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ABCs of Teaching Analytical Science

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Basic Mathematics and Physics for Undergraduate Chemistry Students According to the Eurobachelor[®] Curriculum

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Introduction

Many subjects of mathematics and physics are relevant to teaching analytical chemistry (AC) but a few key topics are essential preparing students to the master level [1-4]. Mathematics and physics are important to understand the operation of advanced apparatus and for the interpretation of data. The overall aim of introducing 10 ECTS credit points of mathematics and 10 ECTS credit points of physics in addition to 15 ECTS credit points for AC is to maintain the education in AC at a high level to benefit science and the progress of AC. The European Association for Chemical and Molecular Science Division of Analytical Chemistry (EuCheMS-DAC) have suggested a curriculum for the bachelor degree [4].

As the language of science is mathematics, similarly physics promotes the understanding of basic mechanisms and chemical interactions. AC requires a multidisciplinary approach to understanding the art of quantifying chemical species in various mixtures and matrices [2]. Thus, students of chemistry pursuing competence in AC are faced with numerous topics such as physics, computing, interfacing, electronics etc. at a relatively high level in order to devise new methods of analysis using advanced apparatus.

Organizing a curriculum of mathematics

The initial interest in teaching mathematics and physics arose for "self defense" reasons after it became clear that the students could not cope with statistics of repeated measurements and propagation of uncertainties. Items such as the Gauss law of propagation of uncertainties and its application to analytical measurements caused them problems due to lack of knowledge of partial derivatives. Many students were also often deficient in the physics of classical mechanics and optics some of which also require familiarity with aspects of geometry.

Discussions with colleagues confirmed similar difficulties in teaching thermodynamics and reaction kinetics. The items of basic mathematics and physics that chemistry staff regarded as essential for chemistry students in the first two years of an undergraduate course were prepared. Lists from the various areas of chemistry had 95% of the items in common. The problem of lack of adequate background in mathematics was not unique to chemistry students in Belfast, for example, the Royal

Society of Chemistry published guidelines, "Mathematics in Chemistry Degree Courses" [5], two years later after our first course. The content was remarkably similar to our (Burns & Hu) list, thus a national consensus existed of what was required as prior knowledge or that needed to be imparted via remedial/revision teaching.

Given the topics, the problem to be solved was how to produce a logical sequence for the items so as to avoid giving too much on trust and also too many back tracks to items already dealt with. Reported here are the content sequences that were found to be effective and indications of when and how to connect the mathematical items to specific aspects of chemistry (details of which are given in the supplementary material). The content of each section of the proposed mathematics course was prepared in detail and the flow of concepts through the various possible sequences of sections examined. The sequence reported here was chosen by consensus as optimum.

Year I module, "Chemical Computation" (see Fig. 1), started with the section on stoichiometry, for which simple algebra was a sufficient background, this was included to deal with demonstrable weakness and/or lack of students' confidence in basic chemical arithmetic. This was followed by the basic mathematics section, then by repeated measurements and estimation of uncertainties. Students were given exercises/problems in stoichiometry, mathematical manipulations, and the evaluation of analytical data, prior to seminar/discussion classes on each set of topics. The computing lectures/demonstrations and practice sessions were run in parallel to the mathematical material and included calculations using spread sheets.

Organising the Curriculum of physics

In the recommendations by EuCheMS-DAC about essential physics for students of chemistry, it is recognised that this subject is of considerable difficulty but recognises the necessity of physics to the understanding of fundamental mechanisms of chemistry [6]. In order to maintain the progression in intellectual challenges it is important to make use of the relations between physics and chemistry when treating advanced topics. Understanding of physics relies on a simultaneous education in mathematics and both subjects should be offered in basic modules, to shape the students' intellectual development. The 10 ECTS credit points allocated to physics imposes limitations to the number of topics in basic modules [6, 7]. From among the wealth of available subjects EuCheMS-DAC recommends a number of priority topics from classical mechanics, liquid-

flow dynamics, optics and electromagnetism thermodynamics, and quantum mechanics, as indicated in the supplementary material, Tables 1-5. These topics support the understanding and operation of modern technical apparatus and interpretation of the data.

