Executive Summary

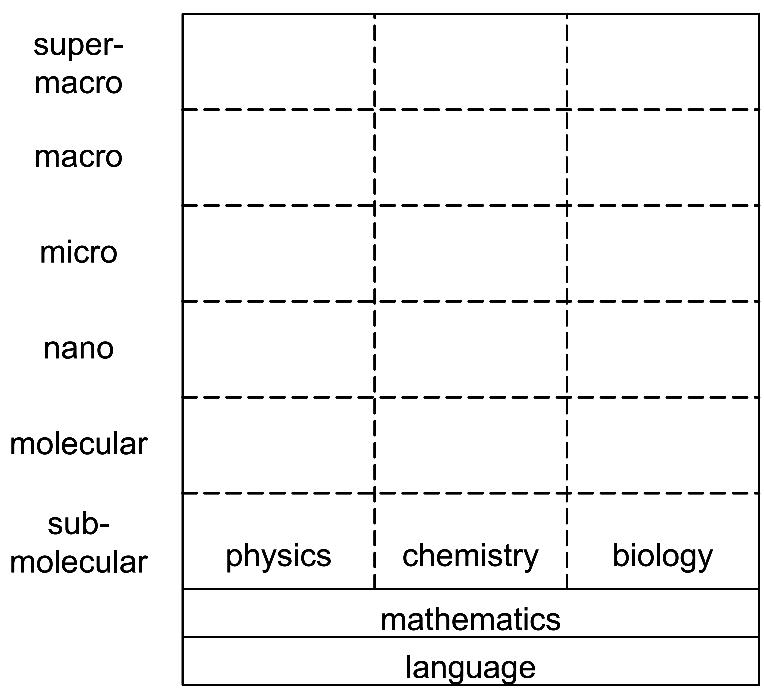
New Frontiers Workshop I in Orlando explored ways to arrange the subject matter of chemical engineering, looking beyond the traditional categories. Workshop II concluded this process by defining three Organizing Principles:

- Molecular Processes
- Multiscale Analysis
- Systems Analysis and Synthesis

Each principle has coherent content and intersects the others in useful ways. Based on this understanding of chemical engineering, the participants then addressed how the material might be presented to students – a curriculum.

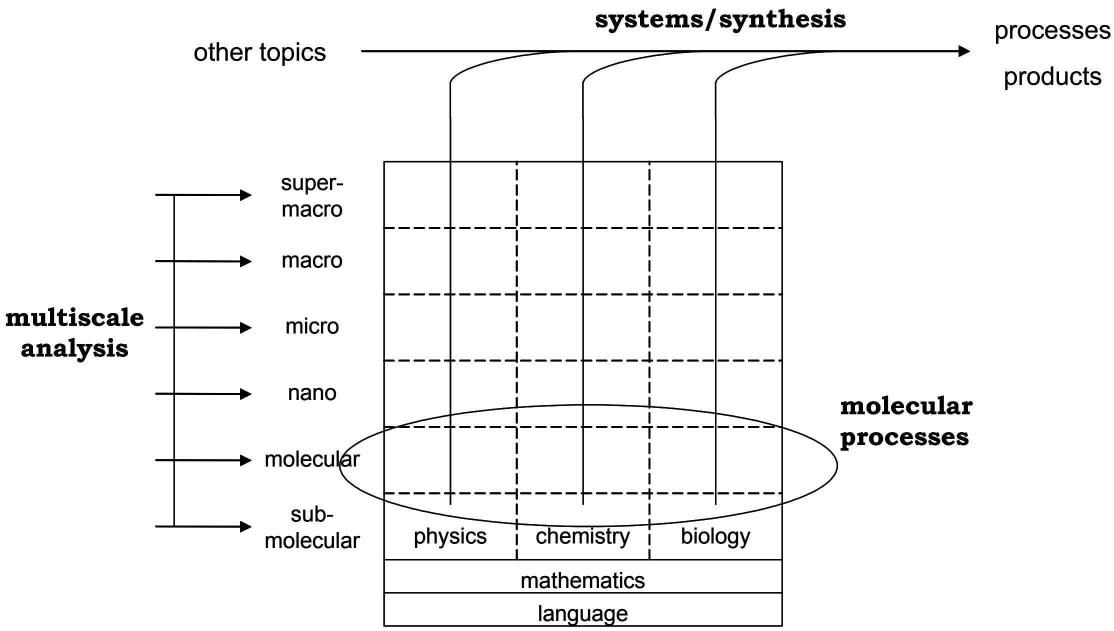
The Subject Matter of Chemical Engineering

