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Chemical And Environmental Engineering Units And Quantities.

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Abstract

Among other places, the International System of Quantities (ISQ) will be utilized in textbooks and instruction, scientific and engineering publications, conference proceedings and papers, and industry.The International Organization for Standardization publishes the 13-part ISO 80000 Quantities and Units standard, which includes the names of quantities along with their symbols and units.The majority of the components are made up of mathematics and the natural sciences, including physics, light and radiation, acoustics, physical chemistry, atomic and nuclear physics, and condensed matter physics. Furthermore discussed are characteristic numbers and a few technical specialties, including mechanics, thermodynamics, and electromagnetic. The International System of Units (SI) serves as the basis for the units. Regretfully, the standard does not address chemical and process engineering, environmental engineering, or engineering economics. . This article suggests adding them to the ISO standard under the provisional heading of “Chemical and Environmental Engineering.” The standard is proposed to include the following additional sections: (a) reaction and separation engineering along with mass transfer and reaction kinetics; (b) process design, control, and optimization; (c) process economics, mathematical modeling, and operational research; and (d) environmental engineering with regard to pollution reduction, climate change, resource efficiency, zero waste, and the circular economy. Approximately 70 pieces, or the average of ISO 80000 parts, are planned but not required. The SI unit, the quantity name and definition (with an equation if applicable), and the notes (running number will be added later) are all included in each quantity item. The standards are outlined in ISO 80000-1 General Rules, and the other ISO 80000 parts' practices are followed; the amounts that are already mentioned in the other parts are not duplicated. The Green Book guidelines of the International Union of Pure and Applied Chemistry (IUPAC) are also followed. Traditional textbooks, encyclopedias, and handbooks from the environmental and chemical engineering disciplines were among the works consulted. The following list includes some typical errors made while printing quantity and unit symbols.

Keywords : *chemical; environmental; engineering; quantities; standard; symbols; units.*

INTRODUCTION

The system of quantities was the final one to be created and established worldwide, following the letters, numbers, and units. When a phenomena, body, or substance has a magnitude that can be represented by a number and a reference (unit), that property is said to have quantity. The worldwide Union of Pure and Applied Physics (IUPAP), founded in 1922, and the International Union of Pure and Applied Chemistry (IUPAC), founded in 1919, were the first worldwide organizations to attempt standardizing chemical and physical quantities. For official usage only, IUPAP developed the first edition of Symbols, Units and Nomenclature in Physics in 1961. The 1987 revision is accessible online [1]. The Manual of Symbols' first edition was released by IUPAC. The first edition of the international standards ISO 31 Quantities and units in 13 sections [4] and ISO 1000 SI units and guidelines for usage [5] were released in 1988 by the International Organization for Standardization (ISO) in collaboration with the International Electrotechnical Commission (IEC). A revised version of both standards was released in 1992. 2009 saw the replacement of the two standards with ISO 80000 Quantities and Units, which contained 13 slightly rearranged sections [6]; the most recent edition was released in 2019, with the exception of the sections indicated in parenthesis (parts 1 and 6 will be revised in 2021):

(1) General (2009)
(2) Mechanics
(3) Thermodynamics
(4) Electromagnetism
(5) Space and time
(6) Mathematics
(7) Radiation and light
(8) Acoustics (2020)
(9) Atomic and nuclear physics
(10) Physical chemistry and molecular physics

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(11), and characteristic numbers
(12) Physics of condensed matter;
(13) Technology and information (2008)
Information on units and amounts, printing guidelines, terminology used in physical quantity names, number rounding, and logarithmic quantities are all included in the general section.
Each subset's quantities, along with the item number, quantity name, symbol and description, unit symbol, and eventual notes, are listed in parts 3–13 (part 14 has been withdrawn).
Since 2019, an alphabetical index of amounts has been included at the conclusion of each section to facilitate item searching. Three more sections are being developed, numbered 15–17 (Logarithmic and related numbers, Printing and Writing Rules, Time Dependency) [7].
The aforementioned list of ISO 80000 components shows that, despite their importance in many ways (turnover, profit, investments, employment, research, etc.), the chemical and process industries (CPI) are not listed. Pharmaceutical, cellulose and paper, metal, ceramic, textile, food and beverage, and other industries are all part of CPI in addition to the chemical industry. Modeling, design, construction, analysis, optimization, operation, control, process economics, safety, hazard assessment, transport phenomena, etc. are all included in this field.Despite the fact that we are experiencing a climatic crisis, species loss, pollution, and a shortage of raw materials, environmental science and engineering do not have a standard for amounts. The ISO 80000 and SI regulations are not being followed by even environmental management quantities in the ISO 14000 family, such as the performance indicators in ISO 14031 [8]. We encounter jargon like "Paris Agreement," "European Green Deal," "Net-zero emissions by 2050," and "sustainable development goals" on a daily basis. They are addressing issues including biodiversity, resource efficiency, zero waste, the circular economy, greenhouse gas emissions, renewable energy, and essential raw resources. As a result, names, symbols, and units for the amounts used in the region must be defined using internationally accepted standards.