Contemporary methods of teaching are encouraged. Lectures, seminars and practical classes should be balanced and offered in appropriate quantities. Individual challenges, team projects, peer-review problems, e-learning, problem-based learning and oral presentations will all assist the student communicating results to wider audiences.

Concepts of physics essential to teaching analytical chemistry

Classical mechanics is needed for understanding statics, motions and interactions (Fig. 2). The treatment of nature by mathematical tools provides an effective description of reality, but one which requires much training to understand. Universities are encouraged to support the use of practical classes, demonstrations and laboratory work that promotes the students insight to the subjects. Teaching of mechanics offers an excellent opportunity to demonstrate the correspondence between simple theoretical modelling and experiment. Since chemists often have to model complicated systems of molecular interactions, it helps to understand their basics in physics, e.g. spheres rolling on a slope or the properties of a spinning top. Such activities are encouraged despite the increase in laboratory hours is also accompanied by an increased use of resources. Some of the concepts, such as angular momentum and moment of inertia, apply directly to understanding of molecular motion.

Despite the obvious links to chemistry, only a limited number of subjects within liquid-flow dynamics (Fig. 2) are normally taught to chemists. Further, as the fundamentals of liquids are traditionally contained in chemical thermodynamics in order not to create duplication, a small number of subjects are attached to physics, e.g. Bernouilli's equation.

In order to allow insight into the world of electronics, a number of topics including electromagnetism (Fig. 2) have to be dealt with. The reason for including electronics is to give students' skills to mend faulty electronic apparatus at a basic level, such as checking fuses, diodes, capacitors and transistors. Further, for safety, the measurement of voltages and currents, both very high and very low, must be taught. Finally, interfacing and automation constitute subjects of increasing importance to AC where programming skills and software skills are also needed. In

parallel to quantum mechanics, electromagnetism is needed to understand the behaviour of electromagnetic radiation and radioactive decay. Although magnetism is not important to chemical reactions, it is of paramount importance to NMR spectroscopy [8], an important analytical tool. Accordingly, topics of spin, magnetism and superconductivity should be available in optional credits of chemistry.

In thermodynamics and statistical thermodynamics (Fig. 2), several topics can with advantage be shared between the teaching of chemistry and of physics. The concepts of energy, heat and work are treated similarly with properties of gases as the common points of origin. However, these concepts may also be used to show the relations between units, which are of great importance to promote the comprehension of new definitions of the fundamental units.

When teaching chemistry and physics, demonstrations, experiments and practices facilitate many inherently difficult issues of understanding and give a unique opportunity to make classes interesting and vivid. Although very demanding on resources, EucheMS-DAC supports application of contemporary means of learning that facilitates the process of learning. Individual work in a competitive environment benefits a scientific trial but 'seasoning' by work in groups using pedagogical tools promotes good profiles for future career prospects.

Conclusions

The mathematics section of the course has run with only minor modifications for 18 years. The lectures are supported by seminars, tutorials, and sets of problems. The items needed for second year physical chemistry, namely, group theory, vectors, matrix algebra were and are introduced as needed within the main chemistry syllabus. The mathematics material (lecture text and copy of slides) have also been used successfully for self-study by individual mature students on ancillary chemistry courses. The various sections of chemical computation are now not given in a single block, the section on stoichiometry is now included in laboratory calculations, the statistics section is incorporated into the second year module, "Instrumental Analysis". The recommended text remains that by Scott [9] or Coelett and Doggett [10].

Teaching physics is a rewarding field of science where demonstrations may be used to demonstrate complicated principles by relatively simple means. The proposed workload of physics may be

considered as an absolute minimum, as recommended by DAC. Universities may offer 10 ECTS compulsory and 10 ECTS elective with a lower number of credits given to exercises [11]. However, application of physics to the Eurobachelor[®] curriculum requires teaching by chemists at a more advanced level including principles of physics demonstrated by means of advanced apparatus. Although more demanding on resources this also brings back the fun of physics. A total of 10 ECTS credits is suggested for the training of physics at the basic level with the aim however to ensure the highest level of competence in AC. For students interested in developing their skills of physics should be offered a platform of elective courses covering 10 ECTS credits. A large amount of knowledge is required for the student if they intend to participate in the science of analytical chemistry, which after all is one of the prime objectives of courses given in a university environment. While the recommendations of mathematics are based on a course run for many years, the recommendations on physics is built on recent experience and observations on that required for students' participation in development of analytical methodology.

