THE PARADIGMS OF CHEMICAL ENGINEERING

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Abstract: It is presented the chemical engineering development, as guided by its four main paradigms: unit operations, transport phenomena, product engineering and sustainable chemical engineering. The starting point is the paradigm definition as "a set of assumptions, concepts, values, and practices that constitutes a way of viewing reality for the community that shares them, especially in an intellectual discipline". Related to the paradigms role in the evolution of chemical engineering, it is relevant that even when paradigms are known to be inadequate, their inadequacies are frequently minimized, or even ignored by the scientific community. Nevertheless, if and when a paradigm reaches a crisis where its technical inadequacies are brought into focus, perhaps driven by social requirements, a new paradigm will arise to explain what the prior paradigm could not. During the evolution of chemical engineering, from its beginning at the end of 19th century up today's, each new paradigm was a step forward which has extended the manifold of the tasks that can be solved. However, no older paradigm is derelict. In fact, almost all paradigms must be used together in order to solve the complex chemical engineering problems.
Keywords: paradigms, unit operations, transport phenomena, product engineering, sustainable chemical engineering

1. INTRODUCTION

The aim of this paper is to present the evolution of chemical engineering pointed to its general *paradigms*. We will start from the paradigm definition given by The American Heritage Dictionary of the English Language: "Paradigm is a set of assumptions, concepts, values, and practices that constitutes a way of viewing reality for the community that shares them, especially in an intellectual discipline". An overuse of the word paradigm has led to some confusion over the meaning of the term. Villermaux (1993) has considered as paradigms: mass, heat, momentum analogies, reaction-transfer coupling, effective media and properties, population balance, residence time distribution, axial dispersion, continuous stirred tank, non-linear dynamics, energy and entropy management, structure of condensed matter, etc. Nevertheless, specific techniques for solving various classes of chemical engineering problems are not new paradigms, they fall within current chemical engineering way of thinking. Related to the overuse and confusion over the meaning of word paradigm, Hill (2009) refers the Dilbert comic strip where every engineer says his project is a paradigm, but no one seems to know what that means!

For the evolution of chemical engineering the definition given by The American Heritage Dictionary of the English Language is useful to be linked with that proposed by Kuhn, which defines a scientific paradigm as: "universally recognized scientific achievements that, for a time, provide model problems and solutions for a community of practitioners" (Kuhn, 1996).

From the ancient times applied chemistry meant an art, a trade for obtaining salt, caustic soda, soap, sulfuric acid, sugar, glass-things in rudimentary workshops. Traditional recipes have been transferred with minor, empirical improvements gained from observation. This period can be considered as the *empirical stage* of chemical engineering.

The development of the variety and the amounts of the chemical products, mainly in the last quarter of the 19th century, imposed a new stage, respectively the *rational stage* of chemical engineering. The empirical rules and practices were abandoned for rational scientific methods. The transition to this stage is especially owing to the great progresses of physical chemistry. In 1885 prof. H.E. Amstrong has taught at Central College of London the first chemical engineering course. In this course fundamental scientific training was combined with technical practice for design of chemical industry equipment. It may be considered that at this moment the rational stage of chemical engineering begins.

In 1887 prof. Geoge Davies from Manchester Technical College has taught a lot of chemical engineering lessons. These lessons were the roots of his further Handbook of Chemical Engineering published in 1901 and next in a second edition consisting in two volumes in 1904 (Fig.1).

The practical value of Davies lessons from this book consists in the variety and abundance of the technical end economical data. Due to the lack of scientific explanations, in fact this book belongs to empirical stage and is a document of what meant chemical engineering at that stage (Bratu, 1976).

