fluid Dynamics (CFD) methods;
- synthesis, optimization, and control of technological schemes within the framework of Process Systems Engineering (PSE);
- prediction, monitoring, and control of technological processes using artificial intelligence, machine learning, and digital twin technologies;
- methodologies for model identification, verification, and validation based on experimental and industrial data.

The scientific significance of modeling methodologies lies in their ability to describe physicochemical systems across multiple scales—from the molecular level to individual process units and entire industrial plants—within a unified methodological framework. According to analyses conducted by the National Academy of Sciences, computational chemistry and chemical engineering are undergoing a qualitative transformation toward the modeling and optimization of processes along the entire "chemical supply chain," linking molecular-scale phenomena with plant-scale operations [7,8]. This approach substantially reduces the number and cost of experimental studies while accelerating the design and development of novel processes and advanced materials.

From an economic perspective, modeling and simulation enable industrial enterprises to minimize design errors, enhance energy and resource efficiency, and improve product quality consistency. Research has demonstrated that the implementation of digital technologies and virtual process replication can reduce production development and optimization time by up to 20% [9]. Such opportunities are directly aligned with the strategic objectives of modernizing the industries of petrochemistry, mineral fertilizer production, and polymer manufacturing in Uzbekistan.

The classical foundations of mathematical modeling of chemical and technological processes are based on mass and energy balance equations, the laws of chemical kinetics, and the theory of transport phenomena. In the monograph *Modeling and Simulation of Chemical Process Systems*, Nasser Ghasem presents methodologies for modeling nonlinear reactor systems, such as Continuous Stirred-Tank Reactors (CSTRs), using fundamental conservation and balance equations as the theoretical basis [10]. Today, this field encompasses a broad spectrum of approaches, including physical, statistical, and experimental–analytical modeling methods, as well as similarity theory and the methodology of design of experiments (DoE) [11].

Computational Fluid Dynamics (CFD) is a powerful computational tool for predicting fluid flow behavior, heat transfer, and mass transport within process equipment through the numerical solution of the conservation equations of mass, momentum, and energy. CFD has already exerted a profound influence on chemical reaction engineering by reducing the extent of experimental investigations required for reactor design and optimization [12]. Industrial case studies have demonstrated the capability of CFD to accurately predict flow patterns in stirred-tank reactors equipped with baffles and mechanical agitators [13]. In recent years, CFD has been extensively applied to the modeling of catalytic hydroprocessing reactors [14], electrochemical reactors [15], and multiphase systems involving gas–liquid–solid interactions [16,17]. In catalytic systems, CFD predictions are increasingly coupled with detailed chemical kinetic models, leading to the development of multiscale modeling frameworks that integrate transport phenomena with reaction mechanisms [18]. CFD has also found broad application in the modeling of biological wastewater treatment systems, where strategies for integrating hydrodynamic simulations with biochemical kinetics have been developed [19].

Process Systems Engineering (PSE) is a scientific discipline that integrates mathematical modeling, data analysis, optimization, and control of physicochemical systems across different scales and levels of complexity [20]. The field was established during the 1960s at Imperial College London by Roger W. H. Sargent, who introduced PSE as an independent subdiscipline of chemical engineering [21]. The foundations of the field were laid through Sargent's seminal 1967 publication *Integrated Design and Optimization of Processes* and through the progressive development of ideas originating from the work of Neal R. Amundson, Rutherford Aris, and Sargent himself, which collectively shaped the future direction of PSE [22]. The system decomposition algorithms developed by Sargent and Arthur W. Westerberg subsequently became an essential component of PSE methodology [23].

The term **"Process Systems Engineering"** was formally adopted at the First International Symposium on Process Systems Engineering held in Kyoto in 1982 [24]. Contemporary studies emphasize the necessity of reinforcing PSE as a central pillar of chemical engineering, given its critical role in the integration of modeling, simulation, optimization, digitalization, and decision-support technologies within modern process industries [25].

In the last decade, chemical process modeling has been integrated with artificial intelligence (AI), machine learning (ML), and digital twin technologies. In the chemical industry, digital twins are fundamentally changing the way processes are optimized, operational efficiency, and safety are managed [26]. Systematic literature reviews analyze the role of artificial intelligence, machine learning, and big data in digital twins [27]. Physics-informed neural networks have been used in dynamic modeling of distillation columns, combining data-driven and physics-based approaches [28]. The above analysis shows that chemical process modeling is a rapidly developing field worldwide, with many leading journals, monographs, and international conferences. However, **this field is not distinguished as a separate**, independent specialty in the classification of scientific degrees in most countries. It usually exists scattered within broader disciplines such as "chemical engineering", "chemical technology" or "process systems engineering".