Details from other academics approaches to the problems discussed are welcomed these will inform the basis of future discussions within DAC and other interested parties about further development of the teaching of analytical chemistry at undergraduate level.

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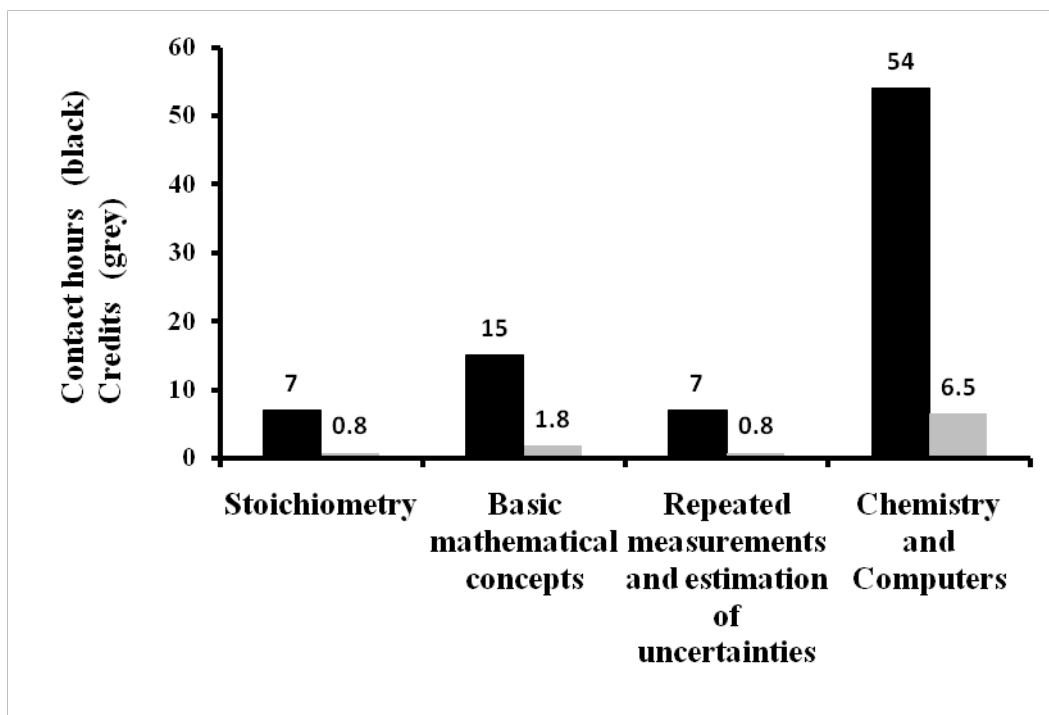


Figure 1. Year I module of mathematics for Chemistry represented by four key areas of effort. The contact hours (black) and credits (grey) includes exercise, seminars and exams. Workload factor = 3 and one ECTS = 25 contact hour per semester week.