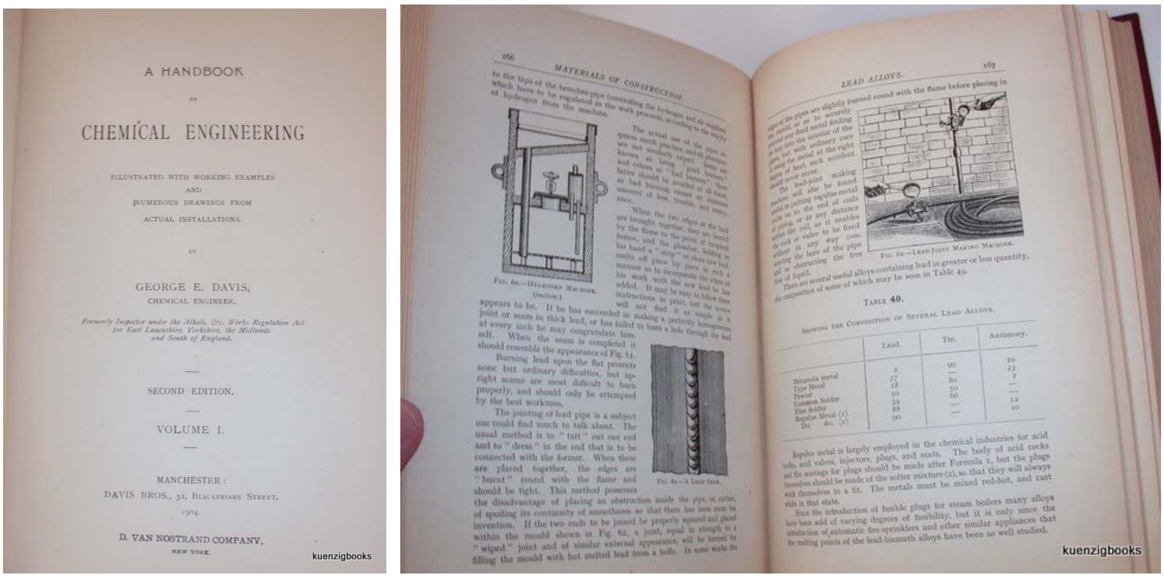

Fig. 1. Second edition (1904) of Davies' Handbook of Chemical Engineering.

2. THE FIRST PARADIGM: UNIT OPERATIONS

The Davies' book contained a novelty, which subsequently it appears to be more important as it incipiently looked: instead to describe each technological process existent at that time, Davies regards an industrial chemical process to be composed by distinct sections which are present - in different sequences and conditions – in many other processes. As this Davies' priority was not explicitly announced, it was assigned to Arthur D. Little, which in a report to Massachusetts Institute of Technology has introduced the notion of *unit operations*. Much more later, in 1958, Davies' priority about the concept of unit operations has been recognized (Bratu, 1976). This concept and its application can be assumed to be the first paradigm of chemical engineering, namely *the unit operations paradigm*. Therefore, the explosion of chemical industrial applications at the end of 19th century and at the beginning of the 20th century imposed the requirements of the process details knowledge systematization. It can be considered that the first paradigm has appeared as a necessity of systematization. The representative book of this paradigm is "Principles of chemical engineering", written by Walker et al., 1923.

The tens thousands industrial chemical processes can't be individually treated to the detailed scale as imposed by design and operation of the corresponding plants. Nonetheless, these processes are made from a much smaller number (about 80) of unit operations. Based on unit operations paradigm, an enormous amount of information concerning both theoretical and experimental studies, as well as results about unit operations is systematized, in a huge literature (books, papers, patents).

For each unit operation there are investigated:

© the fundamental theoretical principles needed by the formulation of phenomena equations ;

© the laboratory and pilot experimental methods needed by the equations which can not be theoretically formulated;

© the ways to equipment scale-up from laboratory or pilot scale to industrial scale.

To achieve the results imposed by process research, design, and operation the unit operation paradigm use the following general theoretical principles:

© momentum, energy and mass balances;

© thermodynamic phase equilibrium relations;

© momentum, energy and mass physical kinetic relations (transfer equations);

© financial conditions and the corresponding equations.

In this way, if the materials physical properties are defined, as well as technological and economic constraints, it is possible to obtain a quantitative solution for each specific industrial chemical process. It may be said that if the chemist is thinking in chemical reactions, the chemical engineer is thinking in unit operations. Subsequently, the paradigm of unit operations was adopted by others process industries, such as food industry or light industry.