Chemical engineers apply the foundation sciences of physics, chemistry, and biology to processes and products. Within each of these sciences, it is useful to consider the length scale of the application. This leads to a 2-dimensional map, in which language and mathematics are shown supporting the whole structure.



Modern chemical engineering ranges over much of this territory. A single topic (such as the rate of a decomposition reaction) might appear as a 'point' on the map. More complex problems (diffusion through cell membranes, a fluidized bed reactor, a polyethylene plant) would be a collection of such points, often spread across more than one foundation science and ranging over multiple length scales.

By using the three Organizing Principles listed above, we collect the phenomena and arrange the tools of chemical engineering. These Principles may be superimposed on the subject map.



First of all, chemical engineers seek to understand the molecular basis of matter, and the molecular-level processes - physical, chemical, and biological – that underlie observed phenomena in nature and technology. **Molecular Processes** is a unified treatment of phenomena at this level, including molecular motion, structure, and transformations, behavior in solution and at phase interfaces, chemical reaction, the contrast between rate processes and the state of equilibrium, the behavior of large molecules, self-assembly, and reproduction in living systems.

Second, chemical engineers have been effective because we have combined macroscopic engineering tools with a molecular understanding of nature. This naturally leads to an Organizing Principle of **Multiscale Analysis**. In this principle we compare and contrast the tools appropriate to a given length scale (molecular dynamics, continuum equations, macroscopic averages), gain an appreciation for the ways in which a given application can depend on phenomena occurring at different scales (the packed bed reactor), and an understanding of the implications of phenomena at one scale for another (molecular structure affects macroscopic properties). Here also we contrast transient and steady processes.

Third, realistic chemical engineering problems (dynamic behavior of batch and continuous processes in nature, technology, and society) feature multiple interacting components and draw from fields outside chemical engineering. The *analysis* of such problems depends on coordinating a variety of tools. Furthermore, chemical engineers design and create things, so that there is a strong component of *synthesis*, as well. Hence we define the Organizing Principle of **Systems Analysis and Synthesis**. Systems topics include modeling and simulation, optimization, dynamics and control, feedback and recycle, financial analysis, process and product design, and plant operation.

In summary, the chemical engineer leverages a knowledge of molecular processes across multiple length scales to analyze and synthesize complex systems describing processes and the products they produce. More detail on the Organizing Principles is given in Sessions 1 and 2 of these Proceedings.

Attributes of the B.S. Chemical Engineer
Organizing the subject matter of a field is a necessary but not sufficient condition for teaching it to the student. Teaching requires that the order of topics be decided, and the materials and methods of delivery prepared. The goal of the curriculum is to prepare a chemical engineer for effective professional performance. In the selection of topics, examples, and teaching methods, the desired attributes of the B.S. graduate must be a primary consideration.

The engineer as problem-solver (both analysis and synthesis activities):

- Keeps it simple
- Makes rational assumptions and estimates
- Communicates qualitative concepts
- Determines important parameters
- Applies skill set to open-ended and novel problems
- Can cope with
    - Incomplete information
    - Multiple (often conflicting) objectives
    - Multiple solutions (and multiple paths to solution)
    - Iterative solution methods
    - Uncertainty and messy data
    - Managing complexity
    - Taking risks
    - Rapid generation and pruning of alternatives
- Understands and works with uncertainty and sensitivity
- Thinks like a molecule

Life-long professional growth

- Knows how to learn
- Desires life-long learning
- Thinks critically
- Receptive to new ideas
- Seeks appropriate connections with other fields