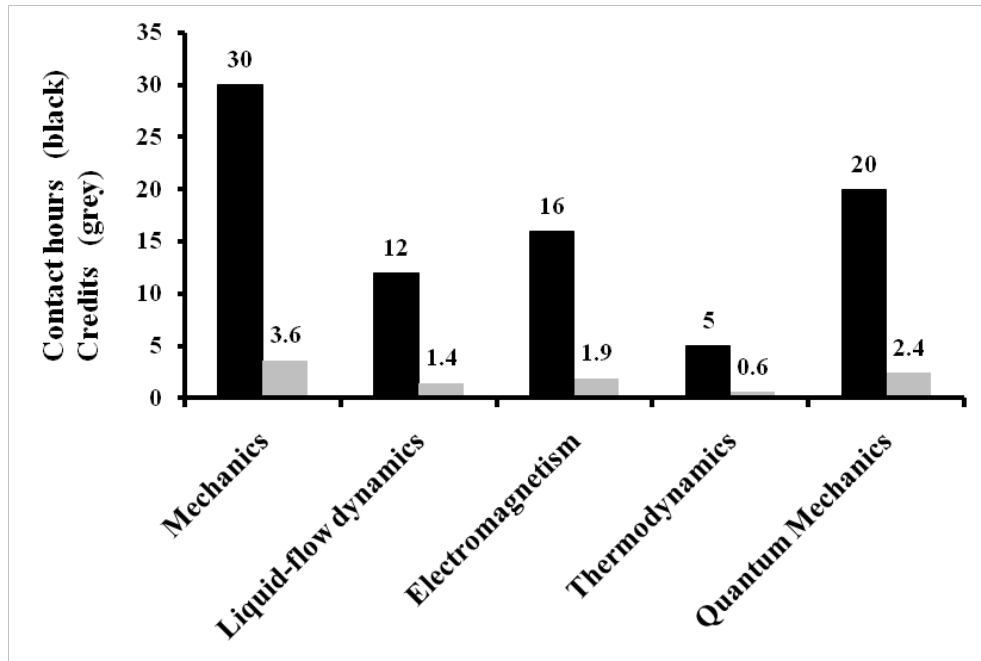


Figure 2. The total workload expressed in contact hours (black) and credits (grey) for a 10 point module (workload factor = 3 and one ECTS = 25 contact hour per semester week) in the bar diagram expresses the weighting of individual subjects, as recommended by DAC.

Supplementary Material

Comment and discussion on the individual lectures on Mathematical Concepts

Year I Module, Chemical Computation

a) Stoichiometry (3 lectures)

Classification of reactions. Methods of balancing equations. Expression of solution and of gaseous concentrations. Calculations involving titrations (acid-base, redox, precipitation and complexometric), gravimetry, elemental analysis and molecular formulae, gas laws and the Beer-Lambert Law.

b) Mathematical concepts for physical and practical chemistry (6 lectures)

Algebraic and geometrical concepts. Series. Variables. Differential calculus. Integral calculus. Equations and Graphs.

c) Repeated measurements and estimation of errors (7 lectures)

Mean, median and mode. Histograms. Gaussian curve of error. Standard deviation and variance. Probability. Tests of significance, t, F, (Chi)². Law of propagation of errors, examples including density, titrimetry, Nernst equation, Beer-Lambert law. Regression.

d) Chemistry and Computers (10 lectures and 20 hrs. workshops)

Detailed Lecture Contents, Comments and Discussion for Mathematical Concepts for Physical and Practical Chemistry

Lecture 1

Topics in detail

- a) aims
- b) Physical Quantities, units, quantity calculus, dimensional analysis
- c) definition and use of logarithms
- d) definition of factorials
- e) tabulation of data, labeling axes of graphs

Comments and discussion

a) The first point made was to explain the aim of the set of lectures, to revise/consolidate/outline the minumum amount of mathematics required in the first two years of a degree course in chemistry. Stress that the material was not difficult and a little could be made to go a long way.

b) Explain, with examples, that, a physical quantity = numerical value x unit, and that the units are manipulated by the rules of simple algebra.

List the 7 SI base units and give their definitions in full and their appoved symbols. Define some of the derived units e.g. the standard atmosphere, the calorie and the litre.

Introduce the IUPAC books of units, symbols and nomenclature for physical and for analytical chemistry.

Rearrange the equation for quantity, $\text{physical quantity/unit} = \text{numerical value}$, to permit taking of logarithms, which is only possible for a pure number.

Note, due to the use of electronic calculators for multiplication and division at school level many students know little, if anything, about logarithms and their uses.

c) Define a logarithm, show their use for multiplication, division and powers, and how to change their base.

d) Factorials were introduced as a convenient short hand way of writing down an item, a number sequence, that occurs quite frequently in physical science.

e) Tabulation appears early, to facilitate the practical course. State the basic rule, when tabulating data and labeling graphs use the quotient of physical quantity and unit. Give as example $\log_e P$ vis $1/T$, stress that the slope of the graph = $-L/R$ is a number, i.e. the units of L and R cancel.

Lastly, to illustrate dimensional analysis, evaluate the gas constant R in a variety of units from $R = PV/nT$.