3. THE SECOND PARADIGM: TRANSPORT PHENOMENA

While still useful to the present day, the unit operations paradigm proved inadequate for solving some important classes of problems (Hill, 2008). This awareness led to the emergence of chemical engineering science as a second paradigm in the late 1950s, as best exemplified by the Birds' textbook Transport Phenomena (Bird et al. 1960, Figure.2).

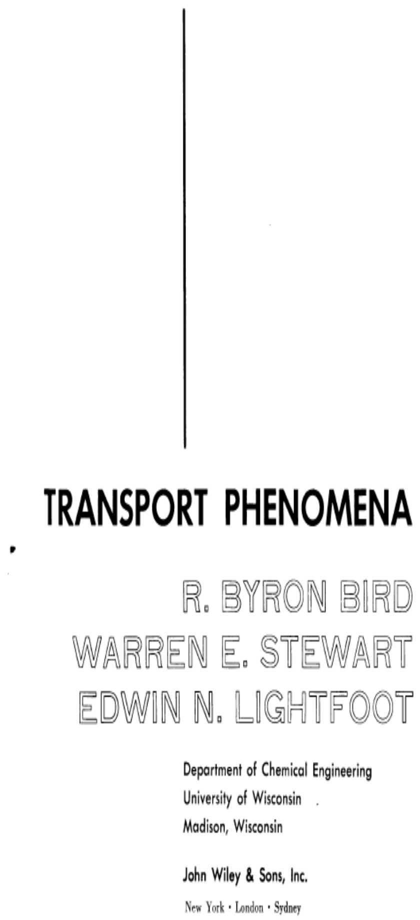

TABLE I. SCHEMATIC DIAGRAM OF THE ORGANIZATION OF TRANSPORT PHENOMENA

Entity Being Transported → / Type of Transport ↓	Momentum	Energy	Mass
TRANSPORT BY MOLECULAR MOTION	1 VISCOSITY μ Newton's law of viscosity Temperature, pressure, and composition dependence of μ Kinetic theory of μ	8 THERMAL CONDUCTIVITY k Fourier's law of heat conduction Temperature, pressure, and composition dependence of k Kinetic theory of k	16 DIFFUSIVITY $\mathfrak{D}_{AB}$ Fick's law of diffusion Temperature, pressure, and composition dependence of $\mathfrak{D}_{AB}$ Kinetic theory of $\mathfrak{D}_{AB}$
TRANSPORT IN LAMINAR FLOW OR IN SOLIDS, IN ONE DIMENSION	2 SHELL MOMENTUM BALANCES Velocity profiles Average velocity Momentum flux at surfaces	9 SHELL ENERGY BALANCES Temperature profiles Average temperature Energy flux at surfaces	17 SHELL MASS BALANCES Concentration profiles Average concentration Mass flux at surfaces
TRANSPORT IN AN ARBITRARY CONTINUUM	3 EQUATIONS OF CHANGE (ISOTHERMAL) Equation of continuity Equation of motion Equation of energy (isothermal)	10 EQUATIONS OF CHANGE (NONISOTHERMAL) Equation of continuity Equation of motion for forced and free convection Equation of energy (nonisothermal)	18 EQUATIONS OF CHANGE (MULTICOMPONENT) Equations of continuity for each species Equation of motion for forced and free convection Equation of energy (multicomponent)
TRANSPORT IN LAMINAR FLOW OR IN SOLIDS, WITH TWO INDEPENDENT VARIABLES	4 MOMENTUM TRANSPORT WITH TWO INDEPENDENT VARIABLES Unsteady viscous flow Two-dimensional viscous flow Ideal two-dimensional flow Boundary-layer momentum transport	11 ENERGY TRANSPORT WITH TWO INDEPENDENT VARIABLES Unsteady heat conduction Heat conduction in viscous flow Two-dimensional heat conduction in solids Boundary-layer energy transport	19 MASS TRANSPORT WITH TWO INDEPENDENT VARIABLES Unsteady diffusion Diffusion in viscous flow Two-dimensional diffusion in solids Boundary-layer mass transport
TRANSPORT IN TURBULENT FLOW	5 TURBULENT MOMENTUM TRANSPORT Time-smoothing of equations of change Eddy viscosity Turbulent velocity profiles	12 TURBULENT ENERGY TRANSPORT Time-smoothing of equations of change Eddy thermal conductivity Turbulent temperature profiles	20 TURBULENT MASS TRANSPORT Time-smoothing of equations of change Eddy diffusivity Turbulent concentration profiles
TRANSPORT BETWEEN TWO PHASES	6 INTERPHASE MOMENTUM TRANSPORT Friction factor f Dimensionless correlations	13 INTERPHASE ENERGY TRANSPORT Heat-transfer coefficient h Dimensionless correlations (forced and free convection)	21 INTERPHASE MASS TRANSPORT Mass-transfer coefficient k_x Dimensionless correlations (forced and free convection)
TRANSPORT BY RADIATION	*Numbers refer to the chapters in this book*	14 RADIANT ENERGY TRANSPORT Planck's radiation law Stefan-Boltzmann law Geometrical problems Radiation through absorbing media	*This book may be studied either by "columns" or by "rows"*
TRANSPORT IN LARGE FLOW SYSTEMS	7 MACROSCOPIC BALANCES (ISOTHERMAL) Mass balance Momentum balance Mechanical energy balance (Bernoulli equation)	15 MACROSCOPIC BALANCES (NONISOTHERMAL) Mass balance Momentum balance Mechanical and total energy balance	22 MACROSCOPIC BALANCES (MULTICOMPONENT) Mass balances for each species Momentum balance Mechanical and total energy balance