METHODS

Textbooks, manuals, standards, lexicons, encyclopedias, and handbooks on chemical and environmental engineering, such as Ullmann's Encyclopaedia [9], Perry's Chemical Engineers' Handbook [10], SI brochure [11], and Google searches, were all included in the literature search.
Due to the restricted number of things, the most significant quantities have been chosen based on their significance and frequency of use, as well as on the references that have been given and the author's own experience.
The proposal begins with quantities related to chemical engineering, moves on to process economics in design, and concludes with environmental considerations. A few typical errors in quantity and unit symbols are listed. The literature also has them [12].The suggested terms will be published in this magazine and discussed at a few professional gatherings. Following modifications, they will be submitted to the American Institute of Chemical Engineers (AIChE), the British Institution of Chemical Engineers (IChemE), the European Federation of Chemical Engineering (EFCE), and the Deutsche Gesellschaft für chemisches Apparatewesen (DECHEMA). They will be required to submit the proposal to the Technical Committee ISO/TC 12 Quantities and Units following its approval.

FINDINGS AND CONVERSATION

Since they span a wide range of issues based on chemistry, physics, mathematics, economics, etc. that deal with a very broad range of materials, procedures, and equipment, chemical and process engineering quantities are quite comprehensive. For example, ([9,10]):
Fundamentals of fluid and particle dynamics, heat and mass transfer, chemical thermodynamics and kinetics, statistics, and optimization techniques; • Heterogeneous gas catalysis, electrolysis, photo-, or plasma-chemistry, fixed or fluidized beds, homogeneous liquid or gas reactions, gas-liquid or gas-liquid solid reactions, etc.;
Process design, construction, operation, control, and development with modeling, costing, simulation, optimization, process safety, pollution, energy integration, waste management, and reuse, circular economy, and renewable energy; • Unit operations like size reduction and classification, transportation, and storage; mechanical, magnetic, and electric separations; mixing and conveying; heating, cooling, adsorption, absorption, extraction, ion exchange, distillation, evaporation, sublimation, refrigeration, crystallization, and drying."
Consequently, there is a genuine need for an ISO standard on numbers and units in these domains.
In addition to that, the IUPAC Green Book [3] would benefit from a few more chapters.

Fundamentals of Chemical Engineering and Unit Functions

Table 1 lists a few fundamental quantities that are not covered in other sections of ISO 80000. Constant values are extracted from CODATA [13] and the SI brochure [11].

Engineering Chemical Reactions

The core of chemical engineering is a chemical reaction, in which reactants enter a reactor, undergo a reaction, and produce products. Consequently, it is necessary to start by talking about amount flow rates. English literature uses the letter F [14], while German literature uses it for Chemical Reaction Engineering [15]. ISO 80000-4-30.2 and 4-31 specify mass flow rate (qm, or kg/s) and volume flow rate (qV, or m3/s), however they do not define quantity-of-substance (or simply "amount" with the unit mol) flow rate, nor does the Green Book [3].Similarly, one may use qn (mol/s) (Table 2). Mass flow, jm, was also specified by ISO 80000-4; as a result, amount flow, jn, is also listed.

The next quantity to be defined is conversion. It is frequently referred to as Umsatzgrad, or fractional conversion. The Green Book and ISO 80000-9 both use the rate of (absolute) conversion and the extent of reaction, ξ (mol).