Lecture 2

Topics in detail

a) Some geometrical items

- i) use of triangular graphs
- ii) definition of circular and solid angles
- iii) deduction of the inverse square law

b) Series

- i) why needed
- ii) geometric series
- iii) exponential series
- iv) binomial series
- v) logarithmic series

c) Dependent and independent variables

Comments and discussion

- a) i) is needed for 3 component phase rule diagrams. The properties of an equilateral triangle, the sum of the relative coordinates of a point = 1, neatly fits the sum of the mole fractions for 3 components.
- ii) introduce angles in radians and define solid angle.
- iii) show that the inverse law follows from the definition of solid angle for a point source of flux (for electrical, magnetic and light flux).
- b) i) needed to evaluate π , e , $\sin\theta$ etc. as they are not expressible by a closed function.
- ii) $S = 1 + x + x^2 + \dots$, how to sum. Note, students will meet this series later, in the quantum theory of specific heats.
- iii) Definition of e^x . Hence the need to explain factorial terminology earlier (lecture 1). That e^x has the unique property of being unchanged upon differentiation. It reappears like the "phoenix".
- This is the only gap in the logic as the student needs to know or be told that $dy/dx = nx^{n-1}$ for $y = x^n$.**
- iv) state that the binomial coefficients appear in the patterns seen in NMR and ESR spectra.
- Use of $(1+x)^n = 1+nx$ as a useful approximation, if x is small.
- v) deduce the series for $\log_e(1+x)$ and $\log_e(1-x)$.
- c) Explain that an independent variable is one that can have any value. Illustrations, expansion of a metal bar, volume of a gas depends on T and on P.
- Deduce the phase rule, $F = C - P + 2$.
- Discuss the choice between (P,T) and (V_m ,T) as the independent variables in physical chemistry:

P,T

V_m, T

experiments are easy if P is fixed

theory is easier if V is fixed

H and G give simplest equations if

U and A give simplest equations if

P and T are the variables

V_m and T are the variables

Lecture 3

Topics

Differential Calculus

i) why needed

ii) notations

iii) dy/dx by first principles for $y = x^n$

iv) logarithmic functions

v) derivative of a function of a function

vi) lists of standard forms of derivatives

vii) maxima, minima and points of inflexion

viii) representation of natural laws by differential equations and the need for integration to compare experiment with theory.

Comments and discussion

i) to relate experimental facts to theory. Experiments when the properties of a system vary with time, pressure, temperature, concentration, surface area etc.

ii) Δ , δ , d , ∂ ,

$dy/dx, y', y^*$

Simple examples of y changing with time,

$\Delta(\text{distance})/\Delta \text{time} = \text{velocity}$

iii) - vii) quite fast, single examples.

viii) Give examples with which they will be familiar,

Hooke's Law,

Radioactive decay etc.

Lecture 4

Topics in detail

Partial Differentiation

- i) demonstration of the concept via changes of the area of a rectangle
- ii) symbols and their meaning
- iii) exact differential equations in chemical thermodynamics
- iv) order of differentiation
- v) cross differentiation.

Comments and discussion

In a similar manner to the material in lecture 3. In iii) the main items were Gibbs' equations and Maxwell's relations.

Lecture 5

Topics in detail

a) Integration

- i) limit of a sum or the inverse of differentiation
- ii) indefinite and definite integrals
- iii) tables of standard forms

b) Partial Fractions

- i) factorisation of algebraic functions to match standard forms prior to integration
- ii) examples from reaction kinetics

Comment

In a similar manner and depth as in lecture 3.

Lecture 6

Topics

- a) Rearranging equations prior to plotting graphs**
- b) "Games" with the equations of state for a perfect gas**

Comments and discussion

The aim was to build confidence in the manipulation of equations. Particularly to manipulate to produce functions to plot to yield straight lines or to make explicit the variable in which you are, or might be, interested.

a) Two or three examples chosen from:

- i) Langmuir's isotherm
- ii) Kohlrausch's law
- iii) Debye equation for molecular dipoles
- iv) conductance of a weak electrolyte
- v) osmotic pressure of a solution of macromolecules
- vi) viscosity of polymer solutions.

b) The 3 tasks were:

- i) If $PV = nRT$,
show $(\partial^2 P / \partial T \partial V)_V = (\partial^2 P / \partial V \partial T)_T$.
- ii) If $f(P, V, T) = 0$,
show $(dV/dT)_P = -(\partial P / \partial T)_V / (\partial P / \partial V)_T$.
- iii) For a perfect gas, $PV = nRT$,
show $dP/P = dT/T - dV/V$

Conclusion and outcomes

The mathematics section of the course has run with only minor modifications for 18 years. The lectures are supported by sets of problems discussed seminars (3) and small group tutorial (2). The items needed for second year physical chemistry, namely, group theory, vectors, matrix algebra were and are introduced as needed within the main syllabus.