Fig. 2. First edition (1960) of Bird et al. Transport Phenomena.

This is the *transport phenomena paradigm*, an upper systematization and synthesis evolution. At the moment of issue of this book, the field of transport phenomena has not been yet recognized as a distinct engineering subject. The authors have considered that it is important to put more emphasis on understanding basic physical principles, than on the blind use of empiricism. Their thought has been that the subject of transport phenomena should rank along thermodynamics, mechanics, and electromagnetism as one of the key "engineering sciences". The paradigm of transport phenomena approaches the three elementary physical processes, which take place in any kind of unit operation: momentum, energy, and mass transport. Thus, unit operations can be considered as specific applications of these three fundamental processes. As combinations of unit operations give technologies, combinations of transport processes give unit operations.

The paradigm of transport processes press for the mechanisms of these processes, on the phenomena, which take place close to the border of two physical phases; the aim of the paradigm consists in the deep understanding of the elementary causes and effects which explain the features and applications of each unit operation. The transport phenomena paradigm extend the content of chemical engineering to a fundamental, theoretical science, closely linked with physics, mathematics, mechanics, thermodynamics, electromagnetism etc, becoming a true "Nucleus of Discovery" (Fig. 3). The birth of the second paradigm was, therefore, the consequence of the need for a deep, scientific knowledge of the phenomena which explain what happened inside of unit operations. Engineering, in the last analysis, depends heavily on heuristics to supplement incomplete knowledge. Transport phenomena can, however, prove immensely helpful by providing useful approximations, starting with order of magnitude estimates, and going on to successively more accurate approximations, such as those provided by boundary layer theory (Bird et al. 2002).

At last, it appears the trend to gather all the three transport phenomena in a single concept, respectively the property transport (Brodkey and Hershey, 1988). This very high systematization is justified by the analogy of the transport phenomena, respectively the structural similitude of differential equations and boundary conditions which describe them. In this treatment, each fundamental transport process becomes a specific case.

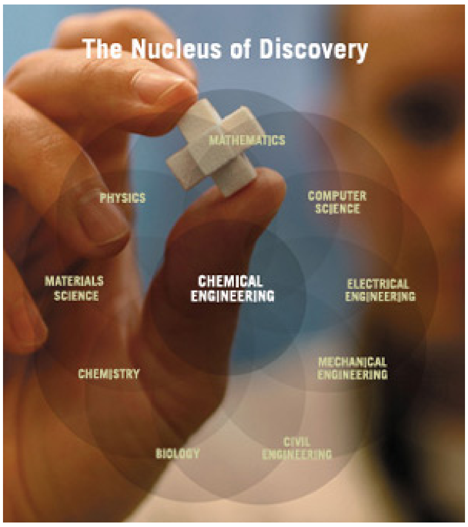

Fig. 3. Nucleus of Discovery: Chemical Engineering.