ξ = dξ/dt (mol/s). The conversion of a reactant A is denoted by the symbols XA, xA, or f A in American textbooks, whereas UA (Umsatz) is used in German ones. Here, XA is adopted. Reactants are represented by the subscripts A, B, C, etc., and reaction products by the subscripts P, R, S, etc. The quantity ratio of the desired product P to all products S generated is known as selectivity, or σP. Reactors with a constant volume can use the definition in Table 2.The quantity ratio of supplied reactant A to desired product P is known as yield (Ausbeute). It can be overall (φ) or instantaneous (φ). As φP = σPXA, yield is always the selectivity times the conversion.

Only ideal gases or fluids with a constant volume may be referred to by the term "rate of reaction." In other situations, it is suggested that the rate of conversion for any species be applied; in fluid-solid systems, the "specific rate of conversion" is used for solids. The "areic rate of conversion" works well on solid catalyst surfaces in gas-solid systems and on interfacial surfaces in two-fluid systems.

Alternatively known as the "rate of production," the term is employed in the context of selectivity, where qn,B = φ qn,A0 = σBXA qn,A0. The "volumic rate of conversion" is based on the volume of a reactor rather than the volume of a fluid.

ISO 80000-9 describes equilibrium constants but not space-time, space velocity, or yield. The time needed to fill a reactor volume with its volume flow rate of feed under specific conditions is known as space-time, or τ (s). The reciprocal between space and time is space velocity, or s (s^{-1}).

The volume flow rate returning to the reactor entrance divided by the volume flow rate exiting the system is known as the recycle ratio, or R (1).

Table 1 only displays a small number of response engineering quantities. The number of molecules (molecularity with distinct orders of reaction) can vary and affect the rate equation, as can single and multiple (series or parallel) reactions, elementary and nonelementary. The reaction may be exothermal or endothermal, and the effects of temperature and pressure may differ. Furthermore, we are aware of several reactor types, including batch, plug flow, mixed flow, and recycle reactors. Both ideal and nonideal flow patterns and contact might occur; in the latter instance, dispersion, convection, or early mixing must be taken into consideration.

Lastly, there are fluid-fluid (liquid or gas), fluid-solid, catalytic, and different biochemical (enzyme or microbial) reactors; in these situations, heat and mass transfer are also crucial. The dispersion coefficient, D (m2/s), mean time of a passage, t (s), and variance, σ 2, are significant numbers in relation to axial dispersion; the Green Book [3] provides information on the probability distribution, statistics, and uncertainties (pp. 151, 152). The rate of conversion equations from Table 2 can be applied to catalytic systems; they can be based on the reactor's void volume, the mass or volume of catalyst pellets, the catalyst surface area, or the reactor's overall volume; a catalyst's activity, a (1), may also be significant.

The standard may include additional measurements for heterogeneous reactions with two or more phases, such as the interfacial area density, a (m2/m3), effectiveness factor (ε or η, 1),

Additional Unit Functions

There are a lot of different types of unit operations. Let's use distillation as an illustration. A flow rate name symbol, such as F for feed flow rate, D for distillate flow rate, S for side-stream flow rate, V for vapor flow rate, etc., is typically used to express amount flow rates (mol/s). In this instance, qn,F, qn,D, qn,S, and qn,V are all subscripts that indicate distinct flow rates and can be used appropriately as a quantity sign. The term "duty," such as condenser duty or reboiler duty, for the heat flow rate (W), while their symbol, is the second instance of disregard for ISO 80000 regulations.

Q complies with the ISO standard. Furthermore, the empty portion.

Design And Development Of Processes

Economic analysis, process optimization, decision-making, process evaluation that includes capacity determination, and process development data—both internal and external—are crucial. The most common quantities in process engineering optimization using economics and mathematics are shown in Table 4. Since statistics are extensively covered in ISO standards, they won't be discussed here. In contrast, the field of economics lacks international coordination and is not standardized, frequently using acronyms in place of symbols [16].The three most popular cost indexes are Nelson-Farrar (since 1946), Chemical Engineering (CE, since 1958), and Marshall and Swift (M&S, since 1926). When added to capital investment, the battery-limits capital investment is obtained. Capital investment comprises equipment expenses, instrumentation, plumbing, insulation, electrical, and engineering costs without any contingencies; contingencies amount to roughly 15% to 20% of capital investment. Funds for wages and salaries, the acquisition of supplies and raw materials, etc., are all included in working capital.