The mathematics material (lecture text and overheads/Powerpoint) have also been used successfully for self-study by individual mature students on ancillary chemistry courses.

The various sections of chemical computation are not now given in a single block, the section on stoichiometry is now included in laboratory calculations, the statistics section incorporated into the second year module, Instrumental Analysis. The recommended text remains that by Scott.

Table 1. Overview of subjects divided in two categories of priority with main focus on modeling for a 3.6 CP module/30 contact hours in Mechanics of the EurobachelorTM in AC.

HIGH PRIORITY	LOWER PRIORITY
• Forces, vectors and scalars	• <i>Relativity</i>
• Newton's laws	• <i>Doppler effect</i>
• Kinematics	• <i>Dynamics</i>
• Work	• <i>Stress</i>
• Velocity	• <i>Strain</i>
• Accelerations	•
• Momentum	
• Angular momentum	
• Moment of inertia	
• Kinetic energy	
• Potential energy	
• Pendulum and oscillations	
• Torsion and rotation	
• Collisions	
• Gravitation	

Table 2. Overview of subjects with main focus on chromatography for a 1.4 CP module/12 contact hours in liquid-flow dynamics of the EurobachelorTM in AC.

<ul style="list-style-type: none">• Ideal liquids
<ul style="list-style-type: none">• Pressure
<ul style="list-style-type: none">• Viscosity
<ul style="list-style-type: none">• Viscous flow
<ul style="list-style-type: none">• Diffusion
<ul style="list-style-type: none">• Bernoulli's equation
<ul style="list-style-type: none">• Boundary layers
<ul style="list-style-type: none">• Hagen-Poiseuille flow
<ul style="list-style-type: none">• Surface tension

Table 3. Overview of subjects divided in two categories of priority with main focus on detectors for a 1.9 CP module/16 contact hours in Electromagnetism of the EurobachelorTM in AC.

HIGH PRIORITY	LOW PRIORITY
• Electrostatics	• Resistor
• Maxwell's equations	• Oersted
• Gauss law for magnetism	• Tesla
• Capacitor	• Biot-Savart
• Transistor	• Dielectric constant
• Diamagnetism	• Superconductivity
• Paramagnetism	• ...

Table 4. List of subjects with main focus on gases and units for a 0.6 CP module/5 contact hours in thermodynamics of the EurobachelorTM in AC.

<ul style="list-style-type: none">• Work
<ul style="list-style-type: none">• Heat
<ul style="list-style-type: none">• Energy
<ul style="list-style-type: none">• Gases
<ul style="list-style-type: none">• Boltzmann statistics
<ul style="list-style-type: none">• Fermi-dirac statistics
<ul style="list-style-type: none">• Rotational energy
<ul style="list-style-type: none">• Vibrational energy
<ul style="list-style-type: none">• Entropy and likelihood
<ul style="list-style-type: none">• Temperature

Table 5. List of subjects divided into two categories of priority with main focus on spectrometry for a 2.4 CP module/20 contact hours in Quantum Mechanics of the EurobachelorTM in AC. Some of the subjects of lower priority are found in basic courses of AC.

HIGH PRIORITY	LOWER PRIORITY
• Planck's law	• Heisenberg uncertainty principle
• Quantum numbers	• Radiation
• Spin	• Scattering
• Bohr atomic model	• Structure of matter
• Rydbergs formula	• Crystallography
• Waves and particles	• Small molecule models
• Schrödinger's equation	• The four fundamental forces
• Wave functions	• Synchrotron
• Single atom models	• Black body radiation
• Periodic table	• Compton effect
• Diffraction	• Millikans experiment
• Elementary particles	• Franck-Hertz experiment
• Fotoelectric effect	• Stern-Gerlach's experiment
• Nuclear physics	• Spin-orbit coupling