4. THE THIRD PARADIGM: CHEMICAL PRODUCT ENGINEERING

In the second part of 20^{th} century the diversity of industrial products (in many cases with close properties and with the same utilization) has a huge growth, and correspondingly, very strong market fights have evolved between producers companies. The same things happened with chemical products. The importance of properties and qualities of chemical products have become essentially. Until recently, the main purpose of chemical engineering has been to obtain the lowest cost process. Even process related issues like reliability, product purity, pollution control, etc. have been ultimately translated into costs that must be minimized. In contrast, chemical product design try to obtain the most added value for a product through enhanced product properties. This is a more complex task than a mathematical treatment to maximize profit. The profit depends in some unidentified way upon the complex set of product properties. Therefore, product engineering problems can't be solved by traditional chemical engineering approaches. Their solution requires not just additional chemical engineering approaches, but even more fundamentally, and that is why *product engineering* should be recognized as a *third paradigm* of chemical engineering, as first hinted in 1988 (Committee on Chemical Engineering Frontiers, 1988). It can be assumed that the third paradigm was imposed by the fight for technical and economical products performances generated by a strong competitive market environment.

New chemical products have been created by combining a wide knowledge of existing chemical products with a big amount of scientific experimentation. A combinational explosion of product options will limit all experimental techniques. Therefore, it is desirable to minimize experimentation through a systematic consideration of product formulation prior to experimentation. Product engineering techniques is largely based on heuristics when data are limited, followed by detailed calculations when data become available, this being the essence of the third paradigm. The basics of the third paradigm were stated in the book of Cussler and Moggridge (1st ed., 2001 and 2nd ed., 2011, Fig.4). Here they have proposed a generic framework for chemical product design, based on a 4-step algorithm: (1) identify customer needs, (2) generate ideas to meet those needs, (3) select among the ideas, and (4) manufacture the product. The step four of chemical product design contains all the following four steps of chemical process design: (1) batch vs. continuous process, (2) inputs and outputs, (3) reactor and recycles, and (4) separations and process integration. The authors admit that this four step algorithm is a major simplification that affects effectiveness in specific cases. But, this procedure can be an excellent starting point, very useful to expand each specific case.

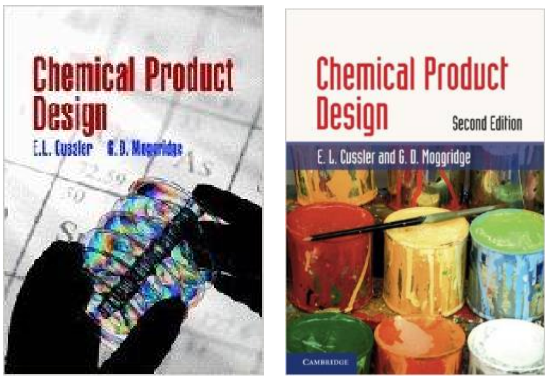

Fig. 4. The first (2001) and second (2011) edition of Cussler and Moggridge book.

Related to the controversy of the key to product design, management or technology, Cussler and Moggridge consider that the application of technology is central to chemical product design.

Hill (2009) proposed a methodology for designing homogeneous chemical products when limited data are available. The methodology has the following eight steps: (1) product definition, (2) technical product requirements, (3) product performance relationships, (4) product candidate generation, (5) product candidate selection, (6) process design, (7) risk analysis, and (8) financial (business case) analysis. This methodology assumes that a homogeneous product can achieve all the required product properties. This approach ignores the class of structured products, which achieve their properties through a microstructure that is determinant by the interaction of its components and the manufacturing process (Edwards, 1998). Product engineering for structured products is significantly more complex, as the product and process must be simultaneously designed (Hill, 2004). Two primary approaches have been proposed: (1) generation and systematic reduction of the number of alternatives through heuristics, and (2) optimization of the set of all potential alternatives through mathematical programming (Hill, 2009).