As emphasized in a report by the National Academy of Sciences, the field currently lacks both sufficient methodological tools and an adequate number of highly trained specialists capable of advancing computational chemistry and chemical engineering across all relevant scales, from the quantum level to the industrial plant level [8]. Leading scholars in the field of **Process Systems Engineering (PSE)** have likewise highlighted the profound transformation of chemical engineering toward a more fundamental scientific and mathematically intensive discipline, emphasizing the necessity of establishing an integrated educational framework to strengthen and ensure the continuity of this research area [21,25]. This can be regarded as an implicit recognition of the need to institutionalize modeling as an independent scientific and educational discipline.

The absence of an independent specialty gives rise to several practical challenges. It complicates the training of researchers within a unified methodological framework, disperses dissertation research across multiple specialties, and hinders the development of standardized qualification requirements and expert evaluation criteria. It was precisely this gap that provided the scientific rationale for the establishment of a new specialty in Uzbekistan.

Taking into account the aforementioned global trends and the growing scientific demand for a dedicated disciplinary framework, the authors developed the specialty passport entitled **“Modeling of Chemical and Technological Processes”** and submitted it to the Higher Attestation Commission of the Republic of Uzbekistan (HAC). Following a comprehensive expert review, the specialty passport was approved by Resolution No. 386/6 dated June 10, 2026, and officially incorporated into the national nomenclature of scientific and scientific -pedagogical specialties under the designation **02.00.20 – Modeling of Chemical and Technological Processes**.

This decision is of considerable historical significance, as it represents one of the first formal initiatives to recognize **Modeling of Chemical and Technological Processes** as an independent scientific specialty. Until now, this field has largely existed within the international scientific landscape as a dispersed research domain embedded within broader disciplines rather than as a distinct academic specialty. In this regard, Uzbekistan has assumed a pioneering role by formally institutionalizing this strategically important field of research.

A particularly noteworthy aspect of the newly established specialty **02.00.20 – Modeling of Chemical and Technological Processes** is that it provides a framework for the award of academic degrees and academic titles in the fields of **chemical sciences, engineering sciences, and pharmaceutical sciences**. This approach fully reflects the inherently interdisciplinary nature of the specialty and enables researchers working in modeling and simulation to pursue academic qualifications within the disciplinary domain most closely aligned with the focus and objectives of their research.

The introduction of a new specialization will provide the following results:

– the opportunity to train highly qualified scientific and scientific-pedagogical personnel on a unified methodological basis in the field will be created;
– a clear scientific field and examination criteria for dissertation research in the field of modeling will be formed;
– the integration of fundamental chemical sciences, computational methods and digital technologies will be encouraged;
– the scientific basis for the digital transformation of the national industry (petroleum and gas chemistry, fertilizers, polymers, pharmaceuticals) will be prepared.

2. Conclusions

Modeling of Chemical and Technological Processes is a rapidly evolving interdisciplinary field that integrates mathematical modeling, Computational Fluid Dynamics (CFD), Process Systems Engineering (PSE), artificial intelligence, and digital twin technologies. The analysis presented in this study demonstrates that, despite the extensive body of research conducted in this area and its growing scientific and industrial significance, the field has not yet been institutionally established as an independent scientific specialty in most countries. Instead, it continues to exist primarily within the framework of broader disciplines, resulting in the fragmentation of research activities, educational programs, and qualification systems.

The specialty 02.00.20 – “Modeling of Chemical and Technological Processes”, proposed by the authors and approved by Resolution No. 386/6 of the Higher Attestation Commission of the Republic of Uzbekistan on June 10, 2026, addresses this important scientific gap. By formally recognizing this field as an independent scientific specialty, Uzbekistan has become one of the first countries to institutionalize this research area within its national system of academic qualifications. This decision is expected to make a significant contribution to strengthening the country's scientific and technological capacity, fostering interdisciplinary research, and supporting the digital modernization of industry in accordance with contemporary global trends in science, engineering, and innovation.

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