Broader context

1. Knows where ChE fits in
- Has social responsibility
- Is driven to add value

Forming a Curriculum
Students may finally achieve an integrated view of chemical engineering, but the material is presented to them one day at a time. Hence the universities must decide both the topical order

and the manner of presentation. Some departments of chemical engineering might choose to arrange the curriculum in traditional lecture courses, others in self-contained modules of varying length, still others as case studies with interacting student teams, or as examples that are repeated in succeeding years in greater levels of complexity. Irrespective of the manner of presentation, however, it seems clear that the subject matter should be arranged so that

- the curriculum is integrated over time within each organizing principle - for example, the student encounters molecular processes each year, and each year's presentation builds on the preceding courses, modules, or cases.
- the curriculum is integrated across organizing principles at any time - for example, in any year, the student should encounter presentations in each of the organizing principles that reinforce the others.
- the curriculum features examples drawn from a wide array of industries and applications, including open-ended and complex problems, illustrating the interplay of science, society, regulation, and economics.

A rough curriculum map is drawn below. In this example, freshmen are introduced to chemical engineering in the context of a simple system, constructed so that the entire scope of the profession is illustrated in outline. In succeeding years, the systems problems and tools become more complex, drawing on the students' increasing sophistication with multiscale analysis tools and molecular descriptions. The laboratory experience, as well, proceeds from basic instruction in instrumentation and data analysis, through practice with demonstration equipment, to open-ended investigations.

In each of the molecular, multiscale, and systems courses, the students can expect to encounter applications of physical, chemical, and biological science. These will range from short examples that illustrate a single point to complicated, open-ended problems that will require significant work. The soft skills of oral, written, and graphic communication, working in teams, creativity techniques, and problem-solving techniques may be woven throughout various courses. Systems courses offer the most obvious platform for consideration of ethics, safety, economics, and social impact.

A good curriculum structure will leave the student at the end of each year feeling capable of practicing engineering at some level. More detail about curriculum proposals is given in Session 3 of these Proceedings.

FRESHMAN	SOPHOMORE	JUNIOR	SENIOR
SYSTEMS 1 introduction	SYSTEMS 2 simple processes	SYSTEMS 3 adv processes	SYSTEMS 4 design
	MULTISCALE 1 cons eqns/p props	MULTISCALE 2 multiphase/rxn	MULTISCALE 3 equipment
MATH through ODEs	MOLEC PROC 1 intro transport/rxn	MOLEC PROC 2 adv transport/rxn	MOLEC PROC 3 surf and structure
PHYSICS mech/electrical	LABORATORY instrument/stats	LABORATORY unit ops demo	LABORATORY research
BIOLOGY general	BIOLOGY cell	BIOLOGY molecular	
CHEMISTRY general	CHEMISTRY organic	CHEMISTRY physical	TECHNICAL electives
HUMANITIES read/write	HUMANITIES read/write	HUMANITIES economics/elect	HUMANITIES electives

Modules or Examples in a Curriculum
Various topics on which examples or modules could be developed are collected here from Session 1:

- water desalination
- hydrogen from biomass
- polystyrene peanuts from raw materials
- design of distillation dolumn → molecular modeling of non-ideal phase equilibria
- catalytic and/or multiphase reactor design
- ethanol fuel
- catalyst design
- synthesis of polyethylene terephthalate
- design for self assembly
    - polymer coating
    - nanotechnology
    - hybrid systems
- design of membranes
    - next generation beer bottles
    - fuel cells
- CO_2 emissions from vehicles
- stationary source emission abatement
- global climate and air pollution
- hydrogen economy
- chemical processes in the human body

- protein expression
- protein folding
- viral infections
- population dynamics
- liposomes
- cell adhesion
- chromatographic separation of proteins – all scales
- biomedicine
- gene therapy
- drug delivery
- drug patch design
- artificial pancreas
- vaccine and drug production
- material processing
- thin film deposition
- atomic layer deposition
- coatings
- controlled particle formation
- nanoparticles
- microelectronics
- design and development of composite materials
- personal care products
- block co-polymers
- metallurgy
- micro-electro-mechanical systems
- chemical and biological sensors
- spectroscopy