Due to major changes in the chemical industry the product design role and merits are continuously increasing, but this is not an argument that process design should disappear. Product design and process design must be used together, in agreement with these changes in the chemical industry.

5. THE FOURTH PARADIGM: SUSTAINABLE CHEMICAL ENGINEERING

Nowadays the concept of sustainability is imposed in al human activities fields, especially in industrial domains. Chemical industry, as a huge materials and energy consumer, and with a strong ecological impact, could not remain outside of sustainability requirements. The basics of the fourth paradigm – *sustainable chemical engineering* – are now formulated. This new paradigm is set on the recognition of limitation of resources, the requirement for inter and transgenerational equity within human society and the need for preservation of life supporting natural systems (Narodoslawskty, 2013). The contemporary discussion around the concept of sustainability started with Brundtland report (World Commission on Environment and Development, 1987). In this report, sustainability or sustainable development is defined as "the development that meets the needs of the present without compromising the ability of the future generations to meet their own needs". This report clearly frames the challenge of sustainability: it requires human society to live within the limitation of our planet in a way that allows infinite development in temporal terms. Sustainability becomes more and more important in the modern economy, and in 1999 the Dow Jones Sustainability Indices were started. Corporate sustainability is considered a business approach that creates long-term shareholder value by embracing opportunities and managing risks deriving from economic, environmental, and social development (Heinzle et al., 2006). Nowadays, these three dimensions constitute sustainability and are considered the three pillars carrying this concept. All these three parts are equally important in sustainable development. They are not independent of each others; on the contrary, there is manifold interaction between them. For the economic assessment there are already a number of books, especially in the chemical engineering field, that cover cost and profitability subjects in detail. From these, Peters et al. (2003) is standard reference book. There are published many methods for environmental assessment. The method proposed by Heinzle and Biwer (2004) provide an approach that allows the scientist or engineer in process development to make an environmental, health, and a safety assessment within a reasonable time. By this method, a global environmental index EI, which indicates the environmental relevance of a whole process, is calculated. The method requires material flows to compute Mass Indices (which is a metric for the material intensity of the process), and the so-called ABC classification (provided by user in order to compute individual Environmental Factors EF_i – a metric for the environmental impact of each component *i*). The environmental index EI is now computed from Mass Indices and Environmental Factors. The identification of relevant social aspects and a corresponding set of indicators is a very complex task. There are important differences between processes and products, countries specificities, national and international legislations, etc. For the social assessment of bioprocesses, by taking into account the results gained from the multi-perspective approach of technology assessment, including the implications of an international stakeholder survey, Heinzle et al. (2006) have identified these eight significant aspects: health and safety; quality of working conditions; impact on employment policy; education and advanced training; knowledge management; innovative potential; customer acceptance and social product benefit; and societal dialogue. A good example of the interaction of the sustainability pillars is given by Heinzle et al. (2006), respectively the use of genetically modified (GM) crops in agriculture. Within environmental dimension there are two opposing aspects. On the one hand the use of GM crops might reduce the use of pesticides and increase the amount of food that can be produced per square meter. On the other hand, there is the risk that GM plants might be distributed in the environment and may cause ecological damage, a hazard which is difficult to predict and quantify. The acceptance of a new technology can strongly affect its economic success. In US the acceptance of crops is relatively high. Although the risks are the same, the acceptance in the EU is low. The fears of a possible direct impact on human health, and also on the environmental quality as an aspect of the quality of life are the reason for this low acceptance. This reduces the possible market size, probably also the price that can be achieved, and may cause additional costs to protect the crops in the field. Furthermore, the low acceptance has led to higher legal constraints for the use of GM crops. Owing to these social factors, the economic advantage of GM crops is substantially reduced and GM crops are used less in the EU compared with the US.

The previous example illustrates the demand to consider all three dimensions of sustainability in all stages of process development. As a consequence process optimization evolves to multi-objective optimization (Rangaiah, 2009). In traditional process optimization the objective function is a scalar one. In multi-objective optimization of sustainable processes the objective function is a vectorial one, with economical, ecological and social components (Taras and Woinaroschy, 2011; 2012).

Chemical engineering, with its strong systemic orientation and its function to link natural sciences, engineering and industrial practice, is in "pole position" among many other engineering sectors to meet the challenges of sustainable development. It is a key engineering discipline for adapting human society towards sustainability (Narodoslawskty, 2013).

A main task of chemical engineering during its entire evolution was to reduce material and energy consumption. Chemical engineering is placed on the first positions among other engineering sectors related to these consumptions. Before sustainability era, reducing of material and energy consumption was imposed by economical reasons (increasing profitability, decreasing products cost). Environmental assessment modifies drastically the material and energy consumption, now these amounts are not the unique objective. The main feature consists in the change of material and energy resources base both in order to preserve the frequently used resources, but also to involve new sources, especially environmentally friendly ones. Related to the use of new raw materials an example in this direction is the book Bioprocessing for Value-Added Products from Renewable Resources (2007). Related to energy resources the limitation of fossil resources adds to the pressure on society to look for other sources. A particular challenge for chemical engineering is providing energy storage in a sustainable way. Renewable sources for energy and material will become more important and will require a massive re-structuring of industrial processes (Narodoslawskty, 2013).

In the field of reducing of material and energy consumption, increasing of research activities and applications of process integration (Klemes, 2011; Kiss, 2013) must not be omitted. Sustainable development will generate formidable challenges and vast chances for chemical engineers in the actual century.

6. CONCLUSIONS

Three paradigms have a paramount importance in the past evolution of chemical engineering. Nowadays, a fourth paradigm, sustainable chemical engineering, must be taken into account. Related to the paradigms role in the evolution of chemical engineering, it is relevant the Kuhn conception (Kuhn, 1996), respectively that even when paradigms are known to be inadequate, their inadequacies are frequently minimized, or even ignored by the scientific community. Nevertheless, if and when a paradigm reaches a crisis where its technical inadequacies are brought into focus, perhaps driven by social requirements, a new paradigm will arise to explain what the prior paradigm could not. During the evolution of chemical engineering each new paradigm was a step forward which has extended the manifold of the tasks that can be solved. However, no older paradigm is derelict. In fact, almost all paradigms must be used together in order to solve the complex chemical engineering problems.

Of course, the discussion about paradigms of chemical engineering cannot avoid the subjectivity. Some personal ideas of the author and the references selection are, doubtlessly, questionable. There are hundreds works that deal with the fundamentals of chemical engineering, with its past, present, and future. Here, we have tried, very briefly, to emphasize the importance of the basic paradigms in chemical engineering evolution.

IN MEMORIAM

The present work is dedicated to the memory of my professor Emilian Bratu (1904–1991), the founder of chemical engineering education in Romania.

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PARDIGMELE INGINERIEI CHIMICE

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Rezumat: Se prezintă dezvoltarea ingineriei chimice călăuzită de cele patru paradigme principale: operaţiile unitare, fenomenele de transport, ingineria de produs, ingineria chimică sustenabilă. Punctul de plecare constă în definiţia paradigmului ca “un set de ipoteze, concepte, valori şi practici ce constituie un mod de reprezentare a realităţii pentru o comunitate care le împărtăşeşte, in special intr-o disciplină intelectuală”. In legătură cu rolul paradigmelor în evoluţia ingineriei chimice, este relevant faptul că chiar şi atunci când paradigmele sunt recunoscute ca inadecvate, respectivele inadecvanţe sunt frecvent minimizate, sau chiar ignorate de comunitatea ştiinţifică. Cu toate acestea, dacă şi când apare criza unui paradigm şi inadecvanţele sale tehnice sunt aduse în prim plan, se va naşte un nou paradigm ce va explica ceeace paradigmul anterior nu o putea face. In cursul evoluţiei ingineriei chimice, pornind de la începuturile sale de la sfârşitul secolului al 19-lea şi pâna în prezent, fiecare nou paradigm a reprezentat un pas înainte ce a extins diversitatea de probleme rezolvabile. Totuşi, nici-un paradigm anterior nu este abandonat. De fapt, aproape toate paradigmele trebuie sa fie utilizate coroborat în scopul rezolvării problematicii complexe a ingineriei chimice.