The total of a product's processing costs plus general, administrative, and selling costs is known as an operating expense. They can be divided into three categories: direct, indirect, and product expenses. Raw materials, utilities, labor, maintenance, supervision, payroll fees, operating supplies, apparel and laundry, royalties, technical services, and environmental control are all considered direct expenses. Plant indirect costs and depreciation are examples of indirect expenses.

Packaging, loading, and shipping costs are added to operational costs to get the total manufacturing expense. The net sales made from a product sale to a customer are known as revenues.

The difference between the product's selling price and the cost of its raw materials is the value added to the product.Inflation is causing money's time worth to decrease. The expected return on borrowed capital is included in the interest rate. Money's present value (Vp) is less than its future value (Vf). A charge is made for the usage of borrowed funds when a business lends money; the interest rate takes into account the borrower's costs, expected inflation, and intended profit. The cost of capital, which is represented by an interest rate, is the total cost to the business of borrowing funds from all sources (stocks, bonds, and loans).There is a tiny distinction between quantity amortization and depreciation, yet both terms are frequently employed. The annual cost is referred to as amortization if the life expectancy is precisely determined. This period of time is referred to as depreciation if it is estimated.

Units, Symbols, And Environmental Quantities

Both the Paris Agreement and the 17 Sustainable Development Goals (SDGs) are becoming more and more important, as are sustainable development and its three pillars—economic, social, and environmental. The biggest issue is the climate disaster brought on by global warming and greenhouse gas (GHG) emissions. Some of the most significant numbers in this field are shown in Table 5, which goes from pollution to GHG emissions and climate change.The most hazardous gases, which are converted into CO2 equivalents, are found in greenhouse gases (GHGs), along with water vapor (H2O). These gases include carbon dioxide (CO2), methane (CH4), nitrous oxide (N2O), ozone (O3), chlorofluorocarbons (CFCs), and hydrofluorocarbons (HFCs). The term "factor" should be used when the two quantities (in this case, electricity and mass) have the same dimension, with a unit of 1; the term "coefficient" should be used when the two quantities have different dimensions. The emissions coefficient of electricity is also known as the "electricity-specific emission factor." The unit used in ecological footprint is the global hectare, represented by the symbol gha. This is incorrect because the area considered is global, but the unit is hectare—global area, Ag, in ha [17]. Since IUPAC does not encourage using units like ppm, ppb (part per billion), etc., the amount (of substance) fraction denoted by the symbol x and unit μmol/mol or nmol/mol, respectively, are used instead.Fossil fuel combustion in transportation, electricity generation, industry, homes, waste fermentation, and agriculture is the source of greenhouse gas emissions. There are other ways to express the CO2 equivalent emissions, such as mass per energy produced (kg/(kW h), or mg/J), mass per fuel volume (mg/L), mass per distance traveled (g/km), and mass of CH4 released or absorbed per agricultural area (kg/ha). They can be computed for each individual, business, city, nation, or planet. There are currently no unique names or symbols available.

CONCLUSION

The 13 sections of the ISO 80000 standard on quantities and units do not include representation from chemical and process engineering, environmental science, or environmental engineering. Sales of the chemical industry alone in 2019 totaled 3.66 trillion euros (1012 EUR), or 4.2% of the global gross domestic product (74.76 TEUR). It differs from the manufacturing sector in that it is highly specialized and multidisciplinary. In the field of sustainable engineering, particularly in environmental sustainability, it is also crucial. As a result, it merits a particular place in the standardization of units and quantities.Numerous amounts and units have names that do not comply with ISO 80000 standards, according to the literature research. In the fields of process economics and chemical and environmental engineering, this work attempted to address and suggest some of the most significant quantities.The acknowledged guidelines in the ISQ and SI systems were attempted to be followed with regard to the names and symbols chosen.Naturally, the selection of quantities is merely an example of the names and symbols that will be used in the proposal. Although there are standards for quality, management, statistics, and health and safety, this does not negate the need for a review of quantity names, units, and symbols in those domains. Furthermore, the fundamental ideas of process modeling, simulation, synthesis, design, integration, and optimization had not yet been covered.Every voyage begins with a single step, yet the area is too vast and complicated to choose specific quantities, names, and symbols.The International Organization for Standardization, as well as national and international associations, must discuss the proposal that includes the list of quantities, their names, symbols, and units. Given that their significance extends beyond the realm of the chemical and process industries, environmental and economic quantities could potentially be examined as distinct standards